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Heat Capacities and Entropies of Organic Compounds in the Condensed Phase. Volume III

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This compilation of data on the heat capacities and entropies of organic compounds in the condensed phase is a cumulative document and includes the following earlier published work on this subject: "Heat Capacities and Entropies of Organic Compounds in the Condensed Phase," E. S. Domalski, W. H. Evans, and E. D. Hearing, J. Phys. Chem. Ref. Data **13**, Suppl. 1 (1984) and "Heat Capacities and Entropies of Organic Compounds in the Condensed Phase, Volume II," E.S. Domalski and E.D. Hearing, J. Phys. Chem. Ref. Data **19**, 881–1047 (1990). In addition, the literature through 1993 has been searched and the pertinent data reported has been included in Volume III. The latter volume provides data on 5332 individual entries for 2503 discrete organic compounds for which over 2200 articles have been examined, evaluated, and referenced. In addition to values for the heat capacity and entropy at 298.15 K, phase transitions for solid/solid, solid/liquid, and in some instances, solid/gas and liquid/gas are tabulated as encountered in the articles examined and evaluated. © *1996 American Institute of Physics and American Chemical Society.*

Key words: condensed phase; entropy; evaluated data; heat capacity; organic compounds; phase transitions; WLN.

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1. Introduction

This compilation provides heat capacity and entropy data on 5332 individual entries for 2503 discrete organic compounds in the liquid and solid phases. Data on the enthalpies and entropies of phase transitions which have been determined from calorimetric measurements are also included. Over 2200 articles have been examined, evaluated, and referenced.

This compilation is a cumulative collection of two earlier documents published in 1984 and 1990 entitled:

"Heat Capacities and Entropies of Organic Compounds in the Condensed Phase," by E. S. Domalski, W. H. Evans, and E. D. Hearing, J. Phys. Chem. Ref. Data **13**, Suppl. 1 (1984)

"Heat Capacities and Entropies of Organic Compounds in the Condensed Phase, Volume II," E.S. Domalski and E.D. Hearing, J. Phys Chem. Ref. Data **19**, 881–1047 (1990)

and also a collection of the pertinent data from the literature through the end of 1993.

Over the period from 1984 through 1993, several large compilations have been published which contain data on the thermodynamic properties of organic compounds in the condensed phase; they are:

"Thermodynamic Properties of Oxygen-Containing Organic Compounds," by I. A. Vasil'ev and V. M. Petrov, Handbook, Leningrad, 240 pages (1984),

"Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C_1 to C_4. Part 1. Properties of Condensed Phases," by R. C. Wilhoit, J. Chao, and K. R. Hall, J. Phys. Chem. Ref. Data **14**, 1–175 (1985),

"Thermodynamic and Thermophysical Properties of Organic Nitrogen Compounds. Part I. Methanamine, Ethanamine, 1- and 2-Propanamine, Benzenamine, 2-, 3-, and 4-Methylbenzenamine" by J. Chao, N.A.M. Gadalla, B.E. Gammon, K.N. Marsh, A.S. Rodgers, G.R. Somayajulu, and R.C. Wilhoit, J. Phys. Chem. Ref. Data **19**, 1547–1615 (1990),

"Thermodynamic and Thermophysical Properties of Organic Nitrogen Compounds. Part II. 1- and 2-Butanamine,

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2-Methyl-1-propanamine, 2-Methyl-2-propanamine, Pyrrole, 1-, 2-, 3-Methylpyrrole, Pyridine, 2-, 3-, and 4-Methylpyridine, Pyrrolidine, Piperidine, Indole, Quinoline, Isoquinoline, Acridine, Carbazole, Phenanthridine, 1- and 2-Naphthalenamine, and 9-Methylcarbazole" by A. Das, M. Frenkel, N.A.M. Gadalla, S. Kudchadker, K.N. Marsh, A.S. Rodgers, and R. C. Wilhoit, J. Phys. Chem. Ref. Data **22**, 659–782 (1993).

The latter compilations were useful in assisting us with the completeness of our search of the literature for papers on heat capacities, entropies, and phase transition properties of various organic compounds. The discussions on specific compounds were especially helpful in the assignment of a rating to our evaluation of those data.

2. Scope of the Search

Our coverage of the chemical literature extends from 1881 through 1993. References containing data on the heat capacities and entropies of organic compounds in the condensed phase were obtained primarily through searching Chemical Abstracts. Additional references were located through searching the files of the Chemical Thermodynamics Data Center of the National Institute of Standards and Technology and the Bulletin of Chemical Thermodynamics. The original papers were examined to obtain the data which has been tabulated, to determine whether corrections should be applied, and to qualitatively evaluate the reported measurements.

The goal of the search has been to obtain heat capacity and entropy data for organic compounds at "room temperature," however, the temperature range included is 200–450 K. This extended range was chosen so that the user would have, whenever possible, values for temperatures close to room temperature even if the measurement range did not include 298.15 K. Usually, the user can extrapolate such data to 298.15 K or to temperatures outside of the reported range if desired. Values of the enthalpy and entropy of phase transitions—solid/solid, solid/liquid, as well as some solid/gas, and liquid/gas transitions—obtained from calorimetric measurements are included along with the data on heat capacity and entropy. No specific search was made for the transition properties. They are included as a by-product of the search for experimental heat capacity data.

Corrections for relative atomic mass (atomic weight) and energy units have been made, where appropriate. Values have been reported at "298 K" with the ice point taken as 273.1, 273.15, or 273.16 K; the correction for this small change is much less than the precision and accuracy of the data. Some researchers did not provide tabulated values of C_p and S as a function of temperature, but gave an equation, such as: $C_p = A + BT + CT^2$. In these cases, a value for C_p and/or S at 298 K was derived from the equation provided. Some researchers have provided only graphs of C_p as a function of temperature. For good quality graphs, estimates of C_p at 298 K were extracted and correspondingly identified. Care was taken to assure that heat capacity data reported in International Steam Table (IT) energy units were converte to the International System of Units (SI Units). Except fo very precise data, corrections involving energy units for mos measurements since about 1930 are often within the uncer tainty of the data. Older data are of lower precision so tha corrections are not needed. In general, transition tempera tures are those reported by the investigator. The effort t convert each investigator's temperature scale to the 1990 In ternational Temperature Scale was not warranted.

3. Arrangement of the Data

The table of heat capacities, entropies, and phase transi tions given in this compilation contains data entries for a variety of organic compounds. The entries here, as in th 1984 and 1990 J. Phys. Chem. Ref. Data publication,[1,2] ar arranged in the order of the empirical formulae of the com pounds; isomers are further separated by their Wiswesse Line Notation.[3] The latter notation system has been used t represent the structure of the organic compound. Under a given organic substance, the data from the pertinent paper are included. The data from each paper form a separate entry complete with identification of the reference source. Whe there are several reference entries for a compound, they ar arranged chronologically by year. For each entry the dat given are: molecular (empirical) formula for the compound physical state, reference code, compound name(s), followe by the values for the heat capacity, entropy, and, where avail able, phase transition data. The entry of information is com pleted by the molecular weight (in units of $g \cdot mol^{-1}$) Wiswesser Line Notation for the compound, and an evalua tion of the presentation of the experimental results and th quality of the data. The formula given is the empirical for mula for the compound; water of hydration is shown as $\cdot (n)H_2O$. The elements are arranged in the order C, H(D, T) followed by the other elements in alphabetical order of thei chemical symbols. One or more names are given for eac compound. No attempt has been made to conform to a rig orously systematic nomenclature. Common names and sys tematic names are used; alternate names have been give freely. All names used appear in the Compound Name-Formula Index in Section 8, which should assist the reade who is aware of the compound name but not its empirica formula. This index also contains the Chemical Abstract Service Registry Number (CASRN) for each compoun listed. Occasionally, a CASRN is not available due to rea sons such as: ambiguous nature of the name of the com pound as reported in the literature, partial deuteration of compound, or poorly defined complex formation. The bibli ography is provided in Section 9. The reference code is c the form XXAAA/BBBN, where XX are the last two digit of the year of publication of the paper, AAA is the first thre letters of the last name of the first author and BBB is the fir three letters of the last name of the second author (if present Authors after the first two are disregarded. N is a digit fro 2 to 9 used to indicate a second, third, ...paper with the sam year and author codes. Thus, 60BRO/SMI2 refers to a pap

by Brown and Smith appearing in 1960, the second one with authors BRO... and SMI...; 44JON is a 1944 paper by Jones. The full citation appears in the bibliography arranged according to the reference codes. For papers published before 1900, all four digits for the year are used.

When authors have given a table of smoothed values for the heat capacity, the value at 298 K (interpolated if necessary) or the value nearest to that temperature is given. If experimental measurements are represented only by a smoothing equation, this is used to calculate the value given. If only the unsmoothed experimental results are given by the authors, one of these is given, with the corresponding temperature. Such a selection is accompanied by a remark.

The third-law entropy is given at 298 K or at the temperature closest to this temperature. The value is that obtained by the authors; we have not reintegrated the heat capacity data to re-evaluate the entropy.

Phases are indicated by g, liq, c, c,I, c,II, etc. In general, no attempt has been made to specify the crystalline form of the solid phases; c,I is used for the form stable at the melting point. For each phase transition, the appropriate process, i.e., c/liq, the temperature in kelvins, the enthalpy and entropy change for the isothermal process, and when appropriate, the pressure, are given. The entropy change ΔS is taken as $\Delta H/T$ unless indicated otherwise. Energy values are given in joules and can be related to the thermochemical calorie by the conversion factor: 4.1840 joules equals one thermochemical calorie. Pressures are given in kilopascals; one standard atmosphere is 101.325 kPa.

The molecular weight is based upon the 1991 IUPAC Table of International Atomic Weights.[4] Three exceptions are made; the atomic weights of hydrogen, nitrogen, and fluorine are taken as 1.0079, 14.0067, and 18.9984 rather than 1.00794, 14.00674, and 18.9984032, respectively. When the molecular weight differs from that originally used by the authors, appropriate corrections to the values have been made.

An indication of our general evaluation of the data reported is given as A (high quality), B (good), C (average), and D (low quality). This rating is based upon the method used, the details of the measurements as reported, the number of measurements, purity of the sample, calibrations, and corrections applied to the data; it is intended as a guide to those data we feel are more reliable. In addition, the number of significant figures given for the numerical values indicates roughly the quality of the data. In general, papers that are rated as being of high quality provide a detailed description of the cryostat used, the experimental procedure, the purity and characterization of the sample, calibration results, both raw and smoothed data for the temperature range over which measurements were made, and comment on the precision and accuracy of their data. An absence of numerical or descriptive information, or poor agreement with a detailed and accurate study can lead to a low rating.

All of the names used to identify the compounds are included in the Compound Name–Formula Index with the appropriate empirical formulae. Prefixes such as *tert-*, *ortho-*, *α-*, 1,2-, (but not *Iso*) are disregarded in the alphabetization of the names.

The sequencing of the compounds is based on the empirical formula. The formulae are sorted alphabetically by the first atomic symbol, then by the number of atoms of this element present (the Hill Indexing System[5]). As was the practice with the 1984 J. Phys. and Chem. Ref. Data publication,[1] C, carbon, is always the first element. This arranged list of formulae is then sorted by the second atomic symbol (H, hydrogen, if present), and then by the number of atoms of this element. The sorting proceeds alphabetically thereafter for each element present. The following list illustrates this scheme:

C

CCl_4

$CHCl_3$

CH_4

CO_2

$C_2Cl_3O_2$

$C_2H_3Cl_2$

C_2H_3Cl

C_2H_4

$C_2H_4O_2$

C_2H_6

C_2H_6O

Isomeric compounds are further sorted by their Wiswesser Line Notation:

$C_4H_{10}O$	2O2	$C_2H_5OC_2H_5$
	3O1	$C_3H_7OCH_3$
	Q1Y1&1	$(CH_3)_2CHCH_2OH$
	QX1&1&1	$(CH_3)_3COH$
	QY2&1	$C_2H_5CH(CH_3)OH$

4. Definitions

Heat Capacity. The heat capacity is defined as the derivative of the energy of the system with respect to the temperature under specified conditions. The heat capacity may be stated as an average value over a temperature range or the limiting value over an infinitesimal temperature change. If the system is maintained at constant volume, the heat capacity, C_v, is given by the derivative of energy with respect to temperature,

$$C_v = (\partial U/\partial T)_v,$$

where U is the internal energy.

If the system is maintained at constant pressure, the heat capacity, C_p, is given by:

$$C_p=(\partial H/\partial T)_p,$$

where H is the enthalpy.

The values of heat capacity reported in this paper are those at constant pressure and correspond to one mole of a specified substance; the units are thus, $J\cdot mol^{-1}\cdot K^{-1}$.

Experimentally, the heat capacity, C_p, is obtained from the enthalpy change at constant pressure over a small temperature change. This value is associated with the temperature at the midpoint of the temperature range:

$$C_p=\Delta H/(T_2-T_1) \quad \text{at } (T_1+T)/2.$$

Actual heat capacity measurements, or C_{sat}, for liquids and solids are normally made with the sample in equilibrium with its own vapor pressure or saturation pressure; the correction from C_{sat} to C_p at the standard pressure, 101.325 kPa (1 atm) is usually negligible for solids and for liquids below their boiling point. For volatile organic compounds in the condensed phase, a correction for the enthalpy of vaporization of the condensed phase as well as the heat capacity of the vapor phase must be applied.

For nonvolatile solid organic compounds, the relationship between C_p and C_{sat} is given by:

$$C_p-C_{sat}=[T(\partial P/\partial T)_{sat}][\partial V/\partial T)_P],$$

where $(\partial P/\partial T)_{sat}$ is the slope of the vapor pressure or saturation pressure curve and $(\partial V/\partial T)_p$ is the volume expansivity of the solid. Again, the magnitude of this correction is usually negligible.

Entropy. For totally reversible processes, the entropy change of a system is equal to the amount of heat, Q absorbed by the system divided by the temperature, T. For an infinitesimal change in entropy:

$$dS=dQ/T.$$

Entropy and heat capacity are related by the following expressions:

$$(\partial S/\partial T)_v=C_v/T, \text{ at constant volume,}$$

$$(\partial S/\partial T)_p=C_p/T, \text{ at constant pressure,}$$

$$(\partial S/\partial T)=C_{sat}/T, \text{ at equilibrium vapor pressure along the two phase line.}$$

The (calorimetric) entropy is obtained by integration of the measured values of C_p/T from the lowest temperature of measurement to the reported temperature. Various methods have been used to extrapolate from the lowest experimental temperature to zero kelvin. Appropriate values of the entropies of phase changes must be added. The entropy at zero kelvin is taken as zero for the stable crystalline state, with the addition of residual (zero point) entropy, not removed by the extrapolation, due to non-random ordering, optical isomerism, or multiple electronic ground states for the molecule. Thus,

$$S^\circ_T=S^\circ(\text{zero point})+\int_0^{T_1}(C_p/T)dT(\text{extrapolation})$$

$$+\int_{T_1}^{T_2}(C_p/T)dT+\Delta H_{T_2}/T_2(\text{phase change})$$

$$+\int_{T_2}^{T_3}(C_p/T)dT+\Delta H_{T_3}/T_3(\text{phase change})$$

$$+\int_{T_3}^{T}(C_p/T)dT.$$

For additional discussions on the concept of entropy, th reader should consult Refs. 6 and 7.

Phase Transitions. A process by which a substance unde goes a change of physical state, i.e., solid–solid, solid liquid, solid–gas, or liquid–gas, is known as a phase trans tion or phase change. The phase change is accompanied by transfer of energy (commonly referred to as latent heat) ar a change in volume while both temperature and pressure r main constant. For a phase change which is carried out r versibly (i.e., under equilibrium conditions) at a consta temperature and pressure, the total Gibbs energy remains u changed. If there is an enthalpy (or heat) change, then follows that there will also be an entropy change for th process, because:

$$\Delta H-\Delta ST=0 \text{ or } \Delta S=\Delta H/T.$$

These equations are applicable only for the temperatu and pressure at which the phases are in equilibrium. F phase changes solid–solid, solid–liquid, solid–gas, liquid gas encountered in the accompanying tables in Section ΔH refers to the isothermal enthalpy change at the transitic temperature. Corrections can be applied to the experiment data for premelting effects to isothermal conditions. Th pressure, unless specified, is the vapor pressure of the sul stance at the transition temperature; the correction to a sta dard state pressure is usually negligible at ordinary pressur for a solid–solid transition and for fusion. The entrop change is taken as $\Delta H/T$ at the equilibrium pressure.

Some investigators have reported the measurement anomalous phase changes in which the volume and entrop are continuous, but the heat capacity is discontinuous. Du ing such phase changes no latent heat is present and th shape of the curve of the heat capacity plotted as a functi of temperature often resembles the Greek letter lambda at th transition point. Such a transition is called a "lambda trans tion." In order to differentiate these anomalous transitio from ordinary phase changes, it has become customary identify normal phase changes as phase changes of the fi order and atypical phase changes as those of the second c der. The discontinuity which occurs in a first order pha transition is a commonly observed phenomenon; howev the discontinuity associated with a second order phase tra sition has been more difficult to identify and/or interpr Sometimes the discontinuous nature of the heat capacity questioned in a second order transition because experimen measurements show a peak or a hump at the transition te perature rather than an unambiguous discontinuity. A pha change which is accompanied by changes in the entropy a

volume and whose first-order derivatives of the Gibbs energy with respect to temperature and pressure change discontinuously is known as a phase change of the first order,

$$S=-(\partial G/\partial T)_P \quad \text{and} \quad V=(\partial G/\partial P)_T.$$

A phase change which is accompanied by changes in the heat capacity, volume expansivity, and isothermal compressibility and whose second order derivatives of the Gibbs energy with respect to temperature and pressure change discontinuously is known as a phase change of the second order,

$$C_p/T=(\partial S/\partial T)_P=-(\partial^2 G/\partial T^2)_P,$$
$$\kappa V=-(\partial V/\partial P)_T=-(\partial^2 G/\partial P^2)_T,$$
$$\beta V=(\partial V/\partial T)_P=(\partial^2 G/\partial T\partial P)_{T,P},$$

where κ is the isothermal compressibility and β is the volume expansivity. The relationship between these quantities and the pressure and temperature is given below by Ehrenfest's Equation.[8]

$$dP/dT=[C_p(f)-C_p(i)]/[TV(\beta(f)-\beta i))],$$
$$dP/dT=[\beta(f)-\beta(f)-\beta(i)]/[K(f)-K(i)],$$

where i and f represent the initial and final states of the phase change.

For additional discussion regarding first and second order phase transitions, the reader should consult Refs. 9, 10, and 11.

5. Acknowledgments

The authors thank Nancy W. Young for her assistance in the search, retrieval, and collection of articles containing information pertinent to this compilation.

6. References for the Introductory Discussion

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7. Table of Heat Capacities, Entropies, and Phase Transition Properties

C (c) 34JAC/PAR
Graphite; Carbon, graphite
Heat Capacity 293.5 K, C_p=8.498 J·mol^{-1}·K^{-1}
Temperature range 93 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=5.69 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 0.761 J·mol^{-1}·K^{-1}.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A(C_p),B(S)
Acheson No. 38 graphite

C (c) 36ROB/FOX
Diamond; Carbon, diamond
Heat Capacity 295 K, C_p=6.081 J·mol^{-1}·K^{-1}
Temperature range 90 to 320 K. Type 1, homogeneous; C_p=5.930 J·mol^{-1}·K^{-1} for Type 2, mosaic structure.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation C

C (c) 38PIT
Diamond; Carbon, diamond
Heat Capacity 287.96 K, C_p=5.669 J·mol^{-1}·K^{-1}
Temperature range 70 to 288 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=2.448 J·mol^{-1}·K^{-1}
Extrapolation below 70.8 K, 0.0322 J·mol^{-1}·K^{-1}.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A(C_p),B(S)

C (c) 53DES
Diamond; Carbon, diamond
Heat Capacity 298.16 K, C_p=6.1149 J·mol^{-1}·K^{-1}
Temperature range 25 to 300 K.
Entropy 298.16 K, S=2.3782 J·mol^{-1}·K^{-1}
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation B

C (c) 53DES/TYL
Graphite, Acheson; Carbon, graphite
Heat Capacity 298.15 K, C_p=8.527 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=5.470 J·mol^{-1}·K^{-1}
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A

C (c) 55DES
Graphite; Carbon, graphite
Heat Capacity 298.15 K, C_p=7.841 J·mol^{-1}·K^{-1}
Temperature range 17 to 300 K.
Entropy 298.15 K, S=5.3953 J·mol^{-1}·K^{-1}
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A

C (c) 57DES/TY
Graphite, Acheson, irradiated; Carbon, irradiated graphite
Heat Capacity 298.15 K, C_p=8.937 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=6.243 J·mol^{-1}·K^{-1}
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A
Stored energy of about 1987 J·g^{-1}.

C (c) 58DES/MO
Diamond; Carbon, diamond
Heat Capacity 277.68 K, C_p=5.3078 J·mol^{-1}·K^{-1}
Temperature range 13 to 277 K. Value is unsmoothed experiment datum.
Entropy 100.00 K, S=0.0720 J·mol^{-1}·K^{-1}
Agreement with DeSorbo (1953) data above 100 K.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A

C (c) 62VI
Diamond; Carbon, diamond
Heat Capacity 298.15 K, C_p=6.117 J·mol^{-1}·K^{-1}
Temperature range 273 to 1073 K.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A

C (c) 65MCI
Graphite; Carbon, graphite
Heat Capacity 300 K, C_p=8.58 J·mol^{-1}·K^{-1}
Temperature range 298 to 1723 K.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A
Special Spectroscopic Electrode Grade SPK.

C (c) 70LUT/VO
Graphite; Carbon, graphite
Heat Capacity 298.15 K, C_p=8.979 J·mol^{-1}·K^{-1}
Temperature range 57 to 320 K.
Entropy 298.15 K, S=5.937 J·mol^{-1}·K^{-1}
T^2 extrapolation below 50 K.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation B
Prepared by electrode technique from petroleum coke and coal tar pitcl Heat treated at 3000°C.

C (c) 70LUT/VC
Graphite; Carbon, graphite
Heat Capacity 298.15 K, C_p=8.473 J·mol^{-1}·K^{-1}
Temperature range 52 to 315 K.
Entropy 298.15 K, S=5.644 J·mol^{-1}·K^{-1}
T^2 extrapolation below 50 K.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation B
Sample with density 2.0 g·cm^{-3} prepared from petroleum coke a coal tar pitch by heat treatment under pressure at 2400°C. Density 2.1 g·cm^{-3} obtained by same process with addition of metal catalys Both heat treated at 3000°C.

C (c) 70LUT/VOL

Graphite, pyrolytic; Carbon, pyrolytic graphite

Heat Capacity 298.15 K, C_p=8.054 J·mol^{-1}·K^{-1}

Temperature range 51 to 311 K.

Entropy 298.15 K, S=5.431 J·mol^{-1}·K^{-1}

T^2 extrapolation below 90 K.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation B

Prepared by deposition from methane on hot graphite surface (2100°C). Heat treated at 3000°C.

C (c) 70LUT/VOL

Graphite, natural Taiguinski; Carbon, natural graphite

Heat Capacity 298.15 K, C_p=8.054 J·mol^{-1}·K^{-1}

Temperature range 51 to 311 K.

Entropy 298.15 K, S=5.431 J·mol^{-1}·K^{-1}

T^2 extrapolation below 50

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation B

Values are taken as those of pyrolytic graphite.

C (c) 70LUT/VOL

Carbon, baked; Baked carbon

Heat Capacity 298.15 K, C_p=9.251 J·mol^{-1}·K^{-1}

Temperature range 52 to 302 K.

Entropy 298.15 K, S=6.201 J·mol^{-1}·K^{-1}

T^2 extrapolation below 50 K.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation B

C (amorp) 70TAK/WES

Carbon, glassy; Glassy carbon

Heat Capacity 298.15 K, C_p=8.598 J·mol^{-1}·K^{-1}

Temperature range 5–350 K.

Entropy 298.15 K, S=5.833 J·mol^{-1}·K^{-1}

Values actually $S-S_0$; there may be a residual entropy.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation A

C (c) 72SHE/BEL

Graphite; Carbon, graphite

Heat Capacity 298 K, C_p=8.12 J·mol^{-1}·K^{-1}

Temperature range 273 to 3650 K. C_p calculated from equation applicable to the temperature range 273 to 1000 K.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation B

C (c) 73BUT/MAD

Graphite; Carbon, graphite

Heat Capacity 300 K, C_p=8.6186 J·mol^{-1}·K^{-1}

Temperature range 200 to 3500 K. Least squares fit of 'best' data gives: C_p=0.538657+9.11129×10^{-6} T−90.2725 T^{-1}−43449.3 T^{-2} +1.59309×10^{7} T^{3} −1.43688×10^{9}T^{-4} cal·g^{-1}·K^{-1} (250 to 3000 K).

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation A

Results from an evaluation of literature data.

C (c) 73MAR/VOL

Graphite; Carbon, graphite, single-crystal

Heat Capacity 298.15 K, C_p=8.11 J·mol^{-1}·K^{-1}

Temperature range 1 to 3000 K. C_p=0.6752 J·g^{-1}·deg^{-1}.

Entropy 298.15 K, S=5.51 J·mol^{-1}·K^{-1}

S°_T=0.4585 J·g^{-1}·deg^{-1}.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation A

Results from an evaluation of literature data.

C (c) 76VOL/BUC

Diamond; Carbon, diamond

Heat Capacity 300 K, C_p=6.57 J·mol^{-1}·K^{-1}

Temperature range 300 to 1200 K. Natural diamond; C_p calculated by extrapolation of value at 350 K.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation C

C (c) 76VOL/BUC

Diamond; Carbon, diamond

Heat Capacity 300 K, C_p=6.61 J·mol^{-1}·K^{-1}

Temperature range 75 to 1200 K. SAM synthetic diamond.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation C

C (c) 76VOL/BUC

Diamond; Carbon, diamond

Heat Capacity 300 K, C_p=6.37 J·mol^{-1}·K^{-1}

Temperature range 75 to 1200 K. Ballas synthetic diamond.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation C

C (c) 80TAY/GRO

Graphite; Carbon, GPCO graphite

Heat Capacity 300 K, C_p=8.43 J·mol^{-1}·K^{-1}

Temperature range 300 to 2400 K.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation A

C (c) 81ISA/WAN

Graphite; Carbon, graphite

Heat Capacity 300 K, C_p=10.05 J·mol^{-1}·K^{-1}

Temperature range 80 to 300 K. C_p=8.729×10^{-4}T + 6.27×10^{-6} T^2+6.309×10^{-9} T^3 J·g^{-1}·K^{-1}. Value calculated from equation.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation B

Poco process graphite: POCO-AXM 5Q1.

C (c) 87DOB/PER

Carbon; Graphite

Heat Capacity 350 K, C_p=10.68 J·mol^{-1}·K^{-1}

Temperature range 300 to 1800 K.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation A

POCO AXM-5Q1 graphite.

C (c) 90MOR/SMI

Diamond; Carbon, diamond

Heat Capacity

Temperature range 220 to 740 K. Data given graphically only.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation B

Synthetic diamond with C^{13} composition of 1.1 and 0.7%.

C (c) 91YIN/LIU

Graphite; Carbon, graphite

Heat Capacity 298 K, C_p=8.23 J·mol^{-1}·K^{-1}

Temperature range 300 to 420 K. C_p value reported at 298 K is 0.685 J/g·K.

Molecular Weight 12.0110

Wiswesser Line Notation C

Evaluation B

$CBrCl_3$ (liq) 59BEN/THO

Bromotrichloromethane

Heat Capacity 298 K, C_p=149.4 J·mol^{-1}·K^{-1}

Mean value 25 to 50 °C.

Molecular Weight 198.2740

Wiswesser Line Notation GXGGE

Evaluation C

$CBrF_3$ (liq) 84STO/CHA

Bromotrifluoromethane

Heat Capacity 293 K, C_p=163.8 J·mol^{-1}·K^{-1}

Temperature range 163 to 293 K.

Molecular Weight 148.9102

Wiswesser Line Notation FXEFF

Evaluation C

CBr_4 (c) 39FRE/HIL

Carbon tetrabromide; Tetrabromomethane

Heat Capacity 298 K, C_p=148.4 J·mol^{-1}·K^{-1}

Temperature range 298 to 423 K.

Phase Changes

c,II/c,I	320.0 K,	ΔH=5941 J·mol^{-1}
		ΔS=18.57 J·mol^{-1} K^{-1}
c,I/liq	363.2 K,	ΔH=3954 J·mol^{-1}
		ΔS=10.89 J·mol^{-1}·K^{-1}

Molecular Weight 331.6270

Wiswesser Line Notation EXEEE

Evaluation B

CBr_4 (c) 56MAR/STA

Carbon tetrabromide; Tetrabromomethane

Heat Capacity 300.6 K, C_p=128.66 J·mol^{-1}·K^{-1}

Temperature range 22 to 84 °C.

Phase Changes

c,II/c,I	320.0 K,	ΔH=6669 J·mol^{-1}
		ΔS=20.84 J·mol^{-1}·K^{-1}

Molecular Weight 331.6270

Wiswesser Line Notation EXEEE

Evaluation B

CBr_4 (c) 84BIC/MIN

Carbon tetrabromide; Tetrabromomethane

Heat Capacity 298.15 K, C_p=145.9 J·mol^{-1}·K^{-1}

One temperature. C_p given as 0.44 J·K^{-1}·g^{-1}.

Molecular Weight 331.6270

Wiswesser Line Notation EXEEE

Evaluation B

CBr_4 (liq) 48KU

Carbon tetrabromide; Tetrabromomethane

Heat Capacity 373 K, C_p=162.3 J·mol^{-1}·K^{-1}

Temperature range 96 to 182 °C. Mean C_p, three temperatures.

Molecular Weight 331.6270

Wiswesser Line Notation EXEEE

Evaluation D

CCl_2F_2 (liq) 31BUF/FI

Dichlorodifluoromethane; Freon 12

Heat Capacity 290 K, C_p=126.8 J·mol^{-1}·K^{-1}

Heat capacity measured at 230 K and 290 K using two differe methods. C_p at 230 K is 106.3 J·mol^{-1}·K^{-1}.

Molecular Weight 120.9138

Wiswesser Line Notation GXGFF

Evaluation C

CCl_2O (liq) 48GIA/JC

Carbonyl chloride; Phosgene

Heat Capacity 280 K, C_p=100.79 J·mol^{-1}·K^{-1}

Temperature range 15 to 280 K.

Entropy 280.71 K, S=198.11 J·mol^{-1}·K^{-1}

A value of S_0 of 6.82 J·mol^{-1}·K^{-1} has been added to the calorimet value of $S_{280}-S_0$.

Phase Changes

c/liq	145.37 K,	ΔH=5736 J·mol^{-1}
		ΔS=39.46 J·mol^{-1}·K^{-1}
liq/g	280.71 K,	ΔH=24401 J·mol^{-1}
		ΔS=86.93 J·mol^{-1}·K^{-1}
		P=101.325 kPa.

Molecular Weight 98.9164

Wiswesser Line Notation GVG

Evaluation A

CCl_2O (liq) 60GIA/O

Carbonyl chloride; Phosgene

Heat Capacity 160.55 K, C_p=102.59 J·mol^{-1}·K^{-1}

Temperature range 13 to 160 K. Value is unsmoothed experimen datum.

Entropy 280.76 K, S=192.80 J·mol^{-1}·K^{-1}

Data for liquid from 48GIA/JON.

Phase Changes

c,III/liq	139.19 K,	ΔH=4732 J·mol^{-1}
		ΔS=34.00 J·mol^{-1}·K^{-1}
c,II/liq	142.09 K,	ΔH=5586 J·mol^{-1}
		ΔS=39.31 J·mol^{-1}·K^{-1}
c,I/liq	145.37 K,	ΔH=5745 J·mol^{-1}
		ΔS=39.52 J·mol^{-1}·K^{-1}

Molecular Weight 98.9164

Wiswesser Line Notation GVG

Evaluation A

CCl_3F (liq) 40BEN/MC

Fluorotrichloromethane; Freon 11

Heat Capacity 298.15 K, C_p=126.7 J·mol^{-1}·K^{-1}

Temperature range 261 to 347 K. Data calculated from equation.

Molecular Weight 137.3684

Wiswesser Line Notation GXFGG

Evaluation B

CCl_3F (liq) 41OSB/GAR
Fluorotrichloromethane; Freon 11
Heat Capacity 298.15 K, C_p=121.55 J·mol^{-1}·K^{-1}
Temperature range 15 to 290 K. Value for saturated liquid.
Entropy 298.15 K, S=225.60 J·mol^{-1}·K^{-1}
Value for saturated liquid.
Phase Changes
c/liq 162.68 K, ΔH=6893.6 J·mol^{-1}
ΔS=42.38 J·mol^{-1}·K^{-1}
liq/g 290.40 K, ΔH=25209 J·mol^{-1}
ΔS=86.81 J·mol^{-1}·K^{-1}
P=80.33 kPA.
Molecular Weight 137.3684
Wiswesser Line Notation GXFGG
Evaluation A

CCl_3F (liq) 82MAR
Fluorotrichloromethane; Freon 11
Phase Changes
c/liq 165.4 K, ΔH=7900 J·mol^{-1}
ΔS=47.8 J·mol^{-1}·K^{-1}
Molecular Weight 137.3684
Wiswesser Line Notation GXFGG
Evaluation C

CCl_3F (liq) 92WIR/BRA2
Fluorotrichloromethane; Freon 11
Heat Capacity 303.15 K, C_p=122.5 J·mol^{-1}·K^{-1}
Temperature range 288 to 503 K. p=0.6 MPa.
Molecular Weight 137.3684
Wiswesser Line Notation GXFGG
Evaluation A

CCl_4 (liq) 22LAT
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 290 K, C_p=133.9 J·mol^{-1}·K^{-1}
Temperature range 39.1 to 290 K.
Entropy 298 K, S=205.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 224.6 K, ΔH=4600 J·mol^{-1}
ΔS=20.5 J·mol^{-1}·K^{-1}
c,I/liq 249 K, ΔH=2694 J·mol^{-1}
ΔS=10.8 J·mol^{-1}·K^{-1}
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 24WIL/DAN
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 303 K, C_p=128.9 J·mol^{-1}·K^{-1}
Temperature range 303 to 330 K. Equation only.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation C

CCl_4 (liq) 25WIL/DAN
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 293.2 K, C_p=128.0 J·mol^{-1}·K^{-1}
Temperature range 20 to 50 °C.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 32RIC/WAL
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.1 K, C_p=130.5 J·mol^{-1}·K^{-1}
Temperature range 293 to 323 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation C

CCl_4 (liq) 33KOL/UDO
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 288.3 K, C_p=126.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation C

CCl_4 (liq) 34KOL/UDO2
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 288.3 K, C_p=126.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation C

CCl_4 (liq) 37STU
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.1 K, C_p=132.63 J·mol^{-1}·K^{-1}
Temperature range 90 to 320 K.
Entropy 298.1 K, S=219.2 J·mol^{-1}·K^{-1}
Extrapolation below 91 K; 74.31 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 225.63 K, ΔH=4602 J·mol^{-1}
ΔS=26.40 J·mol^{-1}·K^{-1}
c,I/liq 250.37 K, ΔH=2431 J·mol^{-1}
ΔS=9.71 J·mol^{-1}·K^{-1}
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B(C_p),C(S)

CCl_4 (liq) 37VOL
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298 K, C_p=133.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 37VOL
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298 K, C_p=133.0 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.2066 cal·deg^{-1}·gram^{-1}.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 39PHI
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 301.2 K, C_p=133.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation C

CCl_4 (liq) 41ZHD
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.1 K, C_p=132.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 46 °C.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation C

CCl_4 (liq) 44HIC/HOO
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.67 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=214.39 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 225.35 K, ΔH=4582 J·mol^{-1}
ΔS=20.33 J·mol^{-1}·K^{-1}
c,I/liq 250.3 K, ΔH=2515 J·mol^{-1}
ΔS=10.05 J·mol^{-1}·K^{-1}
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation A

CCl_4 (liq) 48KUR
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298 K, C_p=128.8 J·mol^{-1}·K^{-1}
Temperature range −20 to 72 °C. Mean C_p, four temperatures.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation D

CCl_4 (liq) 55STA/TUP
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298 K, C_p=132.59 J·mol^{-1}·K^{-1}
Temperature range 295 to 339 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 57HAR/MOE
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 300 K, C_p=130.9 J·mol^{-1}·K^{-1}
Temperature range 243 to 303 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 57HAR/MOE
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 303.3 K, C_p=130.5 J·mol^{-1}·K^{-1}
Temperature range 254 to 303 K. Unsmoothed experimental datum.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation C

CCl_4 (liq) 67RAS/GAN
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 293 K, C_p=131.5 J·mol^{-1}·K^{-1}
Temperature range 293 to 333 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation C

CCl_4 (liq) 70CHA/W
Carbon tetrachloride; Tetrachloromethane
Phase Changes
c,II/c,I 225.35 K, ΔH=4581 J·mol^{-1}
ΔS=20.33 J·mol^{-1}·K^{-1}
c,I/liq 250.3 K, ΔH=2515 J·mol^{-1}
ΔS=10.04 J·mol^{-1}·K^{-1}
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation A

CCl_4 (c) 71ATA/(
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 46 K, C_p=44.22 J·mol^{-1}·K^{-1}
Temperature range 3 to 46 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation A

CCl_4 (liq) 71DES/B
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298 K, C_p=131.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 72ARE/M
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 256.10 K, C_p=131.8 J·mol^{-1}·K^{-1}
Temperature range 243 to 256 K. Value is unsmoothed experime
datum.
Phase Changes
c,II/liq 245.70 K, ΔH=1848 J·mol^{-1}
ΔS=7.52 J·mol^{-1}·K^{-1}
c,I/liq 250.28 K, ΔH=2588 J·mol^{-1}
ΔS=10.22 J·mol^{-1}·K^{-1}
Stable phase.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation A

CCl_4 (liq) 73SUB/E
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=130.8 J·mol^{-1}·K^{-1}
Temperature range 298 to 323 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 74WIL/Z
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 293.15 K, C_p=131.66 J·mol^{-1}·K^{-1}
Temperature range 273 to 323 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 75GRO/E
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 76FOR/BEN
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.36 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 76FOR/BEN2
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.401 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation A

CCl_4 (liq) 76MOR/RIC
Carbon tetrachloride; Tetrachloromethane
Phase Changes
c,II/c,I 225.7 K, ΔH=4631 J·mol^{-1}
ΔS=20.52 J·mol^{-1}·K^{-1}
(c,II/c,Ib)
c,I/liq 250.53 K, ΔH=2562 J·mol^{-1}
ΔS=10.226 J·mol^{-1}·K^{-1}
(c,Ib/liq). Data also given for (c,Ia/liq):
246.00 K, ΔH=1830 J·mol^{-1}
ΔS=7.44 J·mol^{-1}·K^{-1}
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation A

CCl_4 (liq) 77VES/SVO
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.40 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 78GRO/WIL
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.57 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 79VES/ZAB
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.40 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 79WIL/FAR
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.36 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 79GRO/HAM
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 81ATA/ELS
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 293.15 K, C_p=129.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 82TAN
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.34 J·mol^{-1}·K^{-1}
Temperature range 293.15, 298.15, 303.15 K. Data at three temperatures.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation A

CCl_4 (liq) 85NKI/CHA
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=132.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 89LAI/ROD
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=133.35 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 89PET/PES
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=133.0 J·mol^{-1}·K^{-1}
Temperature range 258.15, 278.15, 298.15, 318.15 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CCl_4 (liq) 93SHE
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, C_p=131.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CF_4 (liq) 58KOS/SAM
Carbon tetrafluoride; Tetrafluoromethane; Freon 14
Phase Changes

c,II/c,I	76.09 K,	ΔH=1734.3 J·mol^{-1}
		ΔS=21.38 J·mol^{-1}·K^{-1}
c,I/liq	88.44 K,	ΔH=693.71 J·mol^{-1}
		ΔS=7.74 J·mol^{-1}·K^{-1}

Molecular Weight 88.0046
Wiswesser Line Notatio FXFFF
Evaluation A

CF_4 (liq) 69ENO/SHI2
Carbon tetrafluoride; Tetrafluoromethane; Freon 14
Heat Capacity
Temperature range 4 to 100 K.
Phase Changes

c,II/c,I	76.09 K,	ΔH=1462.3 J·mol^{-1}
		ΔS=19.20 J·mol^{-1}·K^{-1}
c,I/liq	89.529 K,	ΔH=705.4 J·mol^{-1}
		ΔS=7.87 J·mol^{-1}·K^{-1}

Molecular Weight 88.0046
Wiswesser Line Notation FXFFF
Evaluation A

CF_4 (liq) 69SMI/PAC2
Carbon tetrafluoride; Tetrafluoromethane; Freon 14
Heat Capacity 145 K, C_p=80.08 J·mol^{-1}·K^{-1}
Temperature range 12 to 145 K. See also 69SMI/PAC.
Entropy 145.12 K, S=143.97 J·mol^{-1}·K^{-1}
Phase Changes

c,II/c,I	76.27 K,	ΔH=1709.2 J·mol^{-1}
		ΔS=22.41 J·mol^{-1}·K^{-1}
c,I/liq	89.56 K,	ΔH=712.1 J·mol^{-1}
		ΔS=7.95 J·mol^{-1}·K^{-1}
liq/g	145.12 K,	ΔH=11814 J·mol^{-1}
		ΔS=81.41 J·mol^{-1}·K^{-1}
		P=101.325 kPa.

Molecular Weight 88.0046
Wiswesser Line Notation FXFFF
Evaluation A

$(CH)_n$ (c) 83LEI/KAH
Polyacetylene
Heat Capacity 300 K, C_p=60 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K. Cis isomer. C_p=40 J·mol^{-1}·K^{-1} for trans isomer. Data given graphically. Data estimated from graph.
Molecular Weight 13.0189
Wiswesser Line Notation /*YUY*/
Evaluation D

$CHBr_3$ (liq) 32TRE
Tribromomethane; Bromoform
Heat Capacity 298 K, C_p=135.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 252.7309
Wiswesser Line Notation EYEE
Evaluation B

$CHBr_3$ (liq) 48KUR
Tribromomethane; Bromoform
Heat Capacity 298 K, C_p=130.5 J·mol^{-1}·K^{-1}
Temperature range 9 to 147 °C. Mean C_p, four temperatures.
Molecular Weight 252.7309
Wiswesser Line Notation EYEE
Evaluation D

$CHBr_3$ (liq) 84GOL/K(
Tribromomethane; Bromoform
Phase Changes

c/liq	281.84 K,	ΔH=11046 J·mol^{-1}
		ΔS=39.2 J·mol^{-1}·K^{-1}

Molecular Weight 252.7309
Wiswesser Line Notation EYEE
Evaluation A

$CHClF_2$ (liq) 40BEN/MC
Chlorodifluoromethane; Freon 22
Heat Capacity 298.15 K, C_p=114.10 J·mol^{-1}·K^{-1}
Temperature range 256 to 328 K. Data calculated from equation.
Molecular Weight 86.4687
Wiswesser Line Notation GYFF
Evaluation B

$CHClF_2$ (liq) 57NEI/W
Chlorodifluoromethane; Freon 22
Heat Capacity 232.50 K, C_p=93.01 J·mol^{-1}·K^{-1}
Temperature range 16 to 230 K.
Entropy 232.50 K, S=179.91 J·mol^{-1}·K^{-1}
Phase Changes

c,II/c,I	59 K,	ΔH=67 J·mol^{-1}
		ΔS=1.14 J·mol^{-1}·K^{-1}
	Lambda-type transition.	
c,I/liq	115.73 K,	ΔH=4123.3 J·mol^{-1}
		ΔS=35.63 J·mol^{-1}·K^{-1}
liq/g	232.50 K,	ΔH=20217 J·mol^{-1}
		ΔS=86.95 J·mol^{-1}·K^{-1}
		P=101.325 kPa.

Molecular Weight 86.4687
Wiswesser Line Notation GYFF
Evaluation A

$CHCl_2F$ (liq) 40BEN/MC
Dichlorofluoromethane; Freon 21
Heat Capacity 298.15 K, C_p=112.6 J·mol^{-1}·K^{-1}
Temperature range 261 to 338 K. Data calculated from equation.
Molecular Weight 102.9233
Wiswesser Line Notation GYGF
Evaluation B

$CHCl_3$ (liq) 24WIL/D/
Trichloromethane; Chloroform
Heat Capacity 303 K, C_p=116.7 J·mol^{-1}·K^{-1}
Temperature range 295 to 315 K. Equation only.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation C

$CHCl_3$ (liq) 25WIL/D/
Trichloromethane; Chloroform
Heat Capacity 293.2 K, C_p=115.5 J·mol^{-1}·K^{-1}
Temperature range 20 to 50 °C.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 32RIC/WAL
Trichloromethane; Chloroform
Heat Capacity 298.1 K, $C_p = 113.0\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 323 K.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation C

$CHCl_3$ (liq) 39PHI
Trichloromethane; Chloroform
Heat Capacity 303.6 K, $C_p = 139.7\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation C

$CHCl_3$ (liq) 48KUR
Trichloromethane; Chloroform
Heat Capacity 298 K, $C_p = 117.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range −52 to 51 °C. Mean C_p, four temperatures.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation D

$CHCl_3$ (liq) 55STA/TUP
Trichloromethane; Chloroform
Heat Capacity 298 K, $C_p = 114.18\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 284 to 329 K.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 57HAR/MOE
Trichloromethane; Chloroform
Heat Capacity 300 K, $C_p = 113.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 243 to 303 K.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 57HAR/MOE
Trichloromethane; Chloroform
Heat Capacity 303.2 K, $C_p = 114.0\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 245 to 303 K. Unsmoothed experimental datum.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation C

$CHCl_3$ (liq) 67RAS/GAN
Trichloromethane; Chloroform
Heat Capacity 293 K, $C_p = 116.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 333 K.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation C

$CHCl_3$ (liq) 81ING/CAS
Trichloromethane; Chloroform
Heat Capacity 298.15 K, $C_p = 114.26\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 85HEP/KOO
Trichloromethane; Chloroform
Heat Capacity 298.15 K, $C_p = 113.73\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 86ALP/PES
Trichloromethane; Chloroform
Heat Capacity 298.15 K, $C_p = 115.5\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 87GRO/ROU
Trichloromethane; Chloroform
Heat Capacity 298.15 K, $C_p = 113.85\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 89BAR/KOO
Trichloromethane; Chloroform
Heat Capacity 298.15 K, $C_p = 114.35\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 89BAR/KOO2
Trichloromethane; Chloroform
Heat Capacity 298.15 K, $C_p = 114.32\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 89PET/PES
Trichloromethane; Chloroform
Heat Capacity 298.15 K, $C_p = 115.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 258.15, 278.15, 298.15, 318.15 K.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 93GRO/ROU
Trichloromethane; Chloroform
Heat Capacity 298.15 K, $C_p = 114.25\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

$CHCl_3$ (liq) 93SHE
Trichloromethane; Chloroform
Heat Capacity 298.15 K, C_p=113.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation B

CHF_3S (liq) 60DIN/PAC
Trifluoromethanethiol
Heat Capacity 235 K, C_p=113.09 J·mol^{-1}·K^{-1}
Temperature range 12 to 227 K.
Entropy 235.15 K, S=204.60 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 116.04 K, ΔH=4925 J·mol^{-1}
ΔS=42.43 J·mol^{-1}·K^{-1}
Molecular Weight 102.0741
Wiswesser Line Notation HSXFFF
Evaluation A

CHF_3 (liq) 62VAL/BRO
Trifluoromethane; Fluoroform; Freon 23
Heat Capacity 190.97 K, C_p=86.44 J·mol^{-1}·K^{-1}
Temperature range 15 to 190.97 K.
Entropy 190.97 K, S=151.04 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 117.97 K, ΔH=4058 J·mol^{-1}
ΔS=34.40 J·mol^{-1}·K^{-1}
liq/g 190.97 K, ΔH=16711 J·mol^{-1}
ΔS=87.50 J·mol^{-1}·K^{-1}
P=101.325 kPa.
Molecular Weight 70.0141
Wiswesser Line Notation FYFF
Evaluation A

CHI_3 (c) 93CAR/LAY
Triiodomethane; Iodoform
Heat Capacity 298.15 K, C_p=157.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 393.7324
Wiswesser Line Notation IYII
Evaluation A

$CHLiO_2$ (c) 75FER/SAN
Lithium formate
Phase Changes
c,II/c,I 496 K, ΔH=1800 J·mol^{-1}
ΔS=3.6 J·mol^{-1}·K^{-1}
c,I/liq 546 K, ΔH=16190 J·mol^{-1}
ΔS=29.7 J·mol^{-1}·K^{-1}
Molecular Weight 51.9587
Wiswesser Line Notation VHO .LI
Evaluation A

CHN (liq) 39GIA/RU
Hydrogen cyanide
Heat Capacity 300 K, C_p=71.00 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.86 K, S=113.01 J·mol^{-1}·K^{-1}
Phase Changes
near 170 K, ΔH=15.9 J·mol^{-1}
ΔS=0.092 J·mol^{-1}·K^{-1}
Second order transition.
c/liq 259.90 K, ΔH=8406 J·mol^{-1}
ΔS=32.34 J·mol^{-1}·K^{-1}
liq/g 298.85 K, ΔH=25217 J·mol^{-1}
ΔS=84.38 J·mol^{-1}·K^{-1}
P=101.325 kPa.
Molecular Weight 27.0256
Wiswesser Line Notation NCH
Evaluation A

$CHNaO_2$ (c) 60WES/CH
Sodium methanoate; Sodium formate
Heat Capacity 298.15 K, C_p=87.68 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=103.76 J·mol^{-1}·K^{-1}
Molecular Weight 68.0075
Wiswesser Line Notation VHO .NA
Evaluation A

$CHNaO_2$ (c) 75FER/SA
Sodium methanoate; Sodium formate
Heat Capacity 340 K, C_p=88.3 J·mol^{-1}·K^{-1}
Temperature range 340 to 560 K.
Molecular Weight 68.0075
Wiswesser Line Notation VHO .NA
Evaluation B

$CHNaO_2$ (c) 83FRA/PI
Sodium methanoate; Sodium formate
Heat Capacity 298.15 K, C_p=87.68 J·mol^{-1}·K^{-1}
Temperature range 300 to 520 K. C_p data taken from 60WES/CHA temperature range 5 to 350 K.
Entropy 298.15 K, S=103.76 J·mol^{-1}·K^{-1}
S data taken from 60WES/CHA.
Phase Changes
c,II/c,I 491.5 K, ΔH=1214 J·mol^{-1}
ΔS=2.47 J·mol^{-1}·K^{-1}
c,I/liq 530.46 K, ΔH=17710 J·mol^{-1}
ΔS=33.39 J·mol^{-1}·K^{-1}
Molecular Weight 68.0075
Wiswesser Line Notation VHO .NA
Evaluation A

CHO_2Rb (c) 75FER/SA
Rubidium formate
Phase Changes
c,II/c,I 368 K, ΔH=250 J·mol^{-1}
ΔS=0.7 J·mol^{-1}·K^{-1}
Molecular Weight 130.4855
Wiswesser Line Notation VHO .RB
Evaluation C

CHO_2Tl (c) 76MEI/SEY
Thallium formate
Phase Changes
c,I/liq 374 K, $\Delta H = 10878\ J \cdot mol^{-1}$
$\Delta S = 28.9\ J \cdot mol^{-1} \cdot K^{-1}$
Solid-mesophase.
Molecular Weight 249.3877
Wiswesser Line Notation VHO .TL
Evaluation B

$(CH_2)_n$ (c) 57SOC/TRA
Polyethylene
Heat Capacity 270 K, $C_p = 24.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 58 to 270 K. C_p value is unsmoothed experimental datum.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation B

$(CH_2)_n$ (c) 61WAR/PET
Polyethylene
Heat Capacity 300 K, $C_p = 31.69\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 320 K. Interpolated data.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Branched, high pressure polyethylene.

$(CH_2)_n$ (c) 62DAI/EVA3
Polyethylene; Marlex 50 polymer
Heat Capacity 298.15 K, $C_p = 26.29\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 20 to 310 K. Data for "Marlex 50" (low pressure) polythene.
Entropy 298.15 K, $S = 24.72\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A

$(CH_2)_n$ (c) 62DAI/EVA3
Polyethylene; Rigidex 50 polymer
Heat Capacity 298.15 K, $C_p = 26.02\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 20 to 310 K. Data for "Rigidex 50" (low pressure) polythene.
Entropy 298.15 K, $S = 24.53\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A

$(CH_2)_n$ (c) 62DAI/EVA3
Polyethylene; W.N.C. 18 polymer
Heat Capacity 298.15 K, $C_p = 32.47\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 300 K. Data for "W.N.C. 18" (high pressure) polythene.
Entropy 298.15 K, $S = 26.02\ J \cdot mol^{-1} \cdot K^{-1}$
Data extrapolated from 90 K.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A

$(CH_2)_n$ (c) 62WAR/PET
Polyethylene
Heat Capacity 300 K, $C_p = 31.69\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 320 K. Calculated. Conventional high pressure polyethylene.
Entropy 300 K, $S = 25.52\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A

$(CH_2)_n$ (c) 62WUN
Polyethylene
Heat Capacity 300 K, $C_p = 24.53\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 1 to 420 K. Extrapolated value to 100% crystalline phase.
Entropy 300 K, $S = 24.04\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 415 K, $\Delta H = 3879\ J \cdot mol^{-1}$
$\Delta S = 9.35\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A

$(CH_2)_n$ (amorph) 62WUN
Polyethylene
Heat Capacity 300 K, $C_p = 32.85\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 1 to 420 K. Extrapolated value to 100% amorphous phase.
Entropy 300 K, $S = 31.96\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 415 K, $\Delta H = 3879\ J \cdot mol^{-1}$
$\Delta S = 9.35\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A

$(CH_2)_n$ (c) 63PAS/KEV
Polyethylene, branched
Heat Capacity 300 K, $C_p = 29.17\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 415 K.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation B
Branched polyethylene, density, 0.924 at 20°C.

$(CH_2)_n$ (c) 63PAS/KEV
Polyethylene, linear
Heat Capacity 300 K, $C_p = 24.47\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 433 K.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation B
Linear polyethylene, density, 0.968 at 20°C.

$(CH_2)_n$ (c) 65WUN
Polyethylene; Marlex 50 polymer
Heat Capacity 298.15 K, $C_p = 21.88\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 180 to 410 K. Values per gram formula weight.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
99% Crystallinity, extrapolated to 100%. Number-average molecular weight, 9800, weight-average=130000.

$(CH_2)_n$ (c) 73CHA/BES
Polyethylene, branched
Heat Capacity 298.15 K, C_p=30.20 J·mol^{-1}·K^{-1}
Temperature range 2 to 360 K. Values per unit formula weight.
Entropy 298.15 K, S=25.91 J·mol^{-1}·K^{-1}
Values are $S-S_0$.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Branched polyethylene, SRM 1476. Density 0.9247 g·cm^{-3} at 23 °C.

$(CH_2)_n$ (c) 73CHA/BES
Polyethylene, branched, annealed
Heat Capacity 298.15 K, C_p=30.26 J·mol^{-1}·K^{-1}
Temperature range 2 to 360 K.
Entropy 298.15 K, S=25.74 J·mol^{-1}·K^{-1}
Values are $S-S_0$.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Branched polyethylene, SRM 1476, annealed. Density 0.9272 g·cm^{-3} at 23°C.

$(CH_2)_n$ (c) 73CHA/BES
Polyethylene, linear
Heat Capacity 298.15 K, C_p=25.68 J·mol^{-1}·K^{-1}
Temperature range 2 to 360 K. Values per unit formula weight.
Entropy 298.15 K, S=24.52 J·mol^{-1}·K^{-1}
Values are $S-S_0$.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Linear polyethylene, SRM 1475. Density, 0.95 g·cm^{-3} at 23°C.

$(CH_2)_n$ (c) 74CHA
Polyethylene, linear high density
Heat Capacity 298.15 K, C_p=22.60 J·mol^{-1}·K^{-1}
Temperature range 5 to 360 K. Value per monomer unit.
Entropy 298.15 K, S=23.02 J·mol^{-1}·K^{-1}
Value per monomer unit. $S-S_0$.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Extrapolated to 100% crystallinity, from data on other samples.

$(CH_2)_n$ (c) 74CHA
Polyethylene, linear high density
Heat Capacity 298.15 K, C_p=22.98 J·mol^{-1}·K^{-1}
Temperature range 5 to 360 K. Value per monomer unit.
Entropy 298.15 K, S=23.22 J·mol^{-1}·K^{-1}
Value per monomer unit. $S-S_0$.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Density 0.993 g·cm^{-3} at 23°C. Pressure crystallized.

$(CH_2)_n$ (c) 74CHA
Polyethylene, linear high density
Heat Capacity 298.15 K, C_p=23.96 J·mol^{-1}·K^{-1}
Temperature range 5 to 360 K. Value per monomer unit.
Entropy 298.15 K, S=23.64 J·mol^{-1}·K^{-1}
Value per monomer unit. $S-S_0$.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Density 0.981 g·cm^{-3} at 23°C. Slow-melt crystallized.

$(CH_2)_n$ (c) 75CHA/W
Polyethylene, branched, DYNH CT-1660
Heat Capacity 298.15 K, C_p=32.20 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K. Values per CH_2 unit.
Entropy 298.15 K, S=26.37 J·mol^{-1}·K^{-1}
Does not include zero-point entropy.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Branched polyethylene, density 0.91 g·cm^{-3}.

$(CH_2)_n$ (c) 75CHA/W
Polyethylene, linear, Marlex 50 polymer
Heat Capacity 298.15 K, C_p=24.79 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K. Values per CH_2 unit.
Entropy 298.15 K, S=24.04 J·mol^{-1}·K^{-1}
Does not include zero-point entropy.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Linear polyethylene, density 0.973 g·cm^{-3}.

$(CH_2)_n$ (c) 76CI
Polyethylene, linear high molecular weight
Heat Capacity 298.15 K, C_p=24.97 J·mol^{-1}·K^{-1}
Temperature range 5 to 380 K. Value per monomer unit.
Entropy 298.15 K, S=22.04 J·mol^{-1}·K^{-1}
Value per monomer unit. $S-S_0$.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Produced by Ziegler-type vapor polymerization. Molecular wei 2.7–3.0×10^6. Approximately 45% crystalline. Data from quench sample.

$(CH_2)_n$ (c) 78S
Polyethylene
Heat Capacity 298.15 K, C_p=25.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation B

CH_2Br_2 (liq) 48KI
Dibromomethane; Methylene bromide
Heat Capacity 298 K, C_p=127.2 J·mol^{-1}·K^{-1}
Temperature range −22 to 98 °C. Mean Cp, four temperatures.
Molecular Weight 173.8348
Wiswesser Line Notation E1E
Evaluation D

CH_2Br_2 (liq) 57HAR/M
Dibromomethane; Methylene bromide
Heat Capacity 300 K, C_p=105.3 J·mol^{-1}·K^{-1}
Temperature range 243 to 303 K.
Molecular Weight 173.8348
Wiswesser Line Notation E1E
Evaluation B

CH_2Br_2 (liq) 93SHE
Dibromomethane; Methylene bromide
Heat Capacity 298.15 K, C_p=104.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 173.8348
Wiswesser Line Notation E1E
Evaluation B

CH_2Cl_2 (liq) 37PER
Dichloromethane; Methylene dichloride
Heat Capacity 292.5 K, C_p=100.8 J·mol^{-1}·K^{-1}
Temperature range −58 to 19 °C. Value is unsmoothed experimental datum.
Molecular Weight 84.9328
Wiswesser Line Notation G1G
Evaluation B

CH_2Cl_2 (liq) 37PER2
Dichloromethane; Methylene dichloride
Heat Capacity 292.5 K, C_p=100.5 J·mol^{-1}·K^{-1}
Temperature range −58 to 19 °C. Value is unsmoothed experimental datum.
Molecular Weight 84.9328
Wiswesser Line Notation G1G
Evaluation B

CH_2Cl_2 (liq) 40RIE
Dichloromethane; Methylene dichloride
Heat Capacity 298.1 K, C_p=100.0 J·mol^{-1}·K^{-1}
Temperature range −47 to 41 °C.
Molecular Weight 84.9328
Wiswesser Line Notation G1G
Evaluation A

CH_2Cl_2 (liq) 41RIE
Dichloromethane; Methylene dichloride
Heat Capacity 298 K, C_p=100.0 J·mol^{-1}·K^{-1}
Temperature range −47 to 41 °C.
Molecular Weight 84.9328
Wiswesser Line Notation G1G
Evaluation A

CH_2Cl_2 (liq) 48KUR
Dichloromethane; Methylene dichloride
Heat Capacity 298 K, C_p=129.3 J·mol^{-1}·K^{-1}
Temperature range −76 to 41 °C. Mean C_p, four temperatures.
Molecular Weight 84.9328
Wiswesser Line Notation G1G
Evaluation D

CH_2Cl_2 (liq) 57HAR/MOE
Dichloromethane; Methylene dichloride
Heat Capacity 303.2 K, C_p=105.5 J·mol^{-1}·K^{-1}
Temperature range 244 to 303 K. Unsmoothed experimental datum.
Molecular Weight 84.9328
Wiswesser Line Notation G1G
Evaluation C

CH_2Cl_2 (liq) 78MOS/RAB
Dichloromethane; Methylene dichloride
Heat Capacity 298.15 K, C_p=102.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=174.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 178.22 K, ΔH=6160 J·mol^{-1}
Molecular Weight 84.9328
Wiswesser Line Notation G1G
Evaluation A

CH_2I_2 (liq) 48KUR
Diiodomethane; Methylene iodide
Heat Capacity 298 K, C_p=133.9 J·mol^{-1}·K^{-1}
Temperature range 12 to 164 °C. Mean C_p, three temperatures.
Molecular Weight 267.8358
Wiswesser Line Notation I1I
Evaluation D

CH_2I_2 (liq) 93CAR/LAY
Diiodomethane; Methylene iodide
Heat Capacity 298.15 K, C_p=133.81 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 267.8358
Wiswesser Line Notation I1I
Evaluation A

CH_2I_2 (liq) 93SHE
Diiodomethane; Methylene iodide
Heat Capacity 298.15 K, C_p=112.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 267.8358
Wiswesser Line Notation I1I
Evaluation B

CH_2N_2 (c) 83DEW/DEK
Cyanamide
Heat Capacity 300 K, C_p=78.2 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K. Linearly extrapolated.
Phase Changes
c/liq 318.71 K, ΔH=7272 J·mol^{-1}
ΔS=22.82 J·mol^{-1}·K^{-1}
Molecular Weight 42.0402
Wiswesser Line Notation ZCN
Evaluation B(C_p), A(Phase changes).

CH_2N_4 (c) 89HIL/MOU
Tetrazole
Phase Changes
c/liq 430.7 K, ΔH=18400 J·mol^{-1}
Molecular Weight 70.0536
Wiswesser Line Notation T5MNNNJ
Evaluation A

CH_2N_4 (c,I) 93KAB/KOZ
Tetrazole
Heat Capacity 298.15 K, C_p=76.52 J·mol^{-1}·K^{-1}
Temperature range 5 to 320 K.
Entropy 298.15 K, S=96.36 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 242.5 K, ΔH=14.0 J·mol^{-1}
ΔS=0.060 J·mol^{-1}·K^{-1}
c,I/liq 430 K, ΔH=18000 J·mol^{-1}
ΔS=41.9 J·mol^{-1}·K^{-1}
c,I/g 353.1 K, ΔH=88160 J·mol^{-1}
ΔS=250 J·mol^{-1}·K^{-1}
Molecular Weight 70.0536
Wiswesser Line Notation T5MNNNJ
Evaluation A

$(CH_2O)_n$ (c) 59DAI/IVI
Polyoxymethylene
Heat Capacity 300 K, C_p=33.9 J·mol^{-1}·K^{-1}
Temperature range 300 to 333 K, mean value. Value per monomer unit.
Molecular Weight 30.0262
Wiswesser Line Notation /*O1*/
Evaluation B

$(CH_2O)_n$ (c) 62DAI/EVA
Polyoxymethylene
Heat Capacity 300 K, C_p=42.79 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K. Data given for Delrin. Data also given for trioxan copolymer where C_p(300 K)=41.11 J·mol^{-1}·K^{-1}.
Entropy 300 K, S=44.65 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K, Data given for Delrin. Data also given for trioxan copolymer where S(300 K)=43.21 J·mol^{-1}·K^{-1}.
Molecular Weight 30.0262
Wiswesser Line Notation /*O1*/
Evaluation A

CH_2O_2 (liq) 1881REI
Methanoic acid; Formic acid
Heat Capacity 298 K, C_p=95.4 J·mol^{-1}·K^{-1}
Temperature range 291 to 385 K.
Molecular Weight 46.0256
Wiswesser Line Notation VHQ
Evaluation D

CH_2O_2 (liq) 20GIB/LAT
Methanoic acid; Formic acid
Heat Capacity 291.5 K, C_p=98.3 J·mol^{-1}·K^{-1}
Temperature range 71 to 292 K. Value is unsmoothed experimental datum.
Entropy 298 K, S=143.1 J·mol^{-1}·K^{-1}
Used Berthelot's value, 10125 J·mol^{-1} for ΔH fusion. Extrapolation below 70 K, no details.
Molecular Weight 46.0256
Wiswesser Line Notation VHQ
Evaluation B(C_p), C(S)

CH_2O_2 (liq) 29PAR/KEL
Methanoic acid; Formic acid
Entropy 298.1 K, S=128.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 29.7 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 46.0256
Wiswesser Line Notation VHQ
Evaluation C

CH_2O_2 (liq) 34RAD/
Methanoic acid; Formic acid
Heat Capacity 290 K, C_p=100.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0256
Wiswesser Line Notation VHQ
Evaluation C

CH_2O_2 (liq) 36GLA/C
Methanoic acid; Formic acid
Heat Capacity 298.15 K, C_p=98.10 J·mol^{-1}·K^{-1}
Temperature range: 298.15, 333.15, 353.15 K.
Molecular Weight 46.0256
Wiswesser Line Notation VHQ
Evaluation B

CH_2O_2 (liq) 41STO/
Methanoic acid; Formic acid
Heat Capacity 298.15 K, C_p=99.04 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=131.84 J·mol^{-1}·K^{-1}
Includes 2.89 J·mol^{-1}·K^{-1} for zero-point entropy.
Phase Changes
c/liq 281.40 K, ΔH=12678 J·mol^{-1}
ΔS=45.05 J·mol^{-1}·K^{-1}
Molecular Weight 46.0256
Wiswesser Line Notation VHQ
Evaluation A

CH_2S_3 (liq) 63GAT/K
Dihydrosulfide carbon sulfide; Trithiocarbonic acid
Heat Capacity 273 K, C_p=146.5 J·mol^{-1}·K^{-1}
Temperature range −95 to 20 °C.
Entropy 298 K, S=218 J·mol^{-1}·K^{-1}
Extrapolation below −95°C. Estimated uncertainty ± 25 J·mo
K^{-1}.
Phase Changes
c/liq 246.3 K, ΔH=8410 J·mol^{-1}
ΔS=34.1 J·mol^{-1}·K^{-1}
Molecular Weight 110.2068
Wiswesser Line Notation SUYSHSH
Evaluation B(C_p),D(S)

CH_3DO (liq) 49STA/C
Methanol-d_1 ; Methyl alcohol-d_1
Heat Capacity 270 K, C_p=79.66 J·mol^{-1}·K^{-1}
Temperature range 90 to 270 K.
Phase Changes
c,II/c,I 161.1 K, ΔH=651.9 J·mol^{-1}
ΔS=4.05 J·mol^{-1}·K^{-1}
c,I/liq 173.5 K, ΔH=3038 J·mol^{-1}
ΔS=17.51 J·mol^{-1}·K^{-1}
Molecular Weight 33.0500
Wiswesser Line Notation Q1 &1H-2
Evaluation B

CH_3DO (liq) 92FIL/
Methanol-d_1 ; Methyl alcohol-d_1
Heat Capacity 298.15 K, C_p=83.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 33.0500
Wiswesser Line Notation Q1 &1H-2
Evaluation B

CH_3Br (liq) 38EGA/KEM

Bromomethane; Methyl bromide

Heat Capacity	280 K,	C_p=78.83 J·mol^{-1}·K^{-1}
Temperature range 15 to 280 K.		
Entropy	276.71 K,	S=155.14 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/c,I	173.78 K,	ΔH=473 J·mol^{-1}
		ΔS=2.72 J·mol^{-1}·K^{-1}
c,I/liq	179.47 K,	ΔH=5979 J·mol^{-1}
		ΔS=33.3 J·mol^{-1}·K^{-1}
liq/g	276.71 K,	ΔH=23912 J·mol^{-1}
		ΔS=86.42 J·mol^{-1}·K^{-1}
		P=101.325 kPA

Molecular Weight 94.9387
Wiswesser Line Notation E1
Evaluation A

CH_3Br (liq) 48KUR

Bromomethane; Methyl bromide

Heat Capacity 283 K, C_p=114.6 J·mol^{-1}·K^{-1}

Temperature range −67 to 9 °C. Mean C_p, three temperatures.

Molecular Weight 94.9387
Wiswesser Line Notation E1
Evaluation D

CH_3Cl (liq) 24SHO

Chloromethane; Methyl chloride

Heat Capacity 298 K, C_p=81.2 J·mol^{-1}·K^{-1}

Temperature range −30 to 40 °C.

Molecular Weight 50.4877
Wiswesser Line Notation G1
Evaluation C

CH_3Cl (liq) 40AWB/GRI

Chloromethane; Methyl chloride

Heat Capacity 293.15 K, C_p=80.8 J·mol^{-1}·K^{-1}

Temperature range 243 to 303 K. C_p reported at 20 °C=1.598 J·g^{-1}·K^{-1} and at 30°C=1.632 J·g^{-1}·K^{-1}.

Molecular Weight 50.4877
Wiswesser Line Notation G1
Evaluation B

CH_3Cl (liq) 40MES/AST

Chloromethane; Methyl chloride

Heat Capacity	249.67 K,	C_p=75.60 J·mol^{-1}·K^{-1}
Temperature range 12 to 249.67 K. Value is unsmoothed experimental datum.		
Entropy	248.94 K.	S=140.08 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	175.44 K.	ΔH=6431 J·mol^{-1}
		ΔS=36.66 J·mol^{-1}·K^{-1}
liq/g	248.94 K,	ΔH=21535 J·mol^{-1}
		ΔS=86.51 J·mol^{-1}·K^{-1}
		P=101.325 kPA

Molecular Weight 50.4877
Wiswesser Line Notation G1
Evaluation A
Correction in 40MES/AST2.

CH_3ClFOP (liq) 64FUR/REI

Methylphosphonyl chlorofluoride

Heat Capacity	298.15 K,	C_p=153.17 J·mol^{-1}·K^{-1}
Temperature range 15 to 335 K.		
Entropy	398.15 K,	S=216.40 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	250.70 K,	ΔH=11853 J·mol^{-1}
		ΔS=47.28 J·mol^{-1}·K^{-1}

Molecular Weight 116.4593
Wiswesser Line Notation OPGF1
Evaluation A

CH_3Cl_2OP (c) 64FUR/REI

Methylphosphonyl dichloride

Heat Capacity	298.15 K,	C_p=131.12 J·mol^{-1}·K^{-1}
Temperature range 15 to 335 K.		
Entropy	298.15 K,	S=164.84 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	306.14 K,	ΔH=18076 J·mol^{-1}
		ΔS=59.04 J·mol^{-1}·K^{-1}

Molecular Weight 132.9139
Wiswesser Line Notation OPGG1
Evaluation A

CH_3Cl_3Si (liq) 71SAM/KOS2

Trichloromethylsilane

Heat Capacity	298.15 K,	C_p=163.1 J·mol^{-1}·K^{-1}
Temperature range 14 to 307 K. Data deposited VINITI, No 2423-71, 17 December, 1970. C_p(liq)=25.5286 + 0.04132T + 100930T^{-2} (197.37 to 300 K) cal·mol^{-1}·K^{-1}.		
Entropy	298.15 K,	S=262.8 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	197.37 K,	ΔH=8945 J·mol^{-1}
		ΔS=45.31 J·mol^{-1}·K^{-1}

Molecular Weight 149.4792
Wiswesser Line Notation G-SI-GG1
Evaluation A
Debye temperature=98.84 K.

CH_3F_2OP (liq) 64FUR/REI

Methylphosphonyl difluoride

Heat Capacity	298.15 K,	C_p=145.14 J·mol^{-1}·K^{-1}
Temperature range 15 to 335 K.		
Entropy	298.15 K,	S=208.34 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	236.34 K,	ΔH=11878 J·mol^{-1}
		ΔS=50.26 J·mol^{-1}·K^{-1}

Molecular Weight 100.0047
Wiswesser Line Notation OPFF1
Evaluation A

CH_3I (liq) 48KUR

Iodomethane; Methyl iodide

Heat Capacity 298 K, C_p=148.1 J·mol^{-1}·K^{-1}

Temperature range −56 to 35 °C. Mean C_p five temperatures.

Molecular Weight 141.9392
Wiswesser Line Notation I1
Evaluation D

CH_3I (liq) 57HAR/MOE
Iodomethane; Methyl iodide
Heat Capacity 300 K, C_p=82.68 J·mol^{-1}·K^{-1}
Temperature range 243 to 303 K.
Molecular Weight 141.9392
Wiswesser Line Notation I1
Evaluation B

CH_3I (liq) 62LOW/MOE
Iodomethane; Methyl iodide
Heat Capacity 298.2 K, C_p=82.76 J·mol^{-1}·K^{-1}
Temperature range 293 to 308 K.
Molecular Weight 141.9392
Wiswesser Line Notation I1
Evaluation A

CH_3I (liq) 93CAR/LAY
Iodomethane; Methyl iodide
Heat Capacity 298.15 K, C_p=82.75 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 141.9392
Wiswesser Line Notation I1
Evaluation A

CH_3I (liq) 93SHE
Iodomethane; Methyl iodide
Heat Capacity 298.15 K, C_p=82.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 141.9392
Wiswesser Line Notation I1
Evaluation B

CH_3NO (liq) 07WAL
Formamide; Methanamide
Heat Capacity 292 K, C_p=105 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation D

CH_3NO (liq) 65SOM/COO
Formamide; Methanamide
Heat Capacity 298 K, C_p=107.6 J·mol^{-1}·K^{-1}
One temperature
Phase Changes
c/liq 275.72 K, ΔH=7980 J·mol^{-1}
ΔS=28.94 J·mol^{-1}·K^{-1}
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation B

CH_3NO (liq) 67RAS/GAN
Formamide; Methanamide
Heat Capacity 293 K, C_p=105.2 J·mol^{-1}·K^{-1}
Temperature range 293 to 373 K.
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation C

CH_3NO (liq) 74VIS/S
Formamide; Methanamide
Heat Capacity 298.15 K, C_p=108.11 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation A

CH_3NO (liq) 76BON/C
Formamide; Methanamide
Heat Capacity 298.15 K, C_p=107 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation B

CH_3NO (liq) 76SKO/S
Formamide; Methanamide
Heat Capacity 298.15 K, C_p=107.62 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation A

CH_3NO (liq) 77VOR/I
Formamide; Methanamide
Heat Capacity 298.15 K, C_p=108.11 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation A

CH_3NO (liq) 78DEV/H
Formamide; Methanamide
Heat Capacity 298.15 K, C_p=107.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation B

CH_3NO (liq) 83DEW/E
Formamide; Methanamide
Heat Capacity 298.15 K, C_p=107.61 J·mol^{-1}·K^{-1}
Temperature range 90 to 290 K. C_p=89.88 + 0.05947 (T/K) J·mol^{-1}·K^{-1} (275 to 300 K).
Phase Changes
c/liq 275.60 K, ΔH=8667 J·mol^{-1}
ΔS=31.448 J·mol^{-1}·K^{-1}
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation A

CH_3NO_2 (liq) 07V
Nitromethane
Heat Capacity 289 K, C_p=105 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 61.0402
Wiswesser Line Notation WN1
Evaluation D

CH_3NO_2 (liq) 25WIL
Nitromethane
Heat Capacity 298 K, C_p=100 J·mol^{-1}·K^{-1}
Temperature range 288 to 343 K. Equation only.
Molecular Weight 61.0402
Wiswesser Line Notation WN1
Evaluation C

CH_3NO_2 (liq) 47JON/GIA
Nitromethane
Heat Capacity 298.15 K, C_p=105.98 J·mol^{-1}· K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=171.75 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 244.77 K, ΔH=9703 J·mol^{-1}
ΔS=39.64 J·mol^{-1}·K^{-1}
liq/g 298.15 K, ΔH=38271 J·mol^{-1}
ΔS=128.36 J·mol^{-1}·K^{-1}
P=4.89 kPA
Molecular Weight 61.0402
Wiswesser Line Notation WN1
Evaluation A

CH_3NO_2 (liq) 50HOU/MAS
Nitromethane
Heat Capacity 313 K, C_p=108.8 J·mol^{-1}·K^{-1}
Temperature range 313 to 363 K.
Molecular Weight 61.0402
Wiswesser Line Notation WN1
Evaluation B

CH_3NO_2 (liq) 69BER/WES
Nitromethane
Heat Capacity 308 K, C_p=106.22 J·mol^{-1}·K^{-1}
Temperature range 308 to 473 K.
Molecular Weight 61.0402
Wiswesser Line Notation WN1
Evaluation B

CH_3NO_3 (liq) 53GRA/SMI
Methyl nitrate
Heat Capacity 298.2 K, C_p=157.19 J·mol^{-1}·K^{-1}
Temperature range 13 to 295 K.
Entropy 298.2 K, S=216.98 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 190.2 K, ΔH=8242 J·mol^{-1}
ΔS=43.33 J·mol^{-1}·K^{-1}
Molecular Weight 77.0396
Wiswesser Line Notation WNO1
Evaluation A

CH_3NaO (c) 57GRE/WES
Sodium methoxide
Heat Capacity 298.15 K, C_p=69.45 J·mol^{-1}·K^{-1}
Temperature range 5 to 340 K.
Entropy 298.15 K, S=110.58 J·mol^{-1}·K^{-1}
Phase Changes
Anomolous region near 34 K with excess enthalpy of 48.12 J·mol^{-1}, excess entropy of 1.80 J·mol^{-1}·K^{-1}.
Molecular Weight 54.0239
Wiswesser Line Notation O1 .NA
Evaluation A

CH_4 (c) 76VOG/PIT
Methane
Heat Capacity
Temperature range 0.4 to 28 K.
Phase Changes
c,II/c,I 20.53 K, ΔH=93.55 J·mol^{-1}
ΔS=4.557 J·mol^{-1}·K^{-1}
Lambda transition.
c,I/liq 90.67 K, ΔH=939.2 J·mol^{-1}
ΔS=10.36 J·mol^{-1}·K^{-1}
liq/g 99.54 K, ΔH=8519 J·mol^{-1}
ΔS=85.58 J·mol^{-1}·K^{-1}
P=2.81 kPa
Data from 37FRA/CLU and 39FRA/CLU.
Molecular Weight 16.0426
Wiswesser Line Notation 1H
Evaluation A

CH_4N_2O (c) 03MAG
Urea
Heat Capacity 298 K, C_p=80.7 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.321 cal·g^{-1}·K^{-1}.
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation D

CH_4N_2O (c) 20GIB/LAT
Urea
Heat Capacity 298.0 K, C_p=115.5 J·mol^{-1}·K^{-1}
Temperature range 86 to 300 K. Value is unsmoothed experimental datum.
Entropy 298 K, S=172 J·mol^{-1}·K^{-1}
Extrapolation below 86 K, no details.
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation B(C_p),C(S)

CH_4N_2O (c) 33PAR/HUF
Urea
Heat Capacity 298.0 K, C_p=93.64 J·mol^{-1}·K^{-1}
Temperature range 93 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=105.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 33.18 J·mol^{-1}·K^{-1}.
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation B(C_p),C(S)

CH_4N_2O (c) 40CAM/CAM
Urea
Heat Capacity 293 K, C_p=68.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation C

CH_4N_2O (c) 46RUE/HUF
Urea
Heat Capacity 298.15 K, C_p=93.14 J·mol^{-1}·K^{-1}
Temperature range 19 to 318 K.
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation A

CH_4N_2O (c) 66SAS/YOK
Urea
Heat Capacity 298.15 K, C_p=90.0 J·mol^{-1}·K^{-1}
Temperature range 90 to 298 K.
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation A

CH_4N_2O (c) 80VOG/SCH
Urea
Heat Capacity
Temperature range 323 to 493 K. Equation only: C_p=523.38 −265.60×10^{-2}T+41.50×10^{-4} T^2.
Phase Changes
c/liq 405.8 K, ΔH=13610 J·mol^{-1}
ΔS=33.54 J·mol^{-1}·K^{-1}
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation B
Dry sample.

CH_4N_2O (c) 86KOZ/DAL
Urea
Heat Capacity 298.15 K, C_p=93.08 J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K. C_p=38.43 + 4.98×10^{-2}T +7.05×10^{-4}T^2−8.61×10^{-7} T^3 (240 to 400 K).
Entropy 298.15 K, S=104.93 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 405.8 K, ΔH=13900 J·mol^{-1}
ΔS=34.25 J·mol^{-1}·K^{-1}
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation A

CH_4N_2O (c) 87DEL/TER
Urea
Phase Changes
c/liq 406.5 K, ΔH=14790 J·mol^{-1}
ΔS=36.4 J·mol^{-1}·K^{-1}
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation A

CH_4N_2O (c) 88GAM/BRO
Urea
Heat Capacity 304.7 K, C_p=94.0 J·mol^{-1}·K^{-1}
Temperature range 303 to 413 K.
Phase Changes
c/liq 406 K, ΔH=14500 J·mol^{-1}
ΔS=35.7 J·mol^{-1}·K^{-1}
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation B

CH_4N_2O (c) 93AND/MAT
Urea
Heat Capacity 298.15 K, C_p=92.79 J·mol^{-1}·K^{-1}
Temperature range 15 to 310 K.
Entropy 298.15 K, S=104.26 J·mol^{-1}·K^{-1}
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation A

$CH_4N_2O \cdot HNO_3$ (c) 85NUR/E
Urea nitrate
Heat Capacity 298.15 K, C_p=158.6 J·mol^{-1}·K^{-1}
Temperature range 60 to 330 K.
Entropy 298.15 K, S=189.2 J·mol^{-1}·K^{-1}
Molecular Weight 123.0682
Wiswesser Line Notation ZVZ &WNQ
Evaluation A

CH_4N_2S (c) 67WES/C
Thiourea
Heat Capacity 298.15 K, C_p=96.90 J·mol^{-1}·K^{-1}
Temperature range.
Entropy 298.15 K, S=115.8 J·mol^{-1}·K^{-1}
Molecular Weight 76.1160
Wiswesser Line Notation ZYZUS
Evaluation A
Anomalies occur at: 169.3 K, ΔS=0.17 J·mol^{-1}·K^{-1}; 171.2 ΔS=0.04 J·mol^{-1}·K^{-1}; 200 K, ΔS=0.71 J·mol^{-1}·K^{-1}. A slight hi in the heat capacity appears between 210 and 260 K.

CH_4N_2S (c) 82TOR/S
Thiourea
Heat Capacity 298.15 K, C_p=96.90 J·mol^{-1}·K^{-1}
One temperature. C_p data given as 1.273 J·K^{-1}·g^{-1}. Data f 67WES/CHA.
Phase Changes
c/g 298.15 K, ΔH=112000 J·mol^{-1}
ΔS=375.6 J·mol^{-1}·K^{-1}
Molecular Weight 76.1160
Wiswesser Line Notation ZYZUS
Evaluation B

CH_4N_2S (c) 70VAN/V
Ammonium thiocyanate
Heat Capacity 298.15 K, C_p=125.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 340 K.
Entropy 298.15 K, S=140.2 J·mol^{-1}·K^{-1}
Molecular Weight 76.1160
Wiswesser Line Notation NCSH &ZH
Evaluation A

CH_4N_2S (c) 88PET/
Ammonium thiocyanate
Phase Changes
c,II/c,I 360.7 K, ΔH=3200 J·mol^{-1}
ΔS=8.9 J·mol^{-1}·K^{-1}
Molecular Weight 76.1160
Wiswesser Line Notation NCSH &ZH
Evaluation A

$(CH_4N_2S)_3 \cdot C_2H_2Cl_4$ (c) 92SEK/I
Thiourea 1,1,2,2-tetrachloroethane clathrate
Heat Capacity 298.15 K, C_p=414.06 J·mol^{-1}· K^{-1}
Temperature range 13 to 330 K.
Entropy 298.15 K, S=570.71 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 224 K, ΔH=5940 J·mol^{-1}
ΔS=28.1 J·mol^{-1}·K^{-1}
c,II/c,I 248 K, ΔH=2756 J·mol^{-1}
ΔS=11.3 J·mol^{-1}·K^{-1}
Molecular Weight 396.1978
Wiswesser Line Notation ZYZUS 3 &GYGYGG
Evaluation A

$CH_4N_4O_2$ (c) 73KRI/LIC
Nitroguanidine
Heat Capacity 298 K, C_p=129.3 J·mol^{-1}·K^{-1}
Temperature range 200 to 460 K. Equation only.
Molecular Weight 104.0682
Wiswesser Line Notation WNMYZUM
Evaluation C

CD_4O (liq) 92FIL/AFA
Methanol-d_4; Methyl alcohol-d_4
Heat Capacity 298.15 K, C_p=87.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 36.0744
Wiswesser Line Notation QH &1H-2 &2H-2 3
Evaluation B

CHD_3O (liq) 92FIL/AFA
Methanol-d_3; Methyl alcohol-d_3
Heat Capacity 298.15 K, C_p=84.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 35.0663
Wiswesser Line Notation Q1 &2H-2 3
Evaluation B

CH_4O (liq) 1881REI
Methanol; Methyl alcohol
Heat Capacity 298 K, C_p=83.3 J·mol^{-1}·K^{-1}
Temperature range 288 to 335 K.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation D

CH_4O (liq) 07WAL
Methanol; Methyl alcohol
Heat Capacity 291 K, C_p=79 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation D

CH_4O (c) 25MAA/WAL
Methanol; Methyl alcohol
Heat Capacity 173 K, C_p=105 J·mol^{-1}·K^{-1}
Temperature range 93 to 173 K.
Phase Changes
c/liq 176 K, ΔH=2196 J·mol^{-1}
ΔS=12.5 J·mol^{-1}·K^{-1}
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation C

CH_4O (liq) 25PAR
Methanol; Methyl alcohol
Heat Capacity 290.1 K, C_p=79.9 J·mol^{-1}·K^{-1}
Temperature range 89 to 290 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=136.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 40.75 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 161.1 K, ΔH=590 J·mol^{-1}
ΔS=3.66 J·mol^{-1}·K^{-1}
c,I/liq 175.3 K, ΔH=3176 J·mol^{-1}
ΔS=18.12 J·mol^{-1}·K^{-1}
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B(C_p), C(S)

CH_4O (liq) 29KEL5
Methanol; Methyl alcohol
Heat Capacity 292.0 K, C_p=79.9 J·mol^{-1}·K^{-1}
Temperature range 16 to 293 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=126.8 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 157.4 K, ΔH=645.6 J·mol^{-1}
ΔS=4.10 J·mol^{-1}·K^{-1}
c,I/liq 175.2 K, ΔH=3167 J·mol^{-1}
ΔS=18.08 J·mol^{-1}·K^{-1}
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 29PAR/KEL
Methanol; Methyl alcohol
Entropy 298.1 K, S=129.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 34.3 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation C

CH_4O (liq) 29MIT/HAR
Methanol; Methyl alcohol
Heat Capacity 270 K, C_p=78.2 J·mol^{-1}·K^{-1}
Temperature range 190 to 270 K.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 31FIO/GIN
Methanol; Methyl alcohol
Heat Capacity 313.15 K, C_p=83.56 J·mol^{-1}·K^{-1}
Temperature range 40 to 110 °C.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation A

CH_4O (c) 37AHL/BLA
Methanol; Methyl alcohol
Heat Capacity 20.5 K, C_p=5.40 J·mol^{-1}·K^{-1}
Temperature range 5 to 28 K.
Entropy 16.25 K, S=1.117 J·mol^{-1}·K^{-1}
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation A

CH_4O (liq) 39PHI
Methanol; Methyl alcohol
Heat Capacity 300.8 K, C_p=86.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation C

CH_4O (liq) 49STA/GUP
Methanol; Methyl alcohol
Heat Capacity 270 K, C_p=75.77 J·mol^{-1}·K^{-1}
Temperature range 90 to 270 K.
Phase Changes
c,II/c,I 157.8 K, ΔH=711 J·mol^{-1}
ΔS=4.51 J·mol^{-1}·K^{-1}
c,I/liq 175.4 K, ΔH=3159 J·mol^{-1}
ΔS=18.01 J·mol^{-1}·K^{-1}
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 50HOU/MAS
Methanol; Methyl alcohol
Heat Capacity 323 K, C_p=86.2 J·mol^{-1}·K^{-1}
Temperature range 323 to 353 K.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 60SWI/ZIE
Methanol; Methyl alcohol
Heat Capacity 311 K, C_p=80.8 J·mol^{-1}·K^{-1}
Mean value 21 to 56 °C.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation C

CH_4O (liq) 62KAT
Methanol; Methyl alcohol
Heat Capacity 298.2 K, C_p=85.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 60 °C.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (gls) 68SUG/SUG
Methanol; Methyl alcohol
Heat Capacity 120 K, C_p=68.39 J·mol^{-1}·K^{-1}
Temperature range 20 to 120 K.
Phase Changes
c/gls 103 K, ΔH=1540 J·mol^{-1}
ΔS=14.95 J·mol^{-1}·K^{-1}
Glass transition.
c/liq 175 K
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation A

CH_4O (liq) 70PAZ/PAZ
Methanol; Methyl alcohol
Heat Capacity 313.2 K, C_p=85.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 71CAR/W
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=81.13 J·mol^{-1}·K^{-1}
Temperature range 5 to 332 K.
Entropy 298.15 K, S=127.19 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 157.34 K, ΔH=636.0 J·mol^{-1}
ΔS=4.04 J·mol^{-1}·K^{-1}
c,I/liq 175.59 K, ΔH=3215.4 J·mol^{-1}
ΔS=18.31 J·mol^{-1}·K^{-1}
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation A

CH_4O (liq) 71DES/BI
Methanol; Methyl alcohol
Heat Capacity 298 K, C_p=83.7 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 81ATA/E
Methanol; Methyl alcohol
Heat Capacity 293.15 K, C_p=80.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 82BEN/D
Methanol; Methyl alcohol
Heat Capacity 288.15 K, C_p=78.90 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 82VIL/C
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=81.92 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 84ZEG/S
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=81.47 J·mol^{-1}·K^{-1}
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 85COS/
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=80.22 J·mol^{-1}·K^{-1}
Temperature range 298.15, 313.15 K.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 86KOR/KUK
Methanol; Methyl alcohol
Heat Capacity 298 K, C_p=81.32 J·mol^{-1}·K^{-1}
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 86OGA/MUR
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=80.28 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 86TAN/TOY
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=81.56 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation A

CH_4O (liq) 87LAN/CRI
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=81.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 88AND/PAT
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=80.24 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 88OKA/OGA
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=80.35 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 89KHA/ZYK
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=81.11 J·mol^{-1}·K^{-1}
Temperature range 175 to 338 K. Unsmoothed experimental datum.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 92FIL/AFA
Methanol; Methyl alcohol
Heat Capacity 298.15 K, C_p=79.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O_3 (liq) 1881REI
Orthoformic acid
Heat Capacity 298 K, C_p=155.6 J·mol^{-1}·K^{-1}
Temperature range 293 to 406 K.
Molecular Weight 64.0408
Wiswesser Line Notation QYQQ
Evaluation D

CH_4S (liq) 42RUS/OSB
Methanethiol; Methyl mercaptan
Heat Capacity 280 K, C_p=89.04 J·mol^{-1}·K^{-1}
Temperature range 15 to 280 K.
Entropy 279.12 K, S=163.22 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 137.6 K, ΔH=219.7 J·mol^{-1}
ΔS=1.60 J·mol^{-1}·K^{-1}
c,I/liq 150.16 K, ΔH=5904 J·mol^{-1}
ΔS=39.32 J·mol^{-1}·K^{-1}
liq/g 279.12 K, ΔH=24568 J·mol^{-1}
ΔS=88.02 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 48.1026
Wiswesser Line Notation SH1
Evaluation A

CH_5N (liq) 37AST/SIL
Aminomethane; Methylamine
Heat Capacity 259.28 K, C_p=101.80 J·mol^{-1}·K^{-1}
Temperature range 14 to 259 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=150.2 J·mol^{-1}·K^{-1}
For superheated liquid, using extrapolated heat capacities.
Phase Changes
c/liq 179.70 K, ΔH=6134 J·mol^{-1}
ΔS=34.13 J·mol^{-1}·K^{-1}
liq/g 266.84 K, ΔH=25811 J·mol^{-1}
ΔS=96.73 J·mol^{-1}·K^{-1}
Molecular Weight 31.0572
Wiswesser Line Notation Z1
Evaluation A

CH_5N_3O (c) 85NUR/BER
Semicarbazide
Heat Capacity 298.15 K, C_p=110.6 J·mol^{-1}·K^{-1}
Temperature range 60 to 330 K.
Entropy 298.15 K, S=119.6 J·mol^{-1}·K^{-1}
Molecular Weight 75.0700
Wiswesser Line Notation ZVMZ
Evaluation A

CH_5N_3O (c) 86LEB/KUL
Semicarbazide
Heat Capacity 298.15 K, C_p=110.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=119.6 J·mol^{-1}·K^{-1}
Molecular Weight 75.0700
Wiswesser Line Notation ZVMZ
Evaluation A

$CH_5N_3O_3S$ (c) 84NUR/BER
Thiourea nitrate
Heat Capacity 298.15 K, C_p=175.4 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=213.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 265.3 K, ΔH=34.0 J·mol^{-1}
ΔS=0.130 J·mol^{-1}·K^{-1}
Molecular Weight 139.1288
Wiswesser Line Notation ZYZUS &WNQ
Evaluation A

$CH_5N_3O_4$ (c) 85NUR/BER
Urea nitrate
Heat Capacity 298.15 K, C_p=158.6 J·mol^{-1}·K^{-1}
Temperature range 13 to 330 K.
Entropy 298.15 K, S=189.2 J·mol^{-1}·K^{-1}
Molecular Weight 123.0682
Wiswesser Line Notation ZVZ &WNQ
Evaluation A

CH_5N_3S (c) 82TOR/SAB
Thiosemicarbazide
Heat Capacity 298.15 K, C_p=110.9 J·mol^{-1}·K^{-1}
One temperature. C_p data given as 1.217 J·K^{-1}·g^{-1}.
Phase Changes
c/g 298.15 K, ΔH=125800 J·mol^{-1}
ΔS=421.9 J·mol^{-1}·K^{-1}
Molecular Weight 91.1306
Wiswesser Line Notation ZYMZUS
Evaluation B

CH_5N_3S (c) 84NUR/BER
Thiosemicarbazide
Heat Capacity 298.15 K, C_p=114.3 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=128.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 268.9 K, ΔH=70.0 J·mol^{-1}
ΔS=0.250 J·mol^{-1}·K^{-1}
Molecular Weight 91.1306
Wiswesser Line Notation ZYMZUS
Evaluation A

CH_5N_3S (c,I) 85NUR/BER
Thiosemicarbazide
Heat Capacity 298.15 K, C_p=114.3 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=128.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 268.9 K, ΔH=70.0 J·mol^{-1}
ΔS=0.250 J·mol^{-1}·K^{-1}
Molecular Weight 91.1306
Wiswesser Line Notation ZYMZUS
Evaluation A

CD_6IN (c) 92YAM/MAT
Methylammonium iodide-d_6
Heat Capacity
Temperature range 13 to 303 K. Data not given.
Phase Changes
c,II/c,I 164.0 K, ΔS=8.8 J·mol^{-1}·K^{-1}
δ to α' transition.
Molecular Weight 165.0170
Wiswesser Line Notation Z1 &IH &1/2/5/H-2 6
Evaluation B

$CH_6AlNO_8S_2\cdot 12H_2O$ (c) 68ASH/S
Methyl ammonium aluminum alum
Heat Capacity 300 K, C_p=787.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 300 K, S=764.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 176.18 K, ΔS=9.70 J·mol^{-1}·K^{-1}
90 K Anomaly: Schottky type anomaly between 65 and 120 K, maxim
at 90 K, entropy estimated to be between 6 and 9 J·mol^{-1}·K^{-1}. 176
Anomaly: Due to free rotation of methylammonium group (CH_3NH
observed entropy change at 176.18 K is 9.70 J·mol^{-1}·K^{-1}.
Molecular Weight 467.3442
Wiswesser Line Notation AL Z1& S-O4*2 QH-12-
Evaluation A

CH_6ClN (c) 46AST/Z
Methylammonium chloride
Heat Capacity 298.15 K, C_p=90.92 J·mol^{-1}·K^{-1}
Temperature range 12 to 298 K.
Entropy 298 K, S=138.53 J·mol^{-1}·K^{-1}
Using metastable c, II below 220 K gives S=138.70 J·mol^{-1}·K^{-1}.
Phase Changes
c,III/c,II 220.4 K, ΔH=1778 J·mol^{-1}
ΔS=8.07 J·mol^{-1}·K^{-1}
c,II/c,I 264.5 K, ΔH=2820 J·mol^{-1}
ΔS=10.66 J·mol^{-1}·K^{-1}
Molecular Weight 67.5181
Wiswesser Line Notation Z1 &GH
Evaluation A

CH_6BrN (c) 90GEN/L
Methylammoniumbromide
Heat Capacity 300 K, C_p=79.2 J·mol^{-1}·K^{-1}
Temperature range 300 to 480 K. C_p(c)=155.1 −0.514T+8.70×1(
T^2 J·mol^{-1}·K^{-1} (300 to 480 K).
Phase Changes
c,III/c,II 397.7 K, ΔH=1600 J·mol^{-1}
ΔS=4.02 J·mol^{-1}·K^{-1}
c,II/c,I 488.4 K, ΔH=3510 J·mol^{-1}
ΔS=7.18 J·mol^{-1}·K^{-1}
c,I/liq 531.9 K, ΔH=8340 J·mol^{-1}
ΔS=15.69 J·mol^{-1}·K^{-1}
Molecular Weight 111.9691
Wiswesser Line Notation Z1 &EH
Evaluation A

CH_6Br_3NPb (c) 90ONO/M
Methylammonium tribromoplumbate(II)
Heat Capacity 300.44 K, C_p=170.7 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Unsmoothed experimental datum.
Phase Changes
c,IV/c,III 148.8 K, ΔH=1590 J·mol^{-1}
ΔS=11.2 J·mol^{-1}·K^{-1}
c,III/c,II 154.0 K, ΔH=620 J·mol^{-1}
ΔS=4.1 J·mol^{-1}·K^{-1}
c,II/c,I 236.3 K, ΔH=1710 J·mol^{-1}
ΔS=8.2 J·mol^{-1}·K^{-1}
Molecular Weight 478.9771
Wiswesser Line Notation Z1 &-PB-EEE
Evaluation A

CH_6Br_3NSn (c) 91ONO/MAT
Methyl ammonium tin bromide
Heat Capacity 298.15 K, C_p=170.45 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=342.72 J·mol^{-1}·K^{-1}
Phase Changes
c,V/c,IV 46.0 K, ΔH=16 J·mol^{-1}
ΔS=0.37 J·mol^{-1}·K^{-1}
c,IV/c,III 188.2 K, ΔH=1000 J·mol^{-1}
ΔS=6.02 J·mol^{-1}·K^{-1}
c,III/c,II 213.0 K
c,II/c,I 229.4 K, ΔH=4280 J·mol^{-1}
ΔS=18.98 J·mol^{-1}·K^{-1}
c,III/c,II plus c,II/c,I
Molecular Weight 869.8911
Wiswesser Line Notation 1ZH .SN E3
Evaluation A

CH_6ClN_3O (c) 41SAT/SOG4
Semicarbazide hydrochloride
Heat Capacity 323 K, C_p=143.5 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 111.5309
Wiswesser Line Notation ZVMZ &GH
Evaluation C
Same data in 40SAT/SOG5

CH_6Cl_3NPb (c) 90ONO/MAT
Methylammonium trichloroplumbate(II)
Heat Capacity 300.23 K, C_p=170.2 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Unsmoothed experimental datum.
Phase Changes
c,III/c,II 171.5 K, ΔH=2400 J·mol^{-1}
ΔS=14.6 J·mol^{-1}·K^{-1}
c,II/c,I 177.2 K, ΔH=1920 J·mol^{-1}
ΔS=10.0 J·mol^{-1}·K^{-1}
Molecular Weight 345.6241
Wiswesser Line Notation Z1 &-PB-GGG
Evaluation A

CH_6IN (c) 86YAM/OGU
Methylammonium iodide
Heat Capacity 298.15 K, C_p=93.93 J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K.
Entropy 298.15 K, S=160.3 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 166.1 K
Undercooled α' to metastable δ.
Molecular Weight 158.9696
Wiswesser Line Notation Z1 &IH
Evaluation A
Data given for β' phase from 10 to 220 K. β' to α' phase transition at 220 K, ΔH=2970 J·mol^{-1}, ΔS=13.5 J·mol^{-1}·K^{-1}.

CH_6I_3NPb (c) 90ONO/MAT
Methylammonium triiodoplumbate(II)
Heat Capacity 299.14 K, C_p=189.6 J·mol^{-1}·K^{-1}
Temperature range 13 to 365 K. Unsmoothed experimental datum.
Phase Changes
c,III/c,II 161.4 K, ΔH=2980 J·mol^{-1}
ΔS=19.0 J·mol^{-1}·K^{-1}
c,II/c,I 330.4 K, ΔH=2580 J·mol^{-1}
ΔS=9.7 J·mol^{-1}·K^{-1}
Molecular Weight 619.9786
Wiswesser Line Notation Z1 &-PB-III
Evaluation A

CH_6N_2 (liq) 51AST/FIN
Methylhydrazine
Heat Capacity 298.15 K, C_p=134.93 J·mol^{-1}·K^{-1}
Temperature range 15 to 298 K.
Entropy 298.15 K, S=165.94 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 220.79 K, ΔH=10418 J·mol^{-1}
ΔS=47.19 J·mol^{-1}·K^{-1}
liq/g 298.15 K, ΔH=40367 J·mol^{-1}
ΔS=135.39 J·mol^{-1}·K^{-1}
P=6.62 kPa
Molecular Weight 46.0718
Wiswesser Line Notation ZM1
Evaluation A

$CH_6N_2O_2$ (c) 28CLU/HAR
Ammonium carbamate
Heat Capacity 295.5 K, C_p=131.00 J·mol^{-1}·K^{-1}
Temperature range 13 to 296 K.
Molecular Weight 78.0706
Wiswesser Line Notation ZVQ &ZH
Evaluation B

CH_6N_4S (c) 82TOR/SAB
Thiocarbohydrazide
Heat Capacity 298.15 K, C_p=125.3 J·mol^{-1}·K^{-1}
One temperature. C_p data given as 1.180 J·K^{-1}·g^{-1}.
Phase Changes
c/g 298.15 K, ΔH=152100 J·mol^{-1}
ΔS=510.1 J·mol^{-1}·K^{-1}
Molecular Weight 106.1452
Wiswesser Line Notation ZMYMZUS
Evaluation B

CI_4 (c) 93CAR/LAY
Tetraiodomethane
Heat Capacity 298.15 K, C_p=259.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 519.6290
Wiswesser Line Notation IXIII
Evaluation A

CKNS (c) 70VAN/WES
Potassium thiocyanate
Heat Capacity 298.15 K, C_p=88.53 J·mol^{-1}·K^{-1}
Temperature range 5 to 340 K.
Entropy 298.15 K, S=124.3 J·mol^{-1}·K^{-1}
Molecular Weight 97.1760
Wiswesser Line Notation K SCN
Evaluation A

CKNS (c) 92HAM/HOU
Potassium thiocyanate
Phase Changes
c,II/c,I 413 K, ΔH=590–707 J·mol^{-1}
ΔS=1.43–1.71 J·mol^{-1}·K^{-1}
Dependent on heating/cooling rate.
Molecular Weight 97.1760
Wiswesser Line Notation K SCN
Evaluation A

COS (liq) 37KEM/GIA
Carbonyl sulfide
Heat Capacity 220 K, C_p=71.25 J·mol^{-1}·K^{-1}
Temperature range 20 to 220 K.
Entropy 222.91 K, S=136.31 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 134.33 K, ΔH=4728 J·mol^{-1}
ΔS=35.20 J·mol^{-1}·K^{-1}
liq/g 222.91 K, ΔH=18506 J·mol^{-1}
ΔS=83.02 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 60.0704
Wiswesser Line Notation SCO
Evaluation A

CS_2 (liq) 37BRO/MAN
Carbon disulfide
Heat Capacity 297.43 K, C_p=76.02 J·mol^{-1}·K^{-1}
Temperature range 15 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=151.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 161.11 K, ΔH=4389 J·mol^{-1}
ΔS=27.24 J·mol^{-1}·K^{-1}
Molecular Weight 76.1310
Wiswesser Line Notation SCS
Evaluation A

CS_2 (liq) 39MAZ3
Carbon disulfide
Heat Capacity 293 K, C_p=77.8 J·mol^{-1}·K^{-1}
Temperature range −100 to 20 °C.
Molecular Weight 76.1310
Wiswesser Line Notation SCS
Evaluation C

CS_2 (liq) 39PHI
Carbon disulfide
Heat Capacity 301.2 K, C_p=76.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 76.1310
Wiswesser Line Notation SCS
Evaluation C

CS_2 (liq) 45ZHD
Carbon disulfide
Heat Capacity 294.81 K, C_p=74.89 J·mol^{-1}·K^{-1}
Temperature range 7 to 31 °C. Value is unsmoothed experimental datum.
Molecular Weight 76.1310
Wiswesser Line Notation SCS
Evaluation B

CS_2 (liq) 55STA/TUP
Carbon disulfide
Heat Capacity 298 K, C_p=78.99 J·mol^{-1}·K^{-1}
Temperature range 286 to 317 K.
Molecular Weight 76.1310
Wiswesser Line Notation SCS
Evaluation B

CSe_2 (liq) 66GAT/D
Carbon diselenide
Heat Capacity 298 K, C_p=88.7 J·mol^{-1}·K^{-1}
Temperature range −190 to 50 °C.
Entropy 298 K, S=165.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 229.5 K, ΔH=6360 J·mol^{-1}
ΔS=27.7 J·mol^{-1}·K^{-1}
Molecular Weight 169.9310
Wiswesser Line Notation -SE-C-SE-
Evaluation B

$C_2Br_2D_4$ (liq) 49WUY/J
1,2-Dibromoethane-d_4
Heat Capacity 310 K, C_p=149.12 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 191.8864
Wiswesser Line Notation E2E &2/H-2 4
Evaluation C

$C_2Br_2F_4$ (liq) 82KOS/Z
1,2-Dibromotetrafluoroethane
Heat Capacity 298.15 K, C_p=170.8 J·mol^{-1}·K^{-1}
Temperature range 8 to 300 K.
Entropy 298.15 K, S=299.4 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 162.83 K, ΔH=7036.7 J·mol^{-1}
ΔS=43.22 J·mol^{-1}·K^{-1}
Molecular Weight 259.8236
Wiswesser Line Notation FXFEXFFE
Evaluation A

$C_2Br_2F_4$ (liq) 88VES/Z
1,2-Dibromotetrafluoroethane
Heat Capacity 298.15 K, C_p=173.8 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K. C_p(J·mol^{-1}·K^{-1})=13 +0.1420(T/K) (298 to 318 K).
Molecular Weight 259.8236
Wiswesser Line Notation FXFEXFFE
Evaluation A

$C_2CaO_4·H_2O$ (c) 33LAT/S
Calcium oxalate monohydrate
Heat Capacity 299.78 K, C_p=152.4 J·mol^{-1}·K^{-1}
Temperature range 19 to 300 K. C_p value is unsmoothed experime datum.
Entropy 298.1 K, S=156.0 J·mol^{-1}·K^{-1}
Molecular Weight 146.1128
Wiswesser Line Notation OVVO .CA &QH
Evaluation B

C_2ClF_3 (liq) 51OLI/
Chlorotrifluoroethene; Chlorotrifluoroethylene; Trifluorochloroeth Trifluorochloroethylene
Heat Capacity 244.80 K, C_p=122.42 J·mol^{-1}·K^{-1}
Temperature range 16 to 245 K.
Entropy 244.80 K, S=220.66 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 115.0 K, ΔH=5552.6 J·mol^{-1}
ΔS=48.28 J·mol^{-1}·K^{-1}
Molecular Weight 116.4702
Wiswesser Line Notation GYFUYFF
Evaluation A

C_2ClF_3 (liq) 84GOL/KOL

Chlorotrifluoroethene; Chlorotrifluoroethylene; Trifluorochloroethane; Trifluorochloroethylene

Phase Changes

c/liq	118.3 K,	ΔH=5282 J·mol^{-1}
		ΔS=44.6 J·mol^{-1}·K^{-1}

Molecular Weight 116.4702

Wiswesser Line Notation GYFUYFF

Evaluation A

$(C_2ClF_3)_n$ (c) 52HOF

Polytrifluorochloroethylene; Polytrifluorovinyl chloride

Heat Capacity 298 K, C_p=101.7 J·mol^{-1}·K^{-1}

Temperature range 0 to 241 °C. Values given for *air-quenched* and slow-cooled samples. Values per monomer unit slow-cooled samples. Unsmoothed experimental datum.

Molecular Weight 116.4702

Wiswesser Line Notation /*XGFXFF*/

Evaluation B

$(C_2ClF_3)_n$ (liq) 57YAR/KAY

Polytrifluorochloroethylene; Polytrifluorovinyl chloride

Heat Capacity 298 K, C_p=116.3 J·mol^{-1}·K^{-1}

Temperature range 298 to 373 K. Equation only. Values per monomer unit.

Molecular Weight 116.4702

Wiswesser Line Notation /*XGFXFF*/

Evaluation B

$(C_2ClF_3)_n$ (c) 92CHA/WEE

Polytrifluorochloroethylene; Polytrifluorovinyl chloride

Heat Capacity 298.15 K, C_p=97.22 J·mol^{-1}·K^{-1}

Temperature range 2.5 to 620 K.

C_p(amorph, 298.15 K)=103.93 J/mol·K.

Entropy 298.15 K, S=111.00 J·mol^{-1}·K^{-1}

S(amorp, 298.15 K)=110.27 J/mol·K.

Phase Changes

c/liq	497 K,	ΔH=4659 J·mol^{-1}
		ΔS=9.3 J·mol^{-1}·K^{-1}

Molecular Weight 116.4702

Wiswesser Line Notation /*XGFXFF*/

Evaluation A

T(glass)=240 to 400 K. Thermal treatment yields varying degrees of sample cystallinity with related but differing values for Tm and ΔH fusion.

C_2ClF_5 (liq) 55AST/WIL

Pentafluorochloroethane

Heat Capacity 234.04 K, C_p=145.27 J·mol^{-1}·K^{-1}

Temperature range 15 to 234 K. Value is unsmoothed experimental datum.

Entropy 234.04 K, S=248.03 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I	80.24 K,	ΔH=2628 J·mol^{-1}
		ΔS=32.75 J·mol^{-1}·K^{-1}
c,I/liq	173.71 K,	ΔH=1879 J·mol^{-1}
		ΔS=10.82 J·mol^{-1}·K^{-1}
liq/g	234.04 K,	ΔH=19410 J·mol^{-1}
		ΔS=82.93 J·mol^{-1}·K^{-1}
		P=101.325 kPa

Molecular Weight 154.4670

Wiswesser Line Notation GXFFXFFF

Evaluation A

$C_2Cl_2F_4$ (liq) 37PER

1,2-Dichloro-1,1,2,2-tetrafluoroethane: Freon 114

Heat Capacity 293.3 K, C_p=169.9 J·mol^{-1}·K^{-1}

Temperature range −188 to 20 °C. Value is unsmoothed experimental datum.

Molecular Weight 170.9216

Wiswesser Line Notation GXFFXGFF

Evaluation C

Probably a mixture of isomers.

$C_2Cl_2F_4$ (liq) 37PER2

1,2-Dichloro-1,1,2,2-tetrafluoroethane; Freon 114

Heat Capacity 293.3 K, C_p=169.9 J·mol^{-1}·K^{-1}

Temperature range −188 to 20 °C. Value is unsmoothed experimental datum.

Molecular Weight 170.9216

Wiswesser Line Notation GXFFXGFF

Evaluation C

Probably a mixture of isomers. Shows peaks in heat capacity at −180 °C, −140 °C, and −100 °C, which may be glassy transitions.

$C_2Cl_2F_4$ (liq) 81KOL/KOS

1,2-Dichloro-1,1,2,2-tetrafluoroethane; Freon 114

Heat Capacity 98.15 K, C_p=164.0 J·mol^{-1}·K^{-1}

Temperature range 8 to 300 K.

Entropy 298.15 K, S=282.0 J·mol^{-1}·K^{-1}

Phase Changes

c,III/c,II	109.3 K,	ΔH=1212 J·mol^{-1}
		ΔS=11.09 J·mol^{-1}·K^{-1}
c,II/c,I	134.6 K,	ΔH=2628 J·mol^{-1}
		ΔS=19.5 J·mol^{-1}·K^{-1}
c,I/liq	180.62 K,	ΔH=1510 J·mol^{-1}
		ΔS=8.36 J·mol^{-1}·K^{-1}

Molecular Weight 170.9216

Wiswesser Line Notation GXFFXGFF

Evaluation A

$C_2Cl_2F_4$ (liq) 88SAI/SAT

1,2-Dichloro-1,1,2,2-tetrafluoroethane; Freon 114

Heat Capacity

Pressure, temperature study, equation only.

Molecular Weight 170.9216

Wiswesser Line Notation GXFFXGFF

Evaluation A

$C_2Cl_3F_3$ (liq) 38RIE

1,1,2-Trichloro-1,2,2-trifluoroethane; Freon 113

Heat Capacity 98.2 K, C_p=177.0 J·mol^{-1}·K^{-1}

Temperature range −30 to 61 °C.

Molecular Weight 187.3762

Wiswesser Line Notation GXGFXGFF

Evaluation B

$C_2Cl_3F_3$ (liq) 39RIE

1,1,2-Trichloro-1,2,2-trifluoroethane; Freon 113

Heat Capacity 298.2 K, C_p=177.0 J·mol^{-1}·K^{-1}

Temperature range −30 to 61 °C.

Molecular Weight 187.3762

Wiswesser Line Notation GXGFXGFF

Evaluation B

$C_2Cl_3F_3$ (liq) 40BEN/MCH
1,1,2-Trichloro-1,2,2-trifluoroethane; Freon 113
Heat Capacity 98.15 K, C_p=179.8 J·mol^{-1}·K^{-1}
Temperature range 243 to 336 K. Data calculated from equation.
Molecular Weight 187.3762
Wiswesser Line Notation GXGFXGFF
Evaluation B

$C_2Cl_3F_3$ (liq) 81KOL/KOS
1,1,2-Trichloro-1,2,2-trifluoroethane; Freon 113
Heat Capacity 298.15 K, C_p=172.8 J·mol^{-1}·K^{-1}
Temperature range 8 to 300 K.
Entropy 298.15 K, S=289.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 82.5 K, ΔH=830.9 J·mol^{-1}
ΔS=10.1 J·mol^{-1}·K^{-1}
c,I/liq 236.92 K, ΔH=2467 J·mol^{-1}
ΔS=10.4 J·mol^{-1}·K^{-1}
Molecular Weight 187.3762
Wiswesser Line Notation GXGFXGFF
Evaluation A

$C_2Cl_3F_3$ (liq) 84GOL/KOL
1,1,2-Trichloro-1,2,2-trifluoroethane; Freon 113
Phase Changes
c/liq 273.93 K, ΔH=2326 J·mol^{-1}
ΔS=8.49 J·mol^{-1}·K^{-1}
Molecular Weight 187.3762
Wiswesser Line Notation GXGFXGFF
Evaluation A

$C_2Cl_3F_3$ (liq) 88VES/ZAB
1,1,2-Trichloro-1,2,2-trifluoroethane; Freon 113
Heat Capacity 298.15 K, C_p=172.9 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K. C_p(J·mol^{-1}·K^{-1})=113.21 +0.1991(T/K) (240 to 337 K).
Molecular Weight 187.3762
Wiswesser Line Notation GXGFXGFF
Evaluation A

$C_2Cl_3F_3$ (liq) 92WIR/BRA2
1,1,2-Trichloro-1,2,2-trifluoroethane; Freon 113
Heat Capacity 303.15 K, C_p=172.5 J·mol^{-1}·K^{-1}
Temperature range 288 to 503 K. p=0.6 MPa.
Molecular Weight 187.3762
Wiswesser Line Notation GXGFXGFF
Evaluation A

$C_2Cl_3F_3$ (liq) 87OTT/WOO
1,1,1-Trichlorotrifluoroethane
Phase Changes
c,II/c,I 148 K
Solid-plastic crystal.
c,I/liq 287.52 K, ΔH=4110 J·mol^{-1}
ΔS=14 J·mol^{-1}·K^{-1}
Molecular Weight 187.3762
Wiswesser Line Notation GXGGXFFF
Evaluation A

$C_2Cl_3F_3$ (liq) 88SVO/VI
1,1,1-Trichlorotrifluoroethane
Heat Capacity 298.16 K, C_p=168.6 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K. C_p(J·mol^{-1}·K^{-1})=109 +0.200 (T/K) (298 to 318 K).
Molecular Weight 187.3762
Wiswesser Line Notation GXGGXFFF
Evaluation A

C_2Cl_4 (liq) 1881R
Tetrachloroethylene; Tetrachloroethene
Heat Capacity 298 K, C_p=146.9 J·mol^{-1}·K^{-1}
Temperature range 291 to 410 K.
Molecular Weight 165.8340
Wiswesser Line Notation GYGUYGG
Evaluation D

C_2Cl_4 (liq) 48KU
Tetrachloroethylene; Tetrachloroethene
Heat Capacity 298 K, C_p=139.7 J·mol^{-1}·K^{-1}
Temperature range 16 to 119 °C, mean C_p two temperatures.
Molecular Weight 165.8340
Wiswesser Line Notation GYGUYGG
Evaluation D

C_2Cl_4 (liq) 82GRO/IN
Tetrachloroethylene; Tetrachloroethene
Heat Capacity 298.15 K, C_p=146.5 J·mol^{-1}·K^{-1}
Temperature range 298.15 K. One data point given.
Molecular Weight 165.8340
Wiswesser Line Notation GYGUYGG
Evaluation A

C_2Cl_4 (liq) 86NOV/RA
Tetrachloroethylene; Tetrachloroethene
Heat Capacity 298.15 K, C_p=157.9 J·mol^{-1}·K^{-1}
Temperature range 6 to 300 K.
Entropy 298.15 K, S=240.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 125–210 K, ΔH=820 J·mol^{-1}
ΔS=5.26 J·mol^{-1}·K^{-1}
c/liq 250.81 K, ΔH=10880 J·mol^{-1}
ΔS=43.38 J·mol^{-1}·K^{-1}
Molecular Weight 165.8340
Wiswesser Line Notation GYGUYGG
Evaluation A

C_2Cl_4 (liq) 89WIL/L
Tetrachloroethylene; Tetrachloroethene
Heat Capacity 298.15 K, C_p=147.16 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 165.8340
Wiswesser Line Notation GYGUYGG
Evaluation B

$C_2Cl_4F_2$ (c) 84GOL/K
1,1,1,2-Tetrachlorodifluoroethane
Phase Changes
c/liq 314.2 K, ΔH=3990 J·mol^{-1}
ΔS=12.7 J·mol^{-1}·K^{-1}
Molecular Weight 203.8308
Wiswesser Line Notation GXGGXGFF
Evaluation A

$C_2Cl_4F_2$ (liq) 57YAR/KAY
1,1,2,2-Tetrachloro-1,2-difluoroethane
Heat Capacity 298 K, C_p=173.6 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K. Equation only.
Molecular Weight 203.8308
Wiswesser Line Notation GXGFXGGF
Evaluation B

$C_2Cl_4F_2$ (liq) 78KOS/KOL
1,1,2,2-Tetrachloro-1,2-difluoroethane
Heat Capacity 298.15 K, C_p=175.52 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K. Complete data deposited at VINITI, No. 3512-77, 20 Aug 1977.
Entropy 298.15 K, S=273.84 J·mol^{-1}·K^{-1}
Low entropy of fusion indicates possible zero point entropy (disorder).
Phase Changes
c/liq 299.70 K, ΔH=3696.6 J·mol^{-1}
ΔS=12.33 J·mol^{-1}·K^{-1}
Molecular Weight 203.8308
Wiswesser Line Notation GXGFXGGF
Evaluation B

$C_2Cl_4F_2$ (liq) 78KIS/SUG
1,1,2,2-Tetrachloro-1,2-difluoroethane
Heat Capacity 300 K, C_p=178.59 J·mol^{-1}·K^{-1}
Temperature range 13 to 310 K.
Entropy 300 K, S=283.43 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 297.91 K, ΔH=3666 J·mol^{-1}
ΔS=12.31 J·mol^{-1}·K^{-1}
Molecular Weight 203.8308
Wiswesser Line Notation GXGFXGGF
Evaluation A

$C_2Cl_4F_2$ (liq) 92SVO/KUB2
1,1,2,2-Tetrachloro-1,2-difluoroethane
Phase Changes
liq/g 366.2 K, ΔH=35170 J·mol^{-1}
Value obtained by extrapolation.
Molecular Weight 203.8308
Wiswesser Line Notation GXGFXGGF
Evaluation A

C_2Cl_6 (c) 50SEK/MOM
Hexachloroethane
Heat Capacity 298.5 K, C_p=218.0 J·mol^{-1}·K^{-1}
Temperature range 295 to 351 K. Unsmoothed experimental datum.
Phase Changes
c,III/c,II 318 K, ΔH=2565 J·mol^{-1}
ΔS=8.08 J·mol^{-1}·K^{-1}
c,II/c,I 345 K, ΔH=8222 J·mol^{-1}
ΔS=23.8 J·mol^{-1}·K^{-1}
c,I/liq 458 K, ΔH=9749 J·mol^{-1}
ΔS=23.0 J·mol^{-1}·K^{-1}
Molecular Weight 236.7400
Wiswesser Line Notation GXGGXGGG
Evaluation B(C_p), A(Phase changes)

C_2Cl_6 (c) 70MUR/BRE2
Hexachloroethane
Phase Changes
c,III/c,II 320 K, ΔH=2605 J·mol^{-1}
ΔS=8.16 J·mol^{-1}·K^{-1}
c,II/c,I 345 K, ΔH=6310 J·mol^{-1}
ΔS=18.32 J·mol^{-1}·K^{-1}
c,I/liq 454 K
Molecular Weight 236.7400
Wiswesser Line Notation GXGGXGGG
Evaluation A

C_2Cl_6 (c) 75RAK/GUT
Hexachloroethane
Heat Capacity 298.15 K, C_p=198.24 J·mol^{-1}·K^{-1}
Temperature range 13.7 to 360 K.
Entropy 298.15 K, S=237.3 J·mol^{-1}·K^{-1}
Entropy estimated at 13 K to be 3.10 J·mol^{-1}·K^{-1}.
Phase Changes
c,III/c,II 317.4 K, ΔH=2644 J·mol^{-1}
ΔS=8.33 J·mol^{-1}·K^{-1}
c,II/c,I 344.6 K, ΔH=6916 J·mol^{-1}
ΔS=20.1 J·mol^{-1}·K^{-1}
Molecular Weight 236.7400
Wiswesser Line Notation GXGGXGGG
Evaluation A

C_2Cl_6 (c) 88PET/TSY
Hexachloroethane
Phase Changes
c,III/c,II 316.8 K, ΔH=2100 J·mol^{-1}
ΔS=6.6 J·mol^{-1}·K^{-1}
c,II/c,I 345.0 K, ΔH=6300 J·mol^{-1}
ΔS=18.3 J·mol^{-1}·K^{-1}
Molecular Weight 236.7400
Wiswesser Line Notation GXGGXGGG
Evaluation A

$C_2Cl_6D_{12}N_2Sn$ (c) 88MAT/YAN
Bis(methylammonium-d_6) hexachlorostannate (IV)
Heat Capacity 298.15 K, C_p=321.68 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=498.62 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 154.96 K, ΔH=2810 J·mol^{-1}
ΔS=21.8 J·mol^{-1}·K^{-1}
Order/disorder transition.
Molecular Weight 407.6512
Wiswesser Line Notation 1ZH 2 -SN- G6 &1/H-2 3 &2/H-2 3
Evaluation A

$C_2DH_3Br_2$ (liq) 49DHO/JUN
1,2-Dibromoethane-d_1; Ethylene dibromide-d_1
Heat capacity 293 K, C_p=137.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 188.8695
Wiswesser Line Notation E2E &2/H-2
Evaluation B

$C_2DH_3Br_2$ (liq) 49WUY/JUN
1,2-Dibromoethane-d_1; Ethylene dibromide-d_1
Heat Capacity 310 K, C_p=138.28 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 188.8695
Wiswesser Line Notation E2E &2/H-2
Evaluation C

$C_2D_2H_2Br_2$ (liq) 49DHO/JUN
1,2-Dibromoethane-d_2(1,1); Ethylene dibromide-d_2(1,1)
Heat Capacity 293 K, C_p=142.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 189.8774
Wiswesser Line Notation E2E &2-1/H-2 2
Evaluation C

$C_2D_2H_2Br_2$ (liq) 49WUY/JUN
1,2-Dibromoethane-d_2(1,1); Ethylene dibromide-d_2(1,1)
Heat Capacity 310 K, C_p=143.64 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 189.8774
Wiswesser Line Notation E2E &2-1/H-2 2
Evaluation C

$C_2D_2H_2Br_2$ (liq) 49DHO/JUN
1,2-Dibromoethane-d_2(1,2); Ethylene dibromide-d_2(1,2)
Heat Capacity 293 K, C_p=141.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 189.8774
Wiswesser Line Notation E2E &2-1/2-2/H-2 2
Evaluation C

$C_2D_2H_2Br_2$ (liq) 49WUY/JUN
1,2-Dibromoethane-d_2(1,2); Ethylene dibromide-d_2(1,2)
Heat Capacity 310 K, C_p=142.13 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 189.8774
Wiswesser Line Notation E2E &2-1/2-2/H-2 2
Evaluation C

$C_2D_2H_4O_2$ (liq) 62RAB/NIK
1,2-Dihydroxyethane-d_2; 1,2-Ethanediol-d_2; Ethylene glycol-d_2
Heat Capacity 298 K, C_p=155.94 J·mol^{-1}·K^{-1}
Temperature range 10 to 55 °C.
Molecular Weight 64.0806
Wiswesser Line Notation Q2Q &1/3/H-2 2
Evaluation B

$C_2D_2H_4O_2$ (liq) 67NIK/RAB2
1,2-Dihydroxyethane-d_2; 1,2-Ethanediol-d_2; Ethylene glycol-d_2
Heat Capacity 298.15 K, C_p=158.16 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Phase Changes
c/liq 258.8 K, ΔH=9749 J·mol^{-1}
ΔS=37.67 J·mol^{-1}·K^{-1}
Molecular Weight 64.0806
Wiswesser Line Notation Q2Q &1/3/H-2 2
Evaluation B

$C_2D_3HBr_2$ (liq) 49DHO/JU
1,2-Dibromoethane-d_3; Ethylene dibromide-d_3
Heat Capacity 293 K, C_p=144.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 190.8853
Wiswesser Line Notation E2E &2/H-2 3
Evaluation C

$C_2D_3HBr_2$ (liq) 49WUY/JU
1,2-Dibromoethane-d_3; Ethylene dibromide-d_3
Heat Capacity 310 K, C_p=145.14 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 190.8853
Wiswesser Line Notation E2E &2/H-2 3
Evaluation C

$C_2D_4Br_2$ (liq) 49DHO/JU
1,2-Dibromoethane-d_4; Ethylene dibromide-d_4
Heat Capacity 293 K, C_p=147.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 191.8932
Wiswesser Line Notation E2E
Evaluation B

$C_2D_5NO_4$·0.5D_2O (c) 89FUK/MA
Ammonium hydrogen oxalate hemihydrate-d_6
Heat Capacity 298.15 K, C_p=179.97 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=204.45 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 160.1 K, ΔH=0.56 J·mol^{-1}
ΔS=4.12 J·mol^{-1}·K^{-1}
Order-disorder transition.
Molecular Weight 122.1208
Wiswesser Line Notation ZH QVVQ &QH 0.5 &1/H-2 2 &2/4/7/10/1 H-2
Evaluation A

$C_2F_2O_2$ (liq) 71HC
Oxalyl fluoride
Heat Capacity
Temperature range 13 to 270 K.
Phase Changes
c/liq 260.73 K, ΔH=13407 J·mol^{-1}
ΔS=51.4 J·mol^{-1}·K^{-1}
liq/g 270.13 K, ΔH=28255 J·mol^{-1}
ΔS=104.6 J·mol^{-1}·K^{-1}
Molecular Weight 94.0176
Wiswesser Line Notation FVVF
Evaluation A

C_2F_3N (liq) 61PAC/BC
Trifluoroacetonitrile; Trifluoromethyl cyanide
Heat Capacity 205 K, C_p=118.11 J·mol^{-1} K^{-1}
Temperature range 15 to 205 K.
Entropy 205.47 K, S=184.43 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 128.73 K, ΔH=4971 J·mol^{-1}
ΔS=38.62 J·mol^{-1}·K^{-1}
liq/g 205.47 K, ΔH=17832 J·mol^{-1}
ΔS=86.79 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 95.0239
Wiswesser Line Notation NCXFFF
Evaluation Z

C_2F_4 (liq) 53FUR/MCC

Tetrafluorethene; Tetrafluoroethylene

Heat Capacity	200 K,	C_p=112.77 J·mol^{-1}·K^{-1}
Temperature range 6 to 210 K.		
Entropy	197.53 K,	S=184.23 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	142.00 K,	ΔH=7714.5 J·mol^{-1}
		ΔS=54.33 J·mol^{-1}·K^{-1}
liq/g	197.53 K,	ΔH=16821 J·mol^{-1}
		ΔS=85.16 J·mol^{-1}·K^{-1}
		P=101.325 kPa

Molecular Weight 100.0156
Wiswesser Line Notation FYFUYFF
Evaluation A

$(C_2F_4)_n$ (c) 52FUR/MCC

Polytetrafluoroethylene, annealed; Teflon, annealed

Heat Capacity	280 K,	C_p=97.6 J·mol^{-1}·K^{-1}
Temperature range 15 to 370 K. Values per monomer unit.		
Phase Changes		
Transition region 280 to 310 K.		

Molecular Weight 100.0156
Wiswesser Line Notation /*X*FF/
Evaluation A

$(C_2F_4)_n$ (c) 52FUR/MCC

Polytetrafluoroethylene, molded; Teflon, molded

Heat Capacity	280 K,	C_p=101.2 J·mol^{-1}·K^{-1}
Temperature range 15 to 370 K. Values per monomer unit.		
Phase Changes		
Transition region 280 to 310 K.		

Molecular Weight 100.0156
Wiswesser Line Notation /*X*FF/
Evaluation A

$(C_2F_4)_n$ (c) 52FUR/MCC

Polytetrafluoroethylene, powder; Teflon, powder

Heat Capacity	280 K,	C_p=103.6 J·mol^{-1}·K^{-1}
Temperature range 15 to 370 K. Values per monomer unit.		
Phase Changes		
Transition region 280 to 310 K.		

Molecular Weight 100.0156
Wiswesser Line Notation /*X*FF/
Evaluation A

$(C_2F_4)_n$ (c) 55MAR/DOL

Polytetrafluoroethylene, drawn; Teflon, drawn

Heat Capacity	313 K,	C_p=99.29 J·mol^{-1}·K^{-1}
Temperature range 250 to 393 K. Value calculated from equation, valid above 313 K. Values per monomer unit.		

Molecular Weight 100.0156
Wiswesser Line Notation /*X*FF/
Evaluation B

$(C_2F_4)_n$ (c) 55MAR/DOL

Polytetrafluoroethylene, powder; Teflon, powder

Heat Capacity	313 K,	C_p=97.36 J·mol^{-1}·K^{-1}
Temperature range 250 to 393 K. Value calculated from equation, valid above 313 K. Values per monomer unit.		

Molecular Weight 100.0156
Wiswesser Line Notation /*X*FF/
Evaluation B

$(C_2F_4)_n$ (c) 65DOU/HAR

Polytetrafluoroethylene, powder; Teflon, powder

Heat Capacity	350 K,	C_p=101.6 J·mol^{-1}·K^{-1}
Temperature range 350 to 573 K. Values per monomer unit.		

Molecular Weight 100.0156
Wiswesser Line Notation /*X*FF/
Evaluation B

$(C_2F_4)_n$ (c) 65DOU/HAR

Polytetrafluoroethylene, quenched; Teflon, quenched

Heat Capacity	350 K,	C_p=106.4 J·mol^{-1}·K^{-1}
Temperature range 350 to 725 K. Values per monomer unit.		

Molecular Weight 100.0156
Wiswesser Line Notation /*X*FF/
Evaluation B

C_2F_4O (liq) 71HOD

Trifluoroacetyl fluoride

Heat Capacity		
Temperature range 14 to 214 K.		
Phase Changes		
c/liq	113.69 K,	ΔH=4869 J·mol^{-1}
		ΔS=42.83 J·mol^{-1}·K^{-1}
liq/g	214.10 K,	ΔH=19267 J·mol^{-1}
		ΔS=89.99 J·mol^{-1}·K^{-1}

Molecular Weight 116.0150
Wiswesser Line Notation FXFFVF
Evaluation A

C_2F_4O (liq) 72PAC/HOD

Trifluoroacetyl fluoride

Heat Capacity	214.0 K,	C_p=138.95 J·mol^{-1}·K^{-1}
Temperature range 14 to 214 K.		
Entropy	214.1 K,	S=216.48 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	113.69 K,	ΔH=4870 J·mol^{-1}
		ΔS=42.84 J·mol^{-1}·K^{-1}
liq/g	214.10 K,	ΔH=19207 J·mol^{-1}
		ΔS=89.99 J·mol^{-1}·K^{-1}
		P=101.325 kPa

Molecular Weight 116.0150
Wiswesser Line Notation FXFFVF
Evaluation A

C_2F_6 (liq) 48PAC/AST

Hexafluoroethane

Heat Capacity	195 K,	C_p=131.3 J·mol^{-1}·K^{-1}
Temperature range 12 to 195 K.		
Entropy	194.87 K,	S=250.54 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/c,I	103.98 K,	ΔH=3736 J·mol^{-1}
		ΔS=35.93 J·mol^{-1}·K^{-1}
c,I/liq	173.10 K,	ΔH=2686 J·mol^{-1}
		ΔS=15.52 J·mol^{-1}·K^{-1}
liq/g	194.87 K,	ΔH=16150 J·mol^{-1}
		ΔS=82.88 J·mol^{-1}·K^{-1}
		P=101.325 kPA

Molecular Weight 138.0124
Wiswesser Line Notation FXFFXFFF
Evaluation A

$C_2HBrClF_3$ (liq) 84GOL/KOL
2-Bromo-2-chloro-1,1,1-trifluoroethane
Phase Changes
c/liq 157.4 K, $\Delta H = 4840$ J·mol^{-1}
$\Delta S = 30.7$ J·mol^{-1}·K^{-1}
Molecular Weight 197.3821
Wiswesser Line Notation GYEXFFF
Evaluation A

$C_2HBrClF_3$ (liq) 88VES/ZAB
2-Bromo-2-chloro-1,1,1-trifluoroethane
Heat Capacity 298.15 K, $C_p = 156.6$ J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K. C_p(J·mol^{-1}·K^{-1}) = 107.69 +0.1639(T/K) (298 to 318 K).
Molecular Weight 197.3821
Wiswesser Line Notation GYEXFFF
Evaluation A

$C_2HBrClF_3$ (liq) 84GOL/KOL
1-Bromo-2-chloro-1,1,2-trifluoroethane
Phase Changes
c/liq 146.2 K, $\Delta H = 4380$ J·mol^{-1}
$\Delta S = 29.9$ J·mol^{-1}·K^{-1}
Molecular Weight 197.3821
Wiswesser Line Notation GYFXFFE
Evaluation A

$C_2HBrClF_3$ (liq) 88VES/ZAB
1-Bromo-2-chloro-1,1,2-trifluoroethane
Heat Capacity 298.15 K, $C_p = 160.3$ J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K. C_p(J·mol^{-1}·K^{-1}) = 115.64 +0.1501(T/K) (298 to 318 K).
Molecular Weight 197.3821
Wiswesser Line Notation GYFXFFE
Evaluation A

C_2HCl_3 (liq) 33TRE/WAT
Trichloroethene; Trichloroethylene
Heat Capacity 298 K, $C_p = 124.7$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 131.3889
Wiswesser Line Notation GYGU1G
Evaluation B

C_2HCl_3 (liq) 48KUR
Trichloroethene; Trichloroethylene
Heat Capacity 298 K, $C_p = 120.1$ J·mol^{-1}·K^{-1}
Temperature range 12 to 80 °C, mean C_p, three temperatures.
Molecular Weight 131.3889
Wiswesser Line Notation GYGU1G
Evaluation D

C_2HCl_3 (liq) 84GOL/KOL
Trichloroethene; Trichloroethylene
Phase Changes
c/liq 188.5 K, $\Delta H = 8450$ J·mol^{-1}
$\Delta S = 44.8$ J·mol^{-1}·K^{-1}
Molecular Weight 131.3889
Wiswesser Line Notation GYGU1G
Evaluation A

$C_2HCl_3F_2$ (liq) 92LEB/KU
1,2-Difluoro-1,2,2-trichloroethane; Freon-122
Heat Capacity 298.15 K, $C_p = 167.04$ J·mol^{-1}·K^{-1}
Temperature range 13.8 to 330 K.
Entropy 298.15 K, $S = 281.03$ J·mol^{-1}·K^{-1}
Molecular Weight 169.3857
Wiswesser Line Notation GXFGYFG
Evaluation A
T(glass) = 99 K.

C_2HCl_3O (liq) 1881I
2,2,2-Trichloroethanal; Chloral; α,α,α-Trichloroacetaldehyde
Heat Capacity 298 K, $C_p = 151.5$ J·mol^{-1}·K^{-1}
Temperature range 294 to 383 K.
Molecular Weight 147.3883
Wiswesser Line Notation VHXGGG
Evaluation D

$C_2HCl_3O_2$ (c) 1895I
Trichloroacetic acid
Heat Capacity 289–320 K, $C_p = 314$ J·mol^{-1}·K^{-1}
Temperature range 289 to 356 K.
Phase Changes
c/liq 332.25 K, $\Delta H = 5898$ J·mol^{-1}
$\Delta S = 17.75$ J·mol^{-1}·K^{-1}
Molecular Weight 163.3877
Wiswesser Line Notation QVXGGG
Evaluation D

C_2HCl_5 (liq) 48K
Pentachloroethane
Heat Capacity 298 K, $C_p = 196.2$ J·mol^{-1}·K^{-1}
Temperature range 16 to 154 °C, mean C_p, three temperatures.
Molecular Weight 202.2949
Wiswesser Line Notation GYGXGGG
Evaluation D

$C_2H_2Br_2O_2$ (c) 61GLA/T
Dibromoethanoic acid; Dibromoacetic acid
Heat Capacity 301.37 K, $C_p = 124.68$ J·mol^{-1}·K^{-1}
Temperature range −180 to 37 °C. Value is unsmoothed experime datum.
Molecular Weight 217.8446
Wiswesser Line Notation QVYEE
Evaluation B

$C_2H_2Br_4$ (liq) 48K
1,1,2,2 Tetrabromoethane
Heat Capacity 298 K, $C_p = 165.7$ J·mol^{-1}·K^{-1}
Temperature range 15 to 132 °C, mean C_p, three temperatures.
Molecular Weight 345.6538
Wiswesser Line Notation EYEYEE
Evaluation D

$C_2H_2Cl_2$ (liq) 48K
1,2-Dichloroethene; 1,2-Dichloroethylene
Heat Capacity 298 K, $C_p = 112.1$ J·mol^{-1}·K^{-1}
Temperature range −31 to 54 °C, mean C_p, three temperatures.
Molecular Weight 96.9438
Wiswesser Line Notation G1U1G
Evaluation D

$C_2H_2Cl_2$ (liq) 34MEH2
cis-1,2-Dichloroethene; cis-1,2-Dichloroethylene
Heat Capacity 288 K, C_p=113.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 96.9438
Wiswesser Line Notation G1U1G-C
Evaluation C

$C_2H_2Cl_2$ (liq) 34MEH2
trans 1,2 Dichloroethene; trans-1,2-Dichloroethylene
Heat Capacity 288 K, C_p=113.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 96.9438
Wiswesser Line Notation G1U1G-T
Evaluation C

$C_2H_2Cl_2$ (liq) 59HIL/MCD
1,1-Dichloroethene; Vinylidene chloride
Heat Capacity 298.15 K, C_p=111.29 J·mol^{-1}·K^{-1}
Temperature range 13 to 290 K.
Entropy 298.15 K, S=201.54 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 150.59 K, ΔH=6514 J·mol^{-1}
ΔS=43.26 J·mol^{-1}·K^{-1}
liq/g 298.15 K, ΔH=26476 J·mol^{-1}
ΔS=88.80 J·mol^{-1}·K^{-1}
P=80.03 kPa
Molecular Weight 96.9438
Wiswesser Line Notation GYGU1
Evaluation A

$(C_2H_2Cl_2)_n$ (gls) 67LEB/RAB
Polyvinylidene chloride
Heat Capacity 298.15 K, C_p=83.05 J·mol^{-1}·K^{-1}
Temperature range 58 to 300 K.
Entropy 298.15 K, S=86.69 J·mol^{-1}·K^{-1}
Molecular Weight 96.9432
Wiswesser Line Notation /*XGG1*/
Evaluation B

$C_2H_2Cl_2F_2$ (liq) 92LEB/KUL2
1,2-Difluoro-2,2-dichloroethane; Freon-132
Heat Capacity 298.15 K, C_p=151.49 J·mol^{-1}·K^{-1}
Temperature range 13.03 to 310 K.
Entropy 298.15 K, S=253.01 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 162.99 K, ΔH=8192 J·mol^{-1}
ΔS=50.3 J·mol^{-1}·K^{-1}
Molecular Weight 134.9406
Wiswesser Line Notation GXFG1F
Evaluation A
T(glass)=97 K.

$C_2H_2Cl_2O_2$ (liq) 1895PIC
Dichloroacetic acid; Dichloroethanoic acid
Heat Capacity 291–323 K, C_p=207 J·mol^{-1}·K^{-1}
Temperature range 253 to 323 K.
Phase Changes
c/liq 283.95 K, ΔH=7644 J·mol^{-1}
ΔS=26.9 J·mol^{-1}·K^{-1}
Molecular Weight 128.9426
Wiswesser Line Notation QVYGG
Evaluation D

$C_2H_2Cl_2O_2$ (liq) 02LOU
Dichloroacetic acid; Dichloroethanoic acid
Heat Capacity 380 K, C_p=188 J·mol^{-1}·K^{-1}
Temperature range 22 to 196 °C; mean value given.
Molecular Weight 128.9426
Wiswesser Line Notation QVYGG
Evaluation D

$C_2H_2Cl_2O_2$ (c) 61GLA/TIM
Dichloroacetic acid; Dichloroethanoic acid
Heat Capacity 280.31 K, C_p=182.30 J·mol^{-1}·K^{-1}
Temperature range −180 to 7 °C. Value is unsmoothed experimental datum.
Phase Changes
c/liq 286.5 K, ΔH=12340 J·mol^{-1}
ΔS=43.1 J·mol^{-1}·K^{-1}
Molecular Weight 128.9426
Wiswesser Line Notation QVYGG
Evaluation B

$C_2H_2Cl_4$ (liq) 48KUR
1,1,2,2-Tetrachloroethane
Heat Capacity 298 K, C_p=165.3 J·mol^{-1}·K^{-1}
Temperature range 15 to 145 °C, mean C_p four temperatures.
Molecular Weight 167.8498
Wiswesser Line Notation GYGYGG
Evaluation D

$C_2H_2Cl_4$ (liq) 82KOS/KOL
1,1,2,2-Tetrachloroethane
Heat Capacity 298.15 K, C_p=165.4 J·mol^{-1}·K^{-1}
Temperature range 8 to 300 K.
Entropy 298.15 K, S=244.3 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 207.3 K, ΔH=544 J·mol^{-1}
ΔS=2.62 J·mol^{-1}·K^{-1}
c,I/liq 230.8 K, ΔH=9172 J·mol^{-1}
ΔS=39.79 J·mol^{-1}·K^{-1}
Molecular Weight 167.8498
Wiswesser Line Notation GYGYGG
Evaluation A
Data for (c,I).

$C_2H_2Cl_4$ (liq) 82KOS/KOL
1,1,2,2-Tetrachloroethane
Heat Capacity 298.15 K, C_p=165.4 J·mol^{-1}·K^{-1}
Temperature range 8 to 300 K.
Entropy 298.15 K, S=247.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 204.8 K, ΔH=356 J·mol^{-1}
ΔS=1.74 J·mol^{-1}·K^{-1}
c,II/liq 230.3 K, ΔH=9521 J·mol^{-1}
ΔS=41.51 J·mol^{-1}·K^{-1}
Molecular Weight 167.8498
Wiswesser Line Notation GYGYGG
Evaluation A
Data for (c,II).

$C_2H_2Cl_4$ (liq) 89WIL/LAI
1,1,2,2-Tetrachloroethane
Heat Capacity 298.15 K, C_p=168.00 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 167.8498
Wiswesser Line Notation GYGYGG
Evaluation B

$C_2H_2CuO_4 \cdot 4D_2O$ (c) 76MAT/KUM
Copper (II) formate tetradeuterate
Heat Capacity 300.16 K, $C_p = 329.69\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 12 to 300 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 245.64 K, $\Delta H = 936.9\ J \cdot mol^{-1}$
$\Delta S = 3.814\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 233.7054
Wiswesser Line Notation OVH 2 .CU &QH4 &12/13/H-2 8
Evaluation B

$C_2H_2CuO_4 \cdot 4H_2O$ (c) 76MAT/KUM
Copper (II) formate tetrahydrate
Heat Capacity 295.47 K, $C_p = 290.20\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 12 to 300 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 235.78 K, $\Delta H = 836.0\ J \cdot mol^{-1}$
$\Delta S = 3.546\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 225.6422
Wiswesser Line Notation OVH 2 .CU &QH4
Evaluation B

$C_2H_2N_4O_3$ (c) 91FIN/GAR
3-Nitro-1,2,4-triazol-5-one
Heat Capacity 320 K, $C_p = 124.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 320 to 420 K. $C_p(c) = 0.00386(T/K) - 0.278\ J/g \cdot K$.
Molecular Weight 130.0628
Wiswesser Line Notation T5NMVMJ ENW
Evaluation A

$C_2H_2O_4$ (c) 29PAR/KEL
Ethanedioic acid; Oxalic acid
Heat Capacity 298.1 K, $C_p = 120.1\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, 38.49 $J \cdot mol^{-1} \cdot K^{-1}$. Revision of previous data.
Molecular Weight 90.0354
Wiswesser Line Notation QVVQ
Evaluation C

$C_2H_2O_4$ (c) 39SAT/SOG
Ethanedioic acid; Oxalic acid
Heat Capacity 323 K, $C_p = 118.0\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 0 to 100 °C. Mean value given.
Molecular Weight 90.0354
Wiswesser Line Notation QVVQ
Evaluation C

$C_2H_2O_4$ (c) 64DAV
Ethanedioic acid; Oxalic acid
Heat Capacity 340 K, $C_p = 146\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 298 to 373 K. Mean value.
Temperature range uncertain.
Molecular Weight 90.0354
Wiswesser Line Notation QVVQ
Evaluation D

$C_2H_2O_4$ (c) 82LUF/REE
Ethanedioic acid; Oxalic acid
Heat Capacity 298.15 K, $C_p = 105.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 320 K.
Entropy 298.15 K, $S = 115.6\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 90.0354
Wiswesser Line Notation QVVQ
Evaluation A

$C_2H_2O_4$ (c) 88PET/T
Ethanedioic acid; Oxalic acid
Phase Changes
c,II/c,I 393.2 K, $\Delta H = 1300\ J \cdot mol^{-1}$
$\Delta S = 3.3\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 90.0354
Wiswesser Line Notation QVVQ
Evaluation A

C_2H_3Br (liq) 34M
Bromoethene; Vinyl bromide
Heat Capacity 288 K, $C_p = 107.9\ J \cdot mol^{-1} \cdot K^{-1}$
One measurement.
Molecular Weight 106.9497
Wiswesser Line Notation E1U1
Evaluation C

C_2H_3Br (liq) 34ME
Bromoethene; Vinyl bromide
Heat Capacity 288 K, $C_p = 107.5\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 106.9497
Wiswesser Line Notation E1U1
Evaluation C

C_2H_3Cl (liq) 67LEB/R
Vinyl chloride
Heat Capacity 298.15 K, $C_p = 89.45\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 58 to 300 K.
Entropy 298.15 K, $S = 118.0\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 119.31 K, $\Delta H = 4916\ J \cdot mol^{-1}$
$\Delta S = 41.2\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 62.4987
Wiswesser Line Notation G1U1
Evaluation B

$(C_2H_3Cl)_n$ (gls) 55ALF/D
Polyvinyl chloride
Heat Capacity 298 K, $C_p = 59.47\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 253 to 393 K. C_p calculated from equat $C_p(cal \cdot g^{-1} \cdot deg^{-1}) = 0.2092 + 7.29 \times 10^{-4} t$, where $t < 60$ °C for L PVC, $C_p(cal \cdot g^{-1} \cdot deg^{-1}) = 0.2048 + 8.46 \times 10^{-4} t$, where $t < 60$ °C annealed PVC.
Molecular Weight 62.4987
Wiswesser Line Notation /*YG1*/
Evaluation A
T(glass) = 78.5 °C.

$(C_2H_3Cl)_n$ (gls) 67LEB/R
Polyvinyl chloride
Heat Capacity 298.15 K, $C_p = 59.96\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 58 to 300 K. Value per monomer unit.
Entropy 298.15 K, $S = 65.10\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 62.4987
Wiswesser Line Notation /*YG1*/
Evaluation B

$(C_2H_3Cl)_n$ (gls) 77CHA
Polyvinyl chloride
Heat Capacity 298.15 K, C_p=59.03 J·mol^{-1}·K^{-1}
Temperature range 6 to 380 K. Value per monomer unit.
Entropy 298.15 K, S=71.60 J·mol^{-1}·K^{-1}
Per monomer unit. Value is $S-S_0$.
Molecular Weight 62.4987
Wiswesser Line Notation /*YG1*/
Evaluation A
One sample of suspension-polymerized PVC, two samples of bulk-polymerized PVC. Data represent annealed bulk material.

$C_2H_3ClF_2$ (liq) 37PER
1,1-Difluoro-1-chloroethane
Heat Capacity 291.6 K, C_p=130.5 J·mol^{-1}·K^{-1}
Temperature range −180 to 18 °C. Value is unsmoothed experimental datum.
Phase Changes
c/liq 142.4 K, ΔH=2686 J·mol^{-1}
ΔS=18.86 J·mol^{-1}·K^{-1}
Molecular Weight 100.4955
Wiswesser Line Notation GXFF1
Evaluation B

$C_2H_3ClF_2$ (liq) 37PER2
1,1-Difluoro-1-chloroethane
Heat Capacity 291.6 K, C_p=130.5 J·mol^{-1}·K^{-1}
Temperature range −180 to 18 °C. Value is unsmoothed experimental datum for saturated liquid.
Phase Changes
c/liq 142.4 K, ΔH=2686 J·mol^{-1}
ΔS=18.86 J·mol^{-1}·K^{-1}
Molecular Weight 100.4955
Wiswesser Line Notation GXFF1
Evaluation B
Sample probably contains other isomers in small amounts.

$C_2H_3ClF_2$ (liq) 41RIE2
1,1-Difluoro-1-chloroethane
Heat Capacity 294.8 K, C_p=130.5 J·mol^{-1}·K^{-1}
Temperature range −61 to 22 °C. Value is unsmoothed experimental datum.
Molecular Weight 100.4955
Wiswesser Line Notation GXFF1
Evaluation A

$C_2H_3ClF_2$ (liq) 42RIE
1,1-Difluoro-1-chloroethane
Heat Capacity 294.9 K, C_p=130.5 J·mol^{-1}·K^{-1}
Temperature range −61 to 21 °C. Value is unsmoothed experimental datum for saturated liquid.
Molecular Weight 100.4955
Wiswesser Line Notation GXFF1
Evaluation A

$C_2H_3ClF_2$ (liq) 93NAK/HOR
1,1-Difluoro-1-chloroethane
Heat Capacity 300 K, C_p=132.15 J·mol^{-1}·K^{-1}
Temperature range 276 to 350 K. p=0.358 MPa.
Molecular Weight 100.4955
Wiswesser Line Notation GXFF1
Evaluation A

C_2H_3ClO (liq) 1881REI
Acetyl chloride
Heat Capacity 298 K, C_p=117.2 J·mol^{-1}·K^{-1}
Temperature range 289 to 343 K.
Molecular Weight 78.4981
Wiswesser Line Notation GV1
Evaluation D

$C_2H_3ClO_2$ (c) 1895PIC
Monochloroacetic acid; Chloroacetic acid
Heat Capacity 288–318 K, C_p=144 J·mol^{-1}·K^{-1}
Temperature range 288 to 349 K.
Phase Changes
c/liq 334.33 K, ΔH=16296 J·mol^{-1}
ΔS=48.74 J·mol^{-1}·K^{-1}
α-Isomer.
c/liq 329.16 K, ΔH=13933 J·mol^{-1}
ΔS=42.33 J·mol^{-1}·K^{-1}
β-Isomer.
Molecular Weight 94.4975
Wiswesser Line Notation QV1G
Evaluation D

$C_2H_3ClO_2$ (liq) 50URA/SID
Monochloroacetic acid; Chloroacetic acid
Heat Capacity 321.05 K, C_p=179.9 J·mol^{-1}·K^{-1}
Temperature range 47 to 65 °C. Value is unsmoothed experimental datum. Maxima at 50.7, 56.9, and 61.2 °C.
Molecular Weight 94.4975
Wiswesser Line Notation QV1G
Evaluation B

$C_2H_3Cl_3$ (liq) 44RUB/LEV
1,1,1-Trichloroethane; Methyl chloroform
Heat Capacity 299.59 K, C_p=144.31 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=227.48 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 224.20 K, ΔH=7473 J·mol^{-1}
ΔS=33.33 J·mol^{-1}·K^{-1}
c,I/liq 240.2 K, ΔH=1880 J·mol^{-1}
ΔS=7.8 J·mol^{-1}·K^{-1}
ΔH estimated because of errors in C_p above 225 K
Not used in calulation of entropy.
liq/g 286.53 K, ΔH=33313 J·mol^{-1}
ΔS=116.26 J·mol^{-1}·K^{-1}
P=10.26 kPa
Molecular Weight 133.4047
Wiswesser Line Notation GXGG1
Evaluation A

$C_2H_3Cl_3$ (liq) 50CRO/SMY
1,1,1-Trichloroethane; Methyl chloroform
Heat Capacity 257.29 K, C_p=138.9 J·mol^{-1}·K^{-1}
Temperature range 117 to 260 K. Value is unsmoothed experimental datum.
Phase Changes
c,III/c,II 205 K, ΔH=210 J·mol^{-1}
ΔS=1.0 J·mol^{-1}·K^{-1}
c,II/c,I 223.6 K, ΔH=7450 J·mol^{-1}
ΔS=33.3 J·mol^{-1}·K^{-1}
c,I/liq 240.1 K, ΔH=1880 J·mol^{-1}
ΔS=7.8 J·mol^{-1}·K^{-1}
Molecular Weight 133.4047
Wiswesser Line Notation GXGG1
Evaluation C

$C_2H_3Cl_3$ (liq) 73AND/COU
1,1,1-Trichloroethane; Methylchloroform

Heat Capacity	298.15 K,	C_p=144.4 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.		
Entropy	298.15 K,	S=226.7 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/c,I	224.80 K,	ΔH=7490 J·mol^{-1}
		ΔS=33.32 J·mol^{-1}·K^{-1}
c,I/liq	243.13 K,	ΔH=2350 J·mol^{-1}
		ΔS=9.67 J·mol^{-1}·K^{-1}

Molecular Weight 133.4047
Wiswesser Line Notation GXGG1
Evaluation A

$C_2H_3Cl_3$ (liq) 82MAR
1,1,1-Trichloroethane; Methylchloroform

Phase Changes		
c,II/c,I	224.5 K,	ΔH=7470 J·mol^{-1}
		ΔS=33.3 J·mol^{-1}·K^{-1}
c,I/liq	240.9 K,	ΔH=1550 J·mol^{-1}
		ΔS=6.43 J·mol^{-1}·K^{-1}

Molecular Weight 133.4047
Wiswesser Line Notation GXGG1
Evaluation C

$C_2H_3Cl_3$ (c) 88MAR/MON
1,1,1-Trichloroethane; Methylchoroform

Heat Capacity	225 K,	C_p=123 J·mol^{-1}·K^{-1}
Temperature range 10 to 225 K. Data given graphically and estimated from graph.		

Molecular Weight 133.4047
Wiswesser Line Notation GXGG1
Evaluation A

$C_2H_3Cl_3$ (liq) 91HAS/YOS
1,1,1-Trichloroethane; Methylchloroform

Phase Changes	
c,II/c,Ib	225.0 K
c,Ia/liq	236.7 K
c,Ib/liq	242.90 K

Molecular Weight 133.4047
Wiswesser Line Notation GXGG1
Evaluation B

$C_2H_3Cl_3$ (c) 50CRO/SMY
1,1,2-Trichloroethane

Heat Capacity	251.7 K,	C_p=143.1 J·mol^{-1}·K^{-1}
Temperature range 117 to 252 K. Value is unsmoothed experimental datum.		
Phase Changes		
c/liq	237.1 K,	ΔH=11380 J·mol^{-1}
		ΔS=48.0 J·mol^{-1}·K^{-1}

Molecular Weight 133.4047
Wiswesser Line Notation GYG1G
Evaluation C

$C_2H_3Cl_3$ (liq) 84GOL/KOL
1,1,2-Trichloroethane

Phase Changes		
c/liq	237.9 K,	ΔH=10880 J·mol^{-1}
		ΔS=45.7 J·mol^{-1}·K^{-1}

Molecular Weight 145.4157
Wiswesser Line Notation GYG1G
Evaluation A

$C_2H_3F_3$ (liq) 44RUS/G
1,1,1-Trifluoroethane; Freon 143

Heat Capacity	220 K,	C_p=109.66 J·mol^{-1}·K^{-1}
Temperature range 15 to 226 K.		
Entropy	225.85 K,	S=224.10 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/c,I	156.35 K,	ΔH=297 J·mol^{-1}
		ΔS=1.90 J·mol^{-1}·K^{-1}
c,I/liq	161.82 K,	ΔH=6192 J·mol^{-1}
		ΔS=38.26 J·mol^{-1}·K^{-1}
liq/g	224.40 K,	ΔH=19175 J·mol^{-1}
		ΔS=85.45 J·mol^{-1}·K^{-1}
		P=94.54 kPa

Molecular Weight 84.0409
Wiswesser Line Notation FXFF1
Evaluation A

$C_2H_3KO_2$ (c) 75FER/S
Potassium acetate

Phase Changes		
c,II/c,I	423 K,	ΔH=420 J·mol^{-1}
		ΔS=1.0 J·mol^{-1}·K^{-1}
c,I/liq	578.7 K,	ΔH=15230 J·mol^{-1}
		ΔS=26.3 J·mol^{-1}·K^{-1}

Molecular Weight 98.1428
Wiswesser Line Notation OV1 .KA
Evaluation C

$C_2H_3KO_2$ (c) 90HOU/KI
Potassium acetate

Phase Changes		
c,III/c,II	332 K	
c,II/c,I	429.5 K,	ΔH=245.4 J·mol^{-1}
		ΔS=0.577 J·mol^{-1}·K^{-1}

Molecular Weight 98.1428
Wiswesser Line Notation OV1 .KA
Evaluation A

$C_2H_3KO_2$ (c) 90NGE/M
Potassium acetate

Heat Capacity	298.15 K,	C_p=109.38 J·mol^{-1}·K^{-1}
Temperature range 4 to 585 K.		
Entropy	298.15 K,	S=150.82 J·mol^{-1}·K^{-1}
Phase Changes		
hump	300–375 K,	ΔH=229.48 J·mol^{-1}
		ΔS=0.6652 J·mol^{-1}·K^{-1}
Transformation 300 to 375 K.		
c,IIIb/c,IIIa	411 K,	ΔH=346.71 J·mol^{-1}
		ΔS=0.8065 J·mol^{-1}·K^{-1}
c,IIIa/c,II	425 K,	ΔH=189.57 J·mol^{-1}
		ΔS=0.4157 J·mol^{-1}·K^{-1}
c,II/c,I	474 K,	ΔH=1613 J·mol^{-1}
		ΔS=3.3840 J·mol^{-1}·K^{-1}
c,I/liq	582 K,	ΔH=7649 J·mol^{-1}
		ΔS=13.137 J·mol^{-1}·K^{-1}
Crystal to isotropic liquid.		

Molecular Weight 98.1428
Wiswesser Line Notation OV1 .KA
Evaluation A

$C_2H_3LiO_2$ (c) 75FER/S
Lithium acetate

Phase Changes		
c,liq	557 K,	ΔH=11880 J·mol^{-1}
		ΔS=21.3 J·mol^{-1}·K^{-1}

Molecular Weight 65.9855
Wiswesser Line Notation OV1 .LI
Evaluation C

$C_2H_3LiO_2 \cdot 2H_2O$ (c) 84MEI/GRO
Lithium acetate dihydrate
Heat Capacity 298.15 K, C_p=169.7 J·mol^{-1}·K^{-1}
Temperature range 270 to 400 K.
Phase Changes
c/aq 324.71 K, ΔH=24250 J·mol^{-1}
ΔS=74.7 J·mol^{-1}·K^{-1}
Transition of dihydrate to anhydrous salt and aqueous solution.
Molecular Weight 102.0159
Wiswesser Line Notation OV2 .LI &QH 2
Evaluation B

C_2H_3N (liq) 07WAL
Acetonitrile; Ethanenitrile; Methyl cyanide
Heat Capacity 291 K, C_p=88 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation D

C_2H_3N (liq) 65PUT/MCE
Acetonitrile; Ethanenitrile; Methyl cyanide
Heat Capacity 298.15 K, C_p=91.46 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 298.15 K, S=149.62 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 216.9 K, ΔH=897.9 J·mol^{-1}
ΔS=4.14 J·mol^{-1}·K^{-1}
c,I/liq 229.32 K, ΔH=8167 J·mol^{-1}
ΔS=35.61 J·mol^{-1}·K^{-1}
liq/g 298.15 K, ΔH=33225 J·mol^{-1}
ΔS=111.44 J·mol^{-1}·K^{-1}
P=11.83 kPA
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation A

C_2H_3N (liq) 71HAL/BAL
Acetonitrile; Ethanenitrile; Methyl cyanide
Heat Capacity 297 K, C_p=82.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation C

C_2H_3N (liq) 8DEV/HEU
Acetonitrile; Ethanenitrile; Methyl cyanide
Heat Capacity 298.15 K, C_p=91.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation B

C_2H_3N (liq) 79DEV/SOM
Acetonitrile; Ethanenitrile; Methyl cyanide
Heat Capacity 298.15 K, C_p=91.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation B

C_2H_3N (liq) 79VIS/SOM
Acetonitrile; Ethanenitrile; Methyl cyanide
Heat Capacity 298.15 K, C_p=91.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation B

C_2H_3N (liq) 82MAR
Acetonitrile; Ethanenitrile; Methyl cyanide
Phase Changes
c,II/c,I 218.0 K, ΔH=800 J·mol^{-1}
ΔS=3.67 J·mol^{-1}·K^{-1}
c,I/liq 228.7 K, ΔH=6670 J·mol^{-1}
ΔS=29.2 J·mol^{-1}·K^{-1}
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation C

C_2H_3N (liq) 84GUS/MIR
Acetonitrile; Ethanenitrile; Methyl cyanide
Heat Capacity 303.15 K, C_p=81.8 J·mol^{-1}·K^{-1}
Temperature range 303 to 343 K. p=0.1 MPa. Unsmoothed experimental datum given as 1.9930 kJ/kg·K.
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation D

C_2H_3N (liq) 87MIR/SHA
Acetonitrile; Ethanenitrile; Methyl cyanide
Heat Capacity 298.15 K, C_p=77.4 J·mol^{-1}·K^{-1}
Temperature range 253 to 353 K. Unsmoothed experimental datum given as 1.863 kJ/kg·K at 293 K. C_p(liq)=1.2838+0.0004369T/K +5.3125×10^{-6}T^2/K^2 kJ/kg·K (253 to 353 K).
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation C

C_2H_3N (liq) 92KOL/KUL
Acetonitrile; Ethanenitrile; Methyl cyanide
Heat Capacity 298.15 K, C_p=91.69 J·mol^{-1}·K^{-1}
Temperature range 283 to 323 K.
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation B

$(C_2H_3NO)_n$ (c) 80FIN/KUM
Polyglycine I
Heat Capacity 298.15 K, C_p=102.5 J·mol^{-1}·K^{-1}
Temperature range 150 to 375 K. C_p=37.744+0.218T−2.333×10^{-6} T^2.
Molecular Weight 57.0518
Wiswesser Line Notation /*MV1*/
Evaluation B
Same data as in 81FIN/KUM. β-sheet structure.

$(C_2H_3NO)_n$ (c) 80FIN/KUM
Polyglycine II
Heat Capacity 298.15 K, C_p=93.46 J·mol^{-1}·K^{-1}
Temperature range 150 to 375 K. C_p=57.598+0.05T+2.357×10^{-4} T^2.
Molecular Weight 57.0518
Wiswesser Line Notation /*MV1*/
Evaluation B
Same data as in 81FIN/KUM. 3_1 helical structure.

$(C_2H_3NO)_n$ (c) 81FIN/KUM
Polyglycine I
Heat Capacity 298.15 K, C_p=102.5 J·mol^{-1}·K^{-1}
Temperature range 150 to 375 K. Polyglycine I (β-sheet). Data given graphically. C_p calculated from equation.
Molecular Weight 57.0518
Wiswesser Line Notation /*MV1*/
Evaluation B

$(C_2H_3NO)_n$ (c) 81FIN/KUM
Polyglycine II
Heat Capacity 298.15 K, C_p=93.46 J·mol^{-1}·K^{-1}
Temperature range 150 to 375 K. Polyglycine II (3_1helix). Data given graphically. C_p calculated from equation.
Molecular Weight 57.0518
Wiswesser Line Notation /*MV1*/
Evaluation B

$(C_2H_3NO)_n$ (c) 91ROL
Polyglycine
Heat Capacity 300 K, C_p=66.75 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 57.0518
Wiswesser Line Notation /*MV1*/
Evaluation B

$(C_2H_3NO)_n$ (c) 91ROL/WUN
Polyglycine
Heat Capacity 300 K, C_p=66.75 J·mol^{-1}·K^{-1}
Temperature range 230 to 390 K.
Molecular Weight 57.0518
Wiswesser Line Notation /*MV1*/
Evaluation B

$C_2H_3N_3$ (c) 89HIL/MOU
1,2,4-Triazole
Phase Changes
c/liq 393.5 K, ΔH=16100 J·mol^{-1}
Molecular Weight 69.0658
Wiswesser Line Notation T5MN DNJ
Evaluation A

$C_2H_3N_3$ (c) 89JIM/ROU
1,2,4-Triazole
Heat Capacity 298.15 K, C_p=78.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 69.0658
Wiswesser Line Notation T5MN DNJ
Evaluation A

$C_2H_3N_3O$ (c) 91FIN/GAR
1,2,4-Triazol-3-one
Heat Capacity 320 K, C_p=68.9 J·mol^{-1}·K^{-1}
Temperature range 320 to 420 K. C_p(c)=0.00214(T/K)+0.125 J/g·K.
Molecular Weight 85.0652
Wiswesser Line Notation T5NMVMJ
Evaluation A

$C_2H_3NaO_2$ (c) 55
Sodium ethanoate; Sodium acetate
Heat Capacity 291.18 K, C_p=88.07 J·mol^{-1}·K^{-1}
Temperature range 13 to 292 K. Value is unsmoothed experim datum.
Entropy 298.15 K, S=123.09 J·mol^{-1}·K^{-1}
Molecular Weight 82.0343
Wiswesser Line Notation OV1 .NA
Evaluation A

$C_2H_3NaO_2$ (c,IV) 75FER/
Sodium ethanoate; Sodium acetate
Heat Capacity 340 K, C_p=111.7 J·mol^{-1}·K^{-1}
Temperature range 340 to 610 K.
Phase Changes
c,IV/c,III 414 K, ΔH=290 J·mol^{-1}
ΔS=0.7 J·mol^{-1}·K^{-1}
c,III/c,II 465 K, ΔH=420 J·mol^{-1}
ΔS=0.8 J·mol^{-1}·K^{-1}
c,II/c,I 527 K, ΔH=170 J·mol^{-1}
ΔS=0.3 J·mol^{-1}·K^{-1}
c,I/liq 601.3 K. ΔH=17950 J·mol^{-1}
ΔS=29.9 J·mol^{-1}·K^{-1}
Molecular Weight 82.0343
Wiswesser Line Notation OV1 .NA
Evaluation B

$C_2H_3NaO_2$ (c) 83FRA/
Sodium ethanoate; Sodium acetate
Heat Capacity 298.15 K, C_p=100.83 J·mol^{-1}·K^{-1}
Temperature range 7 to 350 K.
Entropy 298.15 K, S=138.10 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 21 K, ΔS=12.5 J·mol^{-1}·K^{-1}
Questionable second-order transition.
Molecular Weight 82.0343
Wiswesser Line Notation OV1 .NA
Evaluation A

$C_2H_3NaO_2 \cdot 3H_2O$ (c) 32
Sodium acetate trihydrate
Heat Capacity 325 K, C_p=322 J·mol^{-1}·K^{-1}
Temperatures above and below melting point.
Phase Changes
c/liq 331.7 K, ΔH=20250 J·mol^{-1}
ΔS=61 J·mol^{-1}·K^{-1}
Molecular Weight 136.0799
Wiswesser Line Notation OV1 .NA &QH3
Evaluation D

$C_2H_3NaO_2 \cdot 3H_2O$ (c) 84MEI/
Sodium acetate trihydrate
Heat Capacity 298.15 K, C_p=229.0 J·mol^{-1}·K^{-1}
Temperature range 270 to 400 K.
Phase Changes
c/aq 331.52 K, ΔH=37860 J·mol^{-1}
ΔS=114.2 J·mol^{-1}·K^{-1}
Transition of trihydrate to anhydrous salt and aqueous solution.
Molecular Weight 136.0799
Wiswesser Line Notation OV1 .NA &QH3
Evaluation B

$C_2H_3O_2Tl$ (c) 76MEI/SEY
Thallium acetate
Phase Changes
c,I/liq 404 K, $\Delta H = 17573\ J \cdot mol^{-1}$
$\Delta S = 43.5\ J \cdot mol^{-1} \cdot K^{-1}$
Solid-mesophase.
Molecular Weight 263.4145
Wiswesser Line Notation OV1 .TL
Evaluation B

C_2H_4 (liq) 37EGA/KEM
Ethylene
Heat Capacity 170 K, $C_p = 67.24\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 15 to 170 K.
Phase Changes
c/liq 103.95 K, $\Delta H = 3351\ J \cdot mol^{-1}$
$\Delta S = 32.23\ J \cdot mol^{-1} \cdot K^{-1}$
liq/g 169.40 K, $\Delta H = 13544\ J \cdot mol^{-1}$
$\Delta S = 79.95\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 28.0536
Wiswesser Line Notation 1U1
Evaluation B

C_2H_4 (liq) 83CHA/HAL
Ethylene
Heat Capacity 170 K, $C_p = 67.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 16 to 169 K.
Entropy 170 K, $S = 117.8\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 103.97 K, $\Delta H = 3351\ J \cdot mol^{-1}$
$\Delta S = 32.23\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 28.0536
Wiswesser Line Notation 1U1
Evaluation A
A reevaluation of the original measured data from: 37EGA/KEM.

C_2H_4BrCl (liq) 92SVO/KUB2
1-Bromo-2-chloroethane
Phase Changes
liq/g 379.8 K, $\Delta H = 38060\ J \cdot mol^{-1}$
Molecular Weight 143.4106
Wiswesser Line Notation G2E
Evaluation A

$C_2H_4Br_2$ (liq) 49DHO/JUN
1,2-Dibromoethane; Ethylene dibromide
Heat Capacity 293 K, $C_p = 134.8\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 187.8616
Wiswesser Line Notation E2E
Evaluation B

$C_2H_4Br_2$ (liq) 92SVO/KUB2
1,2-Dibromoethane; Ethylene dibromide
Phase Changes
liq/g 404.7 K, $\Delta H = 41780\ J \cdot mol^{-1}$
Molecular Weight 187.8616
Wiswesser Line Notation E2E
Evaluation A

$C_2H_4Br_2$ (liq) 93SHE
1,2-Dibromoethane; Ethylene dibromide
Heat Capacity 298.15 K, $C_p = 134.7\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 187.8616
Wiswesser Line Notation E2E
Evaluation B

C_2H_4BrCl (liq) 39RAI
1-Bromo-2-chloroethane
Heat Capacity 300 K, $C_p = 130.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 320 K. Data graphically only. Value read from graph.
Phase Changes
c,II/c,I 182 K, $\Delta H = 3100\ J \cdot mol^{-1}$
$\Delta S = 17.0\ J \cdot mol^{-1} \cdot K^{-1}$
Lambda-type transition. Temperature is maximum in specific heat curve.
c,I/liq 256.4 K, $\Delta H = 9625\ J \cdot mol^{-1}$
$\Delta S = 37.5\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 143.4106
Wiswesser Line Notation G2E
Evaluation C

$C_2H_4Br_2$ (liq) 39RAI
1,2-Dibromoethane; Ethylene dibromide
Heat Capacity 300 K, $C_p = 129.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 320 K. Data graphically only. Value read from graph.
Phase Changes
c,II/c,I 250.6 K, $\Delta H = 1880\ J \cdot mol^{-1}$
$\Delta S = 7.5\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 283.1 K, $\Delta H = 10835\ J \cdot mol^{-1}$
$\Delta S = 38.3\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 187.8616
Wiswesser Line Notation E2E
Evaluation C

$C_2H_4Br_2$ (liq) 40PIT2
1,2-Dibromoethane; Ethylene dibromide
Heat Capacity 298.15 K, $C_p = 136.0\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 15 to 300 K.
Entropy 298.15 K, $S = 223.30\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 249.54 K, $\Delta H = 1940.5\ J \cdot mol^{-1}$
$\Delta S = 7.78\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 283.0 K, $\Delta H = 10944.5\ J \cdot mol^{-1}$
$\Delta S = 38.67\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 187.8616
Wiswesser Line Notation E2E
Evaluation A

$C_2H_4Br_2$ (liq) 48KUR
1,2-Dibromoethane; Ethylene dibromide
Heat Capacity 398 K, $C_p = 134.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 16 to 127 °C, mean C_p, four temperatures.
Molecular Weight 187.8616
Wiswesser Line Notation E2E
Evaluation D

$C_2H_4Br_2$ (liq) 49WUY/JUN
1,2-Dibromoethane; Ethylene dibromide
Heat Capacity 310 K, $C_p = 135.14\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 187.8616
Wiswesser Line Notation E2E
Evaluation C

$C_2H_4Br_2$ (liq) 65FIN/GRU
1,2-Dibromoethane; Ethylene dibromide
Heat Capacity 300 K, $C_p = 136.4\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 187.8616
Wiswesser Line Notation E2E
Evaluation B

$C_2H_4Br_2$ (liq) 69WIL/SCH
1,2-Dibromoethane; Ethylene dibromide
Heat Capacity 298.15 K, C_p=135.0 J·mol^{-1}·K^{-1}
Temperature range 20, 30, 40 °C.
Molecular Weight 187.8616
Wiswesser Line Notation E2E
Evaluation B

$C_2H_4Cl_2$ (liq) 1881REI
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298 K, C_p=122.2 J·mol^{-1}·K^{-1}
Temperature range 290 to 364 K.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation D

$C_2H_4Cl_2$ (liq) 39RAI
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 300 K, C_p=131.0 J·mol^{-1}·K^{-1}
Temperature range 90 to 320 K. Data graphically only. Value read from graph.
Phase Changes
c,II/I 175 K, ΔH=2845 J·mol^{-1}
ΔS=16.2 J·mol^{-1}·K^{-1}
Lambda-type transition. Temperature is maximum in specific heat curve.
c,I/liq 237.6 K, ΔH=8745 J·mol^{-1}
ΔS=36.8 J·mol^{-1}·K^{-1}
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation C

$C_2H_4Cl_2$ (liq) 40PIT2
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298.15 K, C_p=128.9 J·mol^{-1}·K^{-1}
Temperature range 15 to 308 K.
Entropy 298.15 K, S=208.53 J·mol^{-1}·K^{-1}
Phase Changes
Anomalous region at 175 to 180 K, probably a lambda-type transition. No transition heat or temperature given.
c/liq 237.2 K, ΔH=8836.6 J·mol^{-1}
ΔS=37.25 J·mol^{-1}·K^{-1}
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation A

$C_2H_4Cl_2$ (liq) 48KUR
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298 K, C_p=123.0 J·mol^{-1}·K^{-1}
Temperature range −25 to 86°C, mean C_p, four temperatures.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation D

$C_2H_4Cl_2$ (liq) 51SIE/CRU
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 293 K, C_p=124.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation B

$C_2H_4Cl_2$ (liq) 55STA/T
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298 K, C_p=129.70 J·mol^{-1}·K^{-1}
Temperature range 284 to 348 K.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation B

$C_2H_4Cl_2$ (liq) 55R
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298.15 K, C_p=129.54 J·mol^{-1}·K^{-1}
Temperature range 7 to 50°C.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation B

$C_2H_4Cl_2$ (liq) 67RAS/G
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 293 K, C_p=129.2 J·mol^{-1}·K^{-1}
Temperature range 293 to 353 K.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation C

$C_2H_4Cl_2$ (liq) 69WIL/S
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298.15 K, C_p=128.6 J·mol^{-1}·K^{-1}
Temperature range 20, 30 40°C.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation B

$C_2H_4Cl_2$ (liq) 77WIL/G
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298.15 K, C_p=128.99 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.8596
Wiswesser Line Notation G2G
Evaluation B

$C_2H_4Cl_2$ (liq) 79WIL/F
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298.15 K, C_p=128.99 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation B

$C_2H_4Cl_2$ (liq) 79WIL/G
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298.15 K, C_p=129.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation B

$C_2H_4Cl_2$ (liq) 85LAI/ROU
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298.15 K, C_p=128.81 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation B

$C_2H_4Cl_2$ (liq) 93HAL
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298.15 K, C_p=129.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation B

$C_2H_4Cl_2$ (liq) 1881REI
1,1-Dichloroethane; Ethylidene chloride
Heat Capacity 298 K, C_p=120.9 J·mol^{-1}·K^{-1}
Temperature range 287 to 344 K.
Molecular Weight 98.9596
Wiswesser Line Notation GYG1
Evaluation D

$C_2H_4Cl_2$ (liq) 48KUR
1,1-Dichloroethane; Ethylidene chloride
Heat Capacity 298 K, C_p=127.2 J·mol^{-1}·K^{-1}
Temperature range −51 to 55 °C, mean C_p, four temperatures.
Molecular Weight 98.9596
Wiswesser Line Notation GYG1
Evaluation D

$C_2H_4Cl_2$ (liq) 56LI/PIT
1,1-Dichloroethane; Ethylidene chloride
Heat Capacity 298.15 K, C_p=126.27 J·mol^{-1}·K^{-1}
Temperature range 14 to 294 K.
Entropy 298.15 K, S=211.75 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 176.18 K, ΔH=7870 J·mol^{-1}
ΔS=44.67 J·mol^{-1}·K^{-1}
liq/g 293 K, ΔH=31000 J·mol^{-1}
ΔS=105.81 J·mol^{-1}·K^{-1}
P=30.32 kPA
Molecular Weight 98.9596
Wiswesser Line Notation GYG1
Evaluation A

$C_2H_4F_2$ (liq) 82POR/PON
Freon 152a; 1,1-Difluoroethane, Ethylidene difluoride
Heat Capacity 298.17 K, C_p=118.4 J·mol^{-1}·K^{-1}
Temperature range 220 to 425 K. Unsmoothed experimental datum.
C_p data given as 1.793 J·g^{-1}·K^{-1}.
Molecular Weight 66.0504
Wiswesser Line Notation FYF1
Evaluation C

$C_2H_4F_2$ (liq) 93NAK/HOR
Freon 152a; 1,1-Difluoroethane; Ethylidene difluoride
Heat Capacity 300 K, C_p=117.31 J·mol^{-1}·K^{-1}
Temperature range 276 to 360 K. p=0.629 MPa.
Molecular Weight 66.0504
Wiswesser Line Notation FYF1
Evaluation A

$C_2H_4N_2O_2$ (c) 80LEB/KAT
Diformylhydrazine
Heat Capacity 298.15 K, C_p=99.12 J·mol^{-1}·K^{-1}
Temperature range 298 to 350 K. C_p=0.908×10^{-4}T^3−0.0923T^2 +31.3779T−3457.8187 J/mole·K, 298 to 350 K.
Phase Changes
c/g 356 K, ΔH=205100 J·mol^{-1}
ΔS=291 J·mol^{-1}·K^{-1}
Calculated from vapor pressure.
Molecular Weight 88.0658
Wiswesser Line Notation VHMMVH
Evaluation B

$C_2H_4N_2O_2$ (c) 65EGA/WAK
Oxamide
Heat Capacity 298.15 K, C_p=113.89 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S−118.11 J·mol^{-1}·K^{-1}
Molecular Weight 88.0658
Wiswesser Line Notation ZVVZ
Evaluation A
Triclinic form.

$C_2H_4N_4$ (c) 52STE/BER
Dicyandiamide
Heat Capacity 294.63 K, C_p=117.74 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=129.29 J·mol^{-1}·K^{-1}
Molecular Weight 84.0804
Wiswesser Line Notation NCMYZUM
Evaluation A

$C_2H_4N_4$ (c) 64DAV
Dicyandiamide
Heat Capacity 340 K, C_p=142 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K. Mean value.
Temperature range uncertain.
Molecular Weight 84.0804
Wiswesser Line Notation NCMYZUM
Evaluation D

$(C_2H_4O)_n$ (liq) 82ZAR
Polyethylene glycol
Heat Capacity 298 K, C_p=1314 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 600
Wiswesser Line Notation /*O2*/
Evaluation B

$(C_2H_4O)_n$ (liq) 82ZAR
Polyethylene glycol
Heat Capacity 323 K, C_p=3346 J·mol^{-1}·K^{-1}
Temperature range 323, 363 K.
Molecular Weight 1500
Wiswesser Line Notation /*O2*/
Evaluation B

$(C_2H_4O)_n$ (c) 57SOC/TRA
Polyvinyl alcohol
Heat Capacity 245 K, C_p=45.9 J·mol^{-1}·K^{-1}
Temperature range 58 to 245 K. C_p value is unsmoothed experimental datum.
Molecular Weight 44.0530
Wiswesser Line Notation /*QY1*/
Evaluation B
See also 62WAR/BRO

C_2H_4O (liq) 49GIA/GOR
Oxirane; Ethylene oxide
Heat Capacity 285 K, C_p=86.90 J·mol^{-1}·K^{-1}
Temperature range 15 to 283 K.
Entropy 283.60 K, S=149.45 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 160.65 K, ΔH=5173.1 J·mol^{-1}
ΔS=32.20 J·mol^{-1}·K^{-1}
liq/g 283.66 K, ΔH=25527 J·mol^{-1}
ΔS=89.99 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 44.0530
Wiswesser Line Notation T3OTJ
Evaluation A

$C_2H_4O \cdot 7H_2O$ (c) 82LEA/MUR
Ethylene oxide hydrate
Heat Capacity
Temperature range 120 to 260 K. Data given graphically.
Phase Changes
c/liq 283.2 K, ΔH=48000 J·mol^{-1}
ΔS=169.5 J·mol^{-1}·K^{-1}
Molecular Weight 170.1594
Wiswesser Line Notation T3OTJ &QH 7
Evaluation A
Actual formula: $C_2H_4O \cdot 6.89H_0$

$C_2H_4O \cdot 7H_2O$ (liq) 90YAM/HAN
Ethylene oxide hydrate
Heat Capacity 298.15 K, C_p=642.20 J·mol^{-1}·K^{-1}
Temperature range 5 to 298.15 K. Since the melting point is 284.11 K, C_p value at 298.15 is anomolous.
Entropy 298.15 K, S=608.86 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 284.11 K, ΔH=48260 J·mol^{-1}
Molecular Weight 170.1594
Wiswesser Line Notation T3OTJ &QH 7
Evaluation A
Actual formula: $C_2H_4O \cdot 6.86H_2O$. T(glass)=90 K.

C_2H_4O (liq) 47CON/ELV
Ethanal; Acetaldehyde
Heat Capacity 273 K, C_p=96.21 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 44.0530
Wiswesser Line Notation VH1
Evaluation B

C_2H_4O (liq) 88LEB/V
Ethanal; Acetaldehyde
Heat Capacity 298.15 K, C_p=89.05 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=117.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 149.78 K, ΔH=2310 J·mol^{-1}
ΔS=15.43 J·mol^{-1}·K^{-1}
liq/liq 242.9 K, ΔH=1716 J·mol^{-1}
ΔS=7.35 J·mol^{-1}·K^{-1}
Lambda type transition.
Molecular Weight 44.0530
Wiswesser Line Notation VH1
Evaluation A

$C_2H_4O_2$ (liq) 1881R
Acetic acid; Ethanoic acid
Heat Capacity 298 K, C_p=123.5 J·mol^{-1}·K^{-1}
Temperature range 292 to 358 K.
Molecular Weight 60.0524
Wiswesser Line Notation *QV1*
Evaluation D

$C_2H_4O_2$ (liq) 1895P
Acetic acid; Ethanoic acid
Heat Capacity 287–335 K, C_p=137 J·mol^{-1}·K^{-1}
Temperature range 260 to 335 K.
Phase Changes
c/liq 290.06 K, ΔH=11126 J·mol^{-1}
ΔS=38.36 J·mol^{-1}·K^{-1}
Molecular Weight 60.0524
Wiswesser Line Notation QV1
Evaluation D

$C_2H_4O_2$ (c) 03FC
Acetic acid; Ethanoic acid
Heat Capacity 268.5 K, C_p=80 J·mol^{-1}·K^{-1}
Temperature range 251 to 286 K. C_p is the average value over t temperature range.
Phase Changes
c/liq 289.77 K
Molecular Weight 60.0524
Wiswesser Line Notation QV1
Evaluation D

$C_2H_4O_2$ (liq) 25PAR/K
Acetic acid; Ethanoic acid
Heat Capacity 294.7 K, C_p=123.4 J·mol^{-1}·K^{-1}
Temperature range 87 to 295 K. Value is unsmoothed experimen datum.
Entropy 298.1 K, S=193.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K. 76.82 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 289.9 K, ΔH=11728 J·mol^{-1}
ΔS=40.47 J·mol^{-1}·K^{-1}
Molecular Weight 60.0524
Wiswesser Line Notation QV1
Evaluation B(C_p),C(S)

$C_2H_4O_2$ (liq) 29PAR/KEL
Acetic acid; Ethanoic acid
Heat Capacity 298.1 K, C_p=159.8 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 42.68 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 60.0524
Wiswesser Line Notation QV1
Evaluation C

$C_2H_4O_2$ (liq) 32NEU
Acetic acid; Ethanoic acid
Heat Capacity 297.1 K, C_p=121.3 J·mol^{-1}·K^{-1}
Temperature range 23.9 to 80.5 °C. Value is unsmoothed experimental datum.
Molecular Weight 60.0524
Wiswesser Line Notation QV1
Evaluation C

$C_2H_4O_2$ (liq) 34RAD/JUL
Acetic acid; Ethanoic acid
Heat Capacity 298 K, C_p=120.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0524
Wiswesser Line Notation QV1
Evaluation C

$C_2H_4O_2$ (liq) 58SWI/ZIE
Acetic acid; Ethanoic acid
Heat Capacity 332 K, C_p=139.7 J·mol^{-1}·K^{-1}
Mean value 22 to 96 °C.
Molecular Weight 60.0524
Wiswesser Line Notation QV1
Evaluation C

$C_2H_4O_2$ (liq) 82MAR/AND
Acetic acid; Ethanoic acid
Heat Capacity 298.15 K, C_p=123.1 J·mol^{-1}·K^{-1}
Temperature range 13 to 450 K. Data also given by equation.
Entropy 298.15 K, S=158.0 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 298.69 K, ΔH=11720 J·mol^{-1}
ΔS=40.5 J·mol^{-1}·K^{-1}
Molecular Weight 60.0524
Wiswesser Line Notation QV1
Evaluation A

$C_2H_4O_2$ (liq) 1881BER/OGI
Methyl formate; Methyl methanoate
Heat Capacity 298 K, C_p=130 J·mol^{-1}·K^{-1}
Temperature range 286 to 302 K. C_p given as 0.516 cal·g^{-1}·K^{-1}.
Molecular Weight 60.0524
Wiswesser Line Notation VHO1
Evaluation D

$C_2H_4O_2$ (liq) 34MEH2
Methyl formate; Methyl methanoate
Heat Capacity 288 K, C_p=121.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0524
Wiswesser Line Notation VHO1
Evaluation C

$C_2H_4O_2$ (liq) 71HAL/BAL
Methyl formate; Methyl methanoate
Heat Capacity 297 K, C_p=95.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0524
Wiswesser Line Notation VHO1
Evaluation C

$C_2H_4O_2$ (liq) 79FUC
Methyl formate; Methyl methanoate
Heat Capacity 298.15 K, C_p=119.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0524
Wiswesser Line Notation VHO1
Evaluation B

$C_2H_4O_2$ (liq) 87ZAB/HYN
Methyl formate; Methyl methanoate
Heat Capacity 298.75 K, C_p=120.57 J·mol^{-1}·K^{-1}
Temperature range 293 to 299 K. Unsmoothed experimental datum.
Molecular Weight 60.0524
Wiswesser Line Notation VHO1
Evaluation B

C_2H_5DO (liq) 62RAB/NIK
Ethanol-d_1; Ethyl alcohol-d_1
Heat Capacity 298 K, C_p=116.23 J·mol^{-1}·K^{-1}
Temperature range 15 to 55 °C.
Molecular Weight 47.0750
Wiswesser Line Notation Q2 &1/H-2
Evaluation B

C_2H_5DO (liq) 67NIK/RAB
Ethanol-d_1; Ethyl alcohol-d_1
Heat Capacity 250 K, C_p=102.09 J·mol^{-1}·K^{-1}
Temperature range 80 to 250 K.
Phase Changes
c,II/c,I 113.3 K, ΔH=3347 J·mol^{-1}
ΔS=29.54 J·mol^{-1}·K^{-1}
c,I/liq 156.9 K, ΔH=4310 J·mol^{-1}
ΔS=27.47 J·mol^{-1}·K^{-1}
Molecular Weight 47.0750
Wiswesser Line Notation Q2 &1/H-2
Evaluation A

C_2H_5Br (liq) 48KUR
Bromoethane; Ethyl bromide
Heat Capacity 298 K, C_p=100.8 J·mol^{-1}·K^{-1}
Temperature range −50 to 37 °C; mean C_p, five temperatures.
Molecular Weight 108.9655
Wiswesser Line Notation E2
Evaluation D

C_2H_5Br (liq) 93SHE
Bromoethane; Ethyl bromide
Heat Capacity 298.15 K, C_p=105.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 108.9655
Wiswesser Line Notation E2
Evaluation B

C_2H_5Cl (liq) 24JEN/SHO
Chloroethane; Ethyl chloride
Heat Capacity 298 K, C_p=107.70 J·mol^{-1}·K^{-1}
Temperature range −30 to 40 °C.
Molecular Weight 64.5145
Wiswesser Line Notation G2
Evaluation C

C_2H_5Cl (liq) 40RIE
Chloroethane; Ethyl chloride
Heat Capacity 298.1 K, C_p=108.8 J·mol^{-1}·K^{-1}
Temperature range −48 to 46 °C.
Molecular Weight 64.5145
Wiswesser Line Notation G2
Evaluation A

C_2H_5Cl (liq) 41RIE
Chloroethane; Ethyl chloride
Heat Capacity 298 K, C_p=108.8 J·mol^{-1}·K^{-1}
Temperature range −48 to 45 °C.
Molecular Weight 64.5145
Wiswesser Line Notation G2
Evaluation A

C_2H_5Cl (liq) 48GOR/GIA
Chloroethane; Ethyl chloride
Heat Capacity 290 K, C_p=103.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 287 K.
Entropy 285.42 K, S=186.27 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 134.82 K, ΔH=4452 J·mol^{-1}
ΔS=33.02 J·mol^{-1}·K^{-1}
liq/g 285.42 K, ΔH=24652 J·mol^{-1}
ΔS=86.37 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 64.5145
Wiswesser Line Notation G2
Evaluation A

C_2H_5Cl (liq) 48KUR
Chloroethane; Ethyl chloride
Heat Capacity 288 K, C_p=109.6 J·mol^{-1}·K^{-1}
Temperature range −67 to 15 °C; mean C_p, three temperatures.
Molecular Weight 64.5145
Wiswesser Line Notation G2
Evaluation D

$C_2H_5Cl_3Si$ (liq) 69NAG/DZH
Ethyltrichlorosilane
Heat Capacity 298.16 K, C_p=192.6 J·mol^{-1}·K^{-1}
Temperature range 12.5 to 298.16 K.
Entropy 298.16 K, S=307.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 165.26 K, ΔH=6958 J·mol^{-1}
ΔS=42.09 J·mol^{-1}·K^{-1}
Molecular Weight 163.5060
Wiswesser Line Notation G-SI-GG2
Evaluation A

C_2H_5I (liq) 48I
Iodoethane; Ethyl iodide
Heat Capacity 298 K, C_p=115.1 J·mol^{-1}·K^{-1}
Temperature range −37 to 70 °C; mean C_p, three temperatures.
Molecular Weight 155.9660
Wiswesser Line Notation I2
Evaluation D

C_2H_5I (liq) 93
Iodoethane; Ethyl iodide
Heat Capacity 298.15 K, C_p=109.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 155.9660
Wiswesser Line Notation I2
Evaluation B

C_2H_5NO (c) 90STE
Acetaldoxime
Heat Capacity 298.15 K, C_p=241.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation QNUY1
Evaluation B

C_2H_5NO (liq) 74VIS/S
N-Methylformamide; N-Methylmethanamide
Heat Capacity 298.15 K, C_p=126.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation VHM1
Evaluation A

C_2H_5NO (liq) 76BON/
N-Methylformamide; N-Methylmethanamide
Heat Capacity 298.15 K, C_p=122 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation VHM1
Evaluation B

C_2H_5NO (liq) 76SKO/
N-Methylformamide; N-Methylmethanamide
Heat Capacity 298.15 K, C_p=123.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation VHM1
Evaluation A

C_2H_5NO (liq) 79DEV/
N-Methylformamide; N-Methylmethanamide
Heat Capacity 298.15 K, C_p=125.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation VHM1
Evaluation B

C_2H_5NO (liq) 79VIS/SOM
N-Methylformamide; N-Methylmethanamide
Heat Capacity 298.15 K, C_p=125.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation VHM1
Evaluation A

C_2H_5NO (liq) 89KUL/KRE
N-Methylformamide; N-Methylmethanamide
Heat Capacity 308 K, C_p=126.63 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation VHM1
Evaluation B

C_2H_5NO (c) 40CAM/CAM
Acetamide; Ethanamide
Heat Capacity 293 K, C_p=66.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation C

C_2H_5NO (c) 76SKO/SUU
Acetamide; Ethanamide
Heat Capacity 298.15 K, C_p=90.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation A

C_2H_5NO (c) 83DEW/DEK
Acetamide; Ethanamide
Heat Capacity 300 K, C_p=90.00 J·mol^{-1}·K^{-1}
Temperature range 90 to 360 K.
Phase Changes
c/liq 353.33 K, ΔH=15590 J·mol^{-1}
ΔS=44.1 J·mol^{-1}·K^{-1}
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation B(C_p), A(Phase changes).

C_2H_5NO (c) 84NUR/BER
Acetamide; Ethanamide
Heat Capacity 298.15 K, C_p=91.27 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=115.0 J·mol^{-1}·K^{-1}
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation A

C_2H_5NO (c) 85NUR/BER
Acetamide; Ethanamide
Heat Capacity 298.15 K, C_p=91.27 J·mol^{-1}·K^{-1}
Temperature range 13 to 330 K.
Entropy 298.15 K, S=115.0 J·mol^{-1}·K^{-1}
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation A

C_2H_5NO (c) 86EMO/NAU
Acetamide; Ethanamide
Phase Changes
c/liq 342.15 K, ΔH=12522–12877 J·mol^{-1}
ΔS=36.6–37.6 J·mol^{-1}·K^{-1}
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation A
Unstable form.

C_2H_5NO (c) 86EMO/NAU
Acetamide; Ethanamide
Heat Capacity 298 K, C_p=86.65 J·mol^{-1}·K^{-1}
Temperature range 298 to 400 K. C_p data given at 298 K as 1.467 kJ·kg^{-1}·K^{-1} (extrapolated). C_p=1.481+0.0069(T−300) kJ·kg^{-1}·K^{-1} (300 to 330).
Phase Changes
c/liq 353.5 K, ΔH=15606 J·mol^{-1}
ΔS=44.15 J·mol^{-1}·K^{-1}
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation B(C_p), A(Phase changes)
Stable form.

C_2H_5NO (c) 89NIK/TRI
Acetamide; Ethanamide
Phase Changes
c/liq 354.05 K, ΔH=15500 J·mol^{-1}
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation A

$C_2H_5NO \cdot HNO_3$ (c) 85NUR/BER
Acetamide nitrate
Heat Capacity 298.15 K, C_p=175.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 330 K.
Entropy 298.15 K, S=210.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 361 K
Molecular Weight 122.0804
Wiswesser Line Notation ZV1 &WNQ
Evaluation A

$(C_2H_5NO)_3 \cdot HNO_3$ (c) 85NUR/BER
Triacetamide nitrate
Heat Capacity 298.15 K, C_p=383.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 330 K.
Entropy 298.15 K, S=443.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 337 K
Molecular Weight 240.2156
Wiswesser Line Notation ZV1 3 &WNQ
Evaluation A

$C_2H_5NO_2$ (liq) 66LIU/ZIE
Nitroethane
Heat Capacity 298.15 K, C_p=134.22 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Phase Changes
c/liq 183.69 K, ΔH=9853 J·mol^{-1}
ΔS=53.64 J·mol^{-1}·K^{-1}
Molecular Weight 75.0672
Wiswesser Line Notation WN2
Evaluation A

$C_2H_5NO_2$ (c) 33PAR/HUF
Aminoethanoic acid; Glycine
Heat Capacity 299.5 K, C_p=100.50 J·mol^{-1}·K^{-1}
Temperature range 93 to 300 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=109.2 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 31.59 J·mol^{-1}·K^{-1}.
Molecular Weight 75.0670
Wiswesser Line Notation Z1VQ
Evaluation B(C_p),C(S)

$C_2H_5NO_2$ (c) 60HUT/COL
Aminoethanoic acid; Glycine
Heat Capacity 298.15 K, C_p=99.20 J·mol^{-1}·K^{-1}
Temperature range 11 to 305 K.
Entropy 298.15 K, S=103.51 J·mol^{-1}·K^{-1}
Molecular Weight 75.0670
Wiswesser Line Notation Z1VQ
Evaluation A

$C_2H_5NO_2$ (c) 75SPI/WAD
Aminoethanoic acid; Glycine
Heat Capacity 298.15 K, C_p=99.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 75.0670
Wiswesser Line Notation Z1VQ
Evaluation B

$C_2H_5NO_2$ (c) 89KUL/KOZ
Aminoethanoic acid; Glycine
Heat Capacity 298 K, C_p=95.1 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 75.0670
Wiswesser Line Notation Z1VQ
Evaluation C

$C_2H_5NO_2$ (c) 90BAD/KUL
Aminoethanoic acid; Glycine
Heat Capacity 298 K, C_p=95 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 75.0670
Wiswesser Line Notation Z1VQ
Evaluation D

$C_2H_5NO_2$ (c) 76BER/BOU
Methyl carbamate
Phase Changes
c/liq 328.6 K, ΔH=16700 J·mol^{-1}
ΔS=51.0 J·mol^{-1}·K^{-1}
Molecular Weight 75.0670
Wiswesser Line Notation ZVO1
Evaluation A

$C_2H_5NO_3$ (liq) 54GRA/SMI
Ethyl nitrate
Heat Capacity 298 K, C_p=170.3 J·mol^{-1}·K^{-1}
Temperature range 21 to 293 K.
Entropy 298 K, S=247.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 178.6 K, ΔH=8527 J·mol^{-1}
ΔS=47.74 J·mol^{-1}·K^{-1}
Molecular Weight 91.0664
Wiswesser Line Notation WNO2
Evaluation B

$C_2H_5NO_4$ (c) 39SAT/S
Ammonium acid oxalate
Heat Capacity 323 K, C_p=152.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 107.0658
Wiswesser Line Notation QVVQ &ZH
Evaluation C

$C_2H_5NO_4$·0.5H_2O (c) 89FUK/M
Ammonium hydrogen oxalate hemihydrate
Heat Capacity 298.15 K, C_p=166.91 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=189.24 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 145.4 K, ΔH=0.37 J·mol^{-1}
ΔS=3.01 J·mol^{-1}·K^{-1}
Order - disorder transition.
Molecular Weight 116.0734
Wiswesser Line Notation ZH QVVQ &QH 0.5
Evaluation A

$C_2D_5NO_4$·0.5D_2O (c) 89FUK/M
Ammonium hydrogen oxalate hemihydrate-d_6
Heat Capacity 298.15 K, C_p=179.97 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=204.45 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 160.1 K, ΔH=0.56 J·mol^{-1}
ΔS=4.12 J·mol^{-1}·K^{-1}
Order - disorder transition.
Molecular Weight 133.1208
Wiswesser Line Notation ZH QVVQ &QH 0.5 &1/H-2 2 &2/4/7/10/11/H-2
Evaluation A

C_2H_5NS (c) 82SAB/T
Thioacetamide
Heat Capacity 298 K, C_p=100.3 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.335 J·K^{-1}·g^{-1}.
Phase Changes
c/g 298.15 K, ΔH=82800 J·mol^{-1}
ΔS=277.7 J·mol^{-1}·K^{-1}
Molecular Weight 75.1282
Wiswesser Line Notation ZY1&US
Evaluation B

$C_2H_5N_3O_2$ (c) 82LUF/I
Biuret; Carbamylurea
Heat Capacity 298.15 K, C_p=131.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 320 K.
Entropy 298.15 K, S=146.1 J·mol^{-1}·K^{-1}
Molecular Weight 103.0804
Wiswesser Line Notation ZVMVZ
Evaluation A

$C_2H_5N_3O_2$ (c) 88KOZ/
Biuret; Carbamylurea
Heat Capacity 298.15 K, C_p=131.3 J·mol^{-1}·K^{-1}
Temperature range 240 to 450 K.
Entropy 298.15 K, S=146.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 372 K, ΔH=970 J·mol^{-1}
ΔS=2.54 J·mol^{-1}·K^{-1}
Molecular Weight 103.0804
Wiswesser Line Notation ZVMVZ
Evaluation B

C_2H_6 (liq) 30WIE/HUB
Ethane
Heat Capacity 200 K, C_p=74.48 J·mol^{-1}·K^{-1}
Temperature range 67 to 305.2 K. Heat capacity of saturated liquid given to 295 K is 136.1 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 89.50 K, ΔH=2793 J·mol^{-1}
ΔS=31.2 J·mol^{-1}·K^{-1}
liq/g 184.46 K
Molecular Weight 30.0694
Wiswesser Line Notation 2H
Evaluation A

C_2H_6 (liq) 37WIT/KEM
Ethane
Heat Capacity 180 K, C_p=72.22 J·mol^{-1}·K^{-1}
Temperature range 15 to 185 K.
Entropy 184.1 K, S=126.7 J·mol^{-1}·K^{-1}
Entropy from 0 to 15 K calculated using a Debye function.
Phase Changes
c,I/liq 89.87 K, ΔH=2857 J·mol^{-1}
ΔS=31.8 J·mol^{-1}·K^{-1}
liq/g 184.1 K, ΔH=14703 J·mol^{-1}
ΔS=79.87 J·mol^{-1}·K^{-1}
Molecular Weight 30.0694
Wiswesser Line Notation 2H
Evaluation A

C_2H_6 (liq) 76ATA/CHI
Ethane
Heat Capacity 100 K, C_p=68.66 J·mol^{-1}·K^{-1}
Temperature range 50 to 100 K. Data given graphically. C_p=0.69933 (T/K)−2.385 J·mol^{-1}·K^{-1} (50 to 70 K, for solid).
Phase Changes
c,II/c,I 89.813 K, ΔH=2282 J·mol^{-1}
ΔS=25.48 J·mol^{-1}·K^{-1}
c/liq 90.341 K, ΔH=583 J·mol^{-1}
ΔS=6.46 J·mol^{-1}·K^{-1}
Triple point.
Molecular Weight 30.0694
Wiswesser Line Notation 2H
Evaluation A

C_2H_6 (liq) 76ROD
Ethane
Heat Capacity 100.32 K, C_p=68.44 J·mol^{-1}·K^{-1}
Temperature range 93 to 301 K (saturation line), 91 to 330 K, pressures from 0 to 33 MPa.
Molecular Weight 30.0694
Wiswesser Line Notation 2H
Evaluation A

C_2H_6 (liq) 76ROD2
Ethane
Heat Capacity 94 K, C_p=68.5 J·mol^{-1}·K^{-1}
From data 90.3 to 94 K. Average value over range.
Phase Changes
c,II/c,I 89.77 K, ΔH=2437.5 J·mol^{-1}
ΔS=27.15 J·mol^{-1}·K^{-1}
Molecular Weight 30.0694
Wiswesser Line Notation 2H
Evaluation B

C_2H_6Cd (liq) 56LI
Dimethyl cadmium; Cadmium dimethyl
Heat Capacity 298.15 K, C_p=132.01 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=201.88 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 254.35 K, ΔH=1520.9 J·mol^{-1}
ΔS=5.98 J·mol^{-1}·K^{-1}
c,I/liq 270.48 K, ΔH=7837 J·mol^{-1}
ΔS=28.97 J·mol^{-1}·K^{-1}
liq/g 291.5 K, ΔH=38296 J·mol^{-1}
ΔS=131.4 J·mol^{-1}·K^{-1}
P=3.033 kPa
Molecular Weight 142.4794
Wiswesser Line Notation 1-CD-1
Evaluation A

$C_2H_6Cl_2Si$ (liq) 71SAM/KOS2
Dichlorodimethylsilane
Heat Capacity 298.15 K, C_p=171.5 J·mol^{-1}·K^{-1}
Temperature range 21 to 299 K. Data deposited VINITI, No 2423-71, 17 December, 1970. C_p(liq)=18.5676+0.06453T+283310T^{-2} (198.99 to 300 K) cal·mol^{-1}·K^{-1}.
Entropy 298.15 K, S=270.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 198.99 K, ΔH=8828 J·mol^{-1}
ΔS=44.39 J·mol^{-1}·K^{-1}
Molecular Weight 129.0609
Wiswesser Line Notation G-SI-G1&1
Evaluation A
T_{Debye}=100.37 K.

$C_2H_6Cl_4D_6MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(deuteromethylammonium) manganese II
Phase Changes
c,II/c,I 258 K, ΔH=2.6 J·mol^{-1}
ΔS=0.007 J·mol^{-1}·K^{-1}
c,I/liq 389 K, ΔH=14.6 J·mol^{-1}
ΔS=0.036 J·mol^{-1}·K^{-1}
Molecular Weight 266.9278
Wiswesser Line Notation ZH&1 2 .MN G4 &1/H-2 3
Evaluation A

$C_2H_6N_2O$ (c) 87DEL/FER
Methylurea; Monomethylurea
Phase Changes
c/liq 373.8 K, ΔH=15750 J·mol^{-1}
ΔS=42.1 J·mol^{-1}·K^{-1}
Molecular Weight 74.0822
Wiswesser Line Notation ZVM1
Evaluation A

$C_2H_6N_2O$ (c) 93KOZ/KAB
Methylurea; Monomethylurea
Heat Capacity 298.15 K, C_p=114.74 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=138.02 J·mol^{-1}·K^{-1}
Phase Changes
c/g 343 K, ΔH=95730 J·mol^{-1}
Molecular Weight 74.0822
Wiswesser Line Notation ZVM1
Evaluation A

$C_2H_6N_2O_4$ (c) 86MAT/SUG
Hydrazinium hydrogen oxalate
Heat Capacity 299.47 K, C_p=157.6 J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K. Value is unsmoothed experimental datum.
Phase Changes
c,II/c,I 217.6 K, ΔH=1090 J·mol^{-1}
ΔS=4.18 J·mol^{-1}·K^{-1}
Molecular Weight 122.0804
Wiswesser Line Notation QVVQ &ZZ
Evaluation A

$C_2H_6N_2O_4$ (c) 85NUR/BER
Acetamide nitrate
Heat Capacity 298.15 K, C_p=175.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 330 K.
Entropy 298.15 K, S=210.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 361 K
Molecular Weight 122.0804
Wiswesser Line Notation ZV1 &WNQ
Evaluation A

$C_2H_6N_4O_4$ (c) 73KRI/LIC
Ethylenedinitramine
Heat Capacity 298 K, C_p=175.3 J·mol^{-1}·K^{-1}
Temperature range 200 to 448 K. Equation only.
Molecular Weight 150.0938
Wiswesser Line Notation WNM2MNW
Evaluation C

C_2H_6O (liq) 41KEN/SAG
2 Oxapropane; Dimethyl ether; Methoxymethane
Heat Capacity 240 K, C_p=102.30 J·mol^{-1}·K^{-1}
Temperature range 14 to 240 K.
Entropy 200 K, S=146.57 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 131.66 K, ΔH=4936.3 J·mol^{-1}
ΔS=37.49 J·mol^{-1}·K^{-1}
liq/g 248.34 K, ΔH=21510 J·mol^{-1}
ΔS=86.61 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 46.0688
Wiswesser Line Notation 1O1
Evaluation A

C_2H_6O (liq) 1881REI
Ethanol; Ethyl alcohol
Heat Capacity 298 K, C_p=112.1 J·mol^{-1}·K^{-1}
Temperature range 288 to 346 K.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation D

C_2H_6O (liq) 07W
Ethanol; Ethyl alcohol
Heat Capacity 293 K, C_p=109 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation D

C_2H_6O (liq) 20GIB/I
Ethanol; Ethyl alcohol
Heat Capacity 271.4 K, C_p=102.4 J·mol^{-1}·K^{-1}
Temperature range 85 to 271.4 K. Unsmoothed experimental data
Data also given for the glassy state from 85.9 to 96.3 K.
Phase Changes
c/liq 156.2 K, ΔH=4626 J·mol^{-1}
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 24WIL/D
Ethanol; Ethyl alcohol
Heat Capacity 303 K, C_p=115.1 J·mol^{-1}·K^{-1}
Temperature range 303 to 333 K. Equation only.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation C

C_2H_6O (liq) 25I
Ethanol; Ethyl alcohol
Heat Capacity 298.0 K, C_p=113.4 J·mol^{-1}·K^{-1}
Temperature range 87 to 298 K. Value is unsmoothed experime
datum.
Entropy 298.1 K, S=177.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 55.19 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 158.7 K, ΔH=4962 J·mol^{-1}
ΔS=21.22 J·mol^{-1}·K^{-1}
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B(C_p),C(S)

C_2H_6O (liq) 29K
Ethanol; Ethyl alcohol
Heat Capacity 294.31 K, C_p=109.87 J·mol^{-1}·K^{-1}
Temperature range 16 to 298 K. Value is unsmoothed experime
datum.
Entropy 298.15 K, S=160.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 158.5 K, ΔH=5021 J·mol^{-1}
ΔS=31.68 J·mol^{-1}·K^{-1}
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 29MIT/I
Ethanol; Ethyl alcohol
Heat Capacity 270 K, C_p=106.3 J·mol^{-1}·K^{-1}
Temperature range 190 to 270 K.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 29PAR/KEL
Ethanol; Ethyl alcohol
Heat Capacity 298.1 K, C_p=160.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 38.9 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation C

C_2H_6O (liq) 31FIO/GIN
Ethanol; Ethyl alcohol
Heat Capacity 313.15 K, C_p=118.72 J·mol^{-1}·K^{-1}
Temperature range 40 to 110 °C.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A

C_2H_6O (liq) 36ERN/WAT
Ethanol; Ethyl alcohol
Heat Capacity 298 K, C_p=103.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation C

C_2H_6O (liq) 39BYK
Ethanol; Ethyl alcohol
Heat Capacity 298 K, C_p=111.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A

C_2H_6O (liq) 40MAZ
Ethanol; Ethyl alcohol
Heat Capacity 297.8 K, C_p=114.7 J·mol^{-1}·K^{-1}
Temperature range 174 to 298 K. Unsmoothed experimental datum. C_p(liq)=0.5437+0.001858t+0.0000098t^2 cal·g^{-1}·°C^{-1}. C_p(298.15 K)=114.9 J·mol^{-1}·K^{-1}, calculated from equation.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 44YOS
Ethanol; Ethyl alcohol
Phase Changes
c/liq 159 K, ΔH=4973 J·mol^{-1}
ΔS=31.3 J·mol^{-1}·K^{-1}
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 60SWI/ZIE
Ethanol; Ethyl alcohol
Heat Capacity 316 K, C_p=118.8 J·mol^{-1}·K^{-1}
Mean value 21 to 66 °C.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation C

C_2H_6O (liq) 61GRE
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=111.96 J·mol^{-1}·K^{-1}
Temperature range 16 to 350 K.
Entropy 298.15 K, S=161.21 J·mol^{-1}·K^{-1}
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A
Reevaluation of 29KEL2 and 31FIO/GIN.

C_2H_6O (liq) 62RAB/NIK
Ethanol; Ethyl alcohol
Heat Capacity 298 K, C_p=112.26 J·mol^{-1}·K^{-1}
Temperature range 15 to 55 °C.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 66HWA/ZIE
Ethanol; Ethyl alcohol
Heat Capacity 297.359 K, C_p=112.056 J·mol^{-1}·K^{-1}
Temperature range 165 to 304 K. Unsmoothed experimental datum.
Phase Changes
c/liq 159.015 K
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 67NIK/RAB
Ethanol; Ethyl alcohol
Heat Capacity 250 K, C_p=97.53 J·mol^{-1}·K^{-1}
Temperature range 80 to 250 K.
Phase Changes
c,II/c,I 111.4 K, ΔH=3138 J·mol^{-1}
ΔS=28.17 J·mol^{-1}·K^{-1}
c,I/liq 158.8 K, ΔH=4644 J·mol^{-1}
ΔS=29.24 J·mol^{-1}·K^{-1}
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A

C_2H_6O (liq) 70PAZ/PAZ
Ethanol; Ethyl alcohol
Heat Capacity 313.2 K, C_p=118.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 75PED/KAY
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=111.81 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K. C_p(liq)=98.39+0.5368(T/K −273.25) J/K·mol (298 to 348K0.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 76FOR/BEN
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=112.33 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A

C_2H_6O (liq) 76FOR/BEN2
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=112.094 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A
Data from 76FOR/BEN.

C_2H_6O (liq) 77HAI/SUG
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=112.5 J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K. Also glass, supercooled liquid, metastable crystal.
Entropy 298.15 K, S=159.86 J·mol^{-1}·K^{-1}
Phase Changes
c,II/liq 127.5 K, ΔH=659 J·mol^{-1}
ΔS=5.19 J·mol^{-1}·K^{-1}
c,I/liq 159.00 K, ΔH=4931 J·mol^{-1}
ΔS=31.01 J·mol^{-1}·K^{-1}
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A

C_2H_6O (liq) 77VES/SVO
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=112.30 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 79BRO/ZIE
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=112.15 J·mol^{-1}·K^{-1}
Temperature range 159 to 306 K. Results as equation only.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 79VES/ZAB
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=112.30 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 82BEN/DAR
Ethanol; Ethyl alcohol
Heat Capacity 288.15 K, C_p=108.07 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 82VIL/CAS
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=113.75 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 84STE/C
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=115.9 J·mol^{-1}·K^{-1}
Temperature range 266 to 318 K. C_p given as 0.6011 cal·g^{-1}·C^{-1}
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 84ZEG/S(
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=112.67 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A

C_2H_6O (liq) 85OGA/M
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=110.51 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 86OGA/M
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=112.36 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 86TAN/T
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=112.68 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A

C_2H_6O (liq) 88AND/I
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=111.53 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 89PET/I
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p=112.4 J·mol^{-1}·K^{-1}
Temperature range 258.15, 278.15, 298.15, 318.15 K.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6OS (liq) 60KEN/
Dimethyl sulfoxide
Heat Capacity 298.15 K, C_p=149.0 J·mol^{-1}·K^{-1}
Temperature range 298, 343 K.
Molecular Weight 78.1288
Wiswesser Line Notation OS1&1
Evaluation B

C_2H_6OS (liq) 70CLE/WES
Dimethyl sulfoxide
Heat Capacity 298.15 K, C_p=153.18 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=188.78 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 291.67 K, ΔH=14368 J·mol^{-1}
ΔS=49.26 J·mol^{-1}·K^{-1}
Molecular Weight 78.1288
Wiswesser Line Notation OS1&1
Evaluation A

C_2H_6OS (liq) 78DEV/HEU
Dimethyl sulfoxide
Heat Capacity 298.15 K, C_p=155.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1288
Wiswesser Line Notation OS1&1
Evaluation B

C_2H_6OS (liq) 79DEV/SOM
Dimethyl sulfoxide
Heat Capacity 298.15 K, C_p=155.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1288
Wiswesser Line Notation OS1&1
Evaluation B

C_2H_6OS (liq) 79VIS/SOM
Dimethyl sulfoxide
Heat Capacity 298.15 K, C_p=155.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1288
Wiswesser Line Notation OS1&1
Evaluation B

C_2H_6OS (liq) 87LAN/CRI
Dimethyl sulfoxide
Heat Capacity 298.15 K, C_p=153.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1288
Wiswesser Line Notation OS1&1
Evaluation B

C_2H_6OS (liq) 88ROD/MAR
Dimethyl sulfoxide
Heat Capacity 298.15 K, C_p=153.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1288
Wiswesser Line Notation OS1&1
Evaluation B

C_2H_6OS (liq) 89BAR/KOO
Dimethyl sulfoxide
Heat Capacity 298.15 K, C_p=148.28 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1288
Wiswesser Line Notation OS1&1
Evaluation B

C_2H_6OS (liq) 93GRO/ROU
Dimethyl sulfoxide
Heat Capacity 298.15 K, C_p=149.39 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1288
Wiswesser Line Notation OS1&1
Evaluation B

$(C_2H_6OSi)_n$ (liq) 78LEB/MUK
Poly(dimethylsiloxane)
Heat Capacity 298.15 K, C_p=154.6 J·mol^{-1}·K^{-1}
Temperature range 8 to 332 K.
Entropy 298.15 K, S=154.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 246 K, ΔH=4540 J·mol^{-1}
ΔS=18.6 J·mol^{-1}·K^{-1}
Degree of crystallinity is 67%.
Molecular Weight 74.1543
Wiswesser Line Notation /*-SI-O*1&1/
Evaluation A

$(C_2H_6OSi)_n$ (amorph) 89VAR/WES
Poly(dimethylsiloxane)
Heat Capacity 298.15 K, C_p=117.775 J·mol^{-1}·K^{-1}
Temperature range 0.10 to 550 K. C_p(liq)=0.1215T+81.55 J/(K mol) (146 to 340 K).
Entropy 298.15 K, S=150.394 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 219 K, ΔH=2750 J·mol^{-1}
100% crystallinity.
Molecular Weight 74.1543
Wiswesser Line Notation /*-SI-O*1&1/
Evaluation A
T(glass)=146 K.

$(C_2H_6OSi)_n$ (c) 89VAR/WES
Poly(dimethylsiloxane)
Heat Capacity 298.15 K, C_p=120.274 J·mol^{-1}·K^{-1}
Temperature range 0.10 to 550 K. C_p(c)=exp[0.0189189(lnT)^3 −0.402175(lnT)^2+3.35144(lnT)−4.78444] J/(K mol) (5 to 146 K).
Entropy 298.15 K, S=135.769 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 219 K, ΔH=2750 J·mol^{-1}
100% crystallinity.
Molecular Weight 74.1543
Wiswesser Line Notation /*-SI-O*1&1/
Evaluation A
T(glass)=146 K.

$C_2H_6O_2$ (liq) 01FOR
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity C_p=152 J·mol^{-1}·K^{-1}
Temperature range 286 to 332.7 K. Value given over temperature range.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation D

$C_2H_6O_2$ (liq) 25PAR/KEL
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 293.0 K, C_p=149.4 J·mol^{-1}·K^{-1}
Temperature range 88 to 293 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=179.5 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 11.46 cal·mol^{-1}·K^{-1}.
Phase Changes
c/liq 260.8 K, ΔH=11623 J·mol^{-1}
ΔS=44.57 J·mol^{-1}·K^{-1}
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation B(C_p),C(S)

$C_2H_6O_2$ (liq) 29PAR/KEL
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Entropy 298.1 K, S=166.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 8.2 cal·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation C

$C_2H_6O_2$ (liq) 32NEI/KUR
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 293.4 K, C_p=145.6 J·mol^{-1}·K^{-1}
Temperature range 20.2 to 78.4 °C. Value is unsmoothed experimental datum.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation C

$C_2H_6O_2$ (liq) 62RAB/NIK
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 298 K, C_p=148.87 J·mol^{-1}·K^{-1}
Temperature range 10 to 55 °C.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation B

$C_2H_6O_2$ (liq) 65TUN/MIS
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 298 K, C_p=147.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation B

$C_2H_6O_2$ (liq) 67NIK/RAB2
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 298.15 K, C_p=150.33 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Phase Changes
c/liq 260.6 K, ΔH=9958 J·mol^{-1}
ΔS=38.21 J·mol^{-1}·K^{-1}
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation B

$C_2H_6O_2$ (liq) 70PAZ/PAZ
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 301.2 K, C_p=150.6 J·mol^{-1}·K^{-1}
Temperature range 28, 40 °C.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation B

$C_2H_6O_2$ (liq) 72KAW/(
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 303 K, C_p=145.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation B

$C_2H_6O_2$ (liq) 77MUR/S
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 298.15 K, C_p=149.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation B

$C_2H_6O_2$ (liq) 79STE/T
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 298 K, C_p=149.3 J·mol^{-1}·K^{-1}
Temperature range 273 to 493 K.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation B

$C_2H_6O_2$ (liq) 82?
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 298 K, C_p=149.8 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation B

$C_2H_6O_2S$ (c) 70CLE/M
Dimethyl sulfone
Heat Capacity 298.15 K, C_p=125.35 J·mol^{-1}·K^{-1}
Temperature range 5 to 410 K.
Entropy 298.15 K, S=145.48 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 382.01 K, ΔH=18301 J·mol^{-1}
ΔS=47.91 J·mol^{-1}·K^{-1}
Molecular Weight 94.1282
Wiswesser Line Notation WS1&1
Evaluation A

C_2H_6S (liq) 42OSB/
Dimethylsulfide; 2-Thiapropane
Heat Capacity 298.15 K, C_p=118.11 J·mol^{-1}·K^{-1}
Temperature range 11 to 287 K.
Entropy 298.15 K, S=196.40 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 174.85 K, ΔH=7984.7 J·mol^{-1}
ΔS=45.67 J·mol^{-1}·K^{-1}
liq/g 291.06 K, ΔH=27983 J·mol^{-1}
ΔS=96.14 J·mol^{-1}·K^{-1}
P=35.40 kPa
Molecular Weight 62.1294
Wiswesser Line Notation 1S1
Evaluation A

C_2H_6S (liq) 52MCC/SCO
Ethanethiol; Ethyl mercaptan
Heat Capacity 299.05 K, C_p=117.99 J·mol^{-1}·K^{-1}
Temperature range 14 to 315 K. Unsmoothed experimental datum.
Entropy 298.15 K, S=207.02 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 195.26 K, ΔH=4975 J·mol^{-1}
ΔS=25.48 J·mol^{-1}·K^{-1}
Molecular Weight 62.1294
Wiswesser Line Notation SH2
Evaluation A

$C_2H_6S_2$ (liq) 50SCO/FIN
2,3-Dithiabutane; Dimethyl disulfide
Heat Capacity 298.15 K, C_p=146.11 J·mol^{-1}·K^{-1}
Temperature range 13 to 352 K.
Entropy 298.15 K, S=235.39 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 188.44 K, ΔH=9192.7 J·mol^{-1}
ΔS=48.78 J·mol^{-1}·K^{-1}
Molecular Weight 94.1894
Wiswesser Line Notation 1SS1
Evaluation A

C_2H_6Se (liq) 91RAB/SHE
Dimethyl selenium
Heat Capacity 298.15 K, C_p=121.1 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=210.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 185.14 K, ΔH=8499 J·mol^{-1}
ΔS=45.90 J·mol^{-1}·K^{-1}
Molecular Weight 109.0294
Wiswesser Line Notation 1-SE-1
Evaluation A

$C_2H_6Se_2$ (liq) 91RAB/SHE
Dimethyl diselenium
Heat Capacity 298.15 K, C_p=155.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=261.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 190.89 K, ΔH=8545 J·mol^{-1}
ΔS=44.76 J·mol^{-1}·K^{-1}
Molecular Weight 187.9894
Wiswesser Line Notation 1-SE-SE-1
Evaluation A

C_2H_6Zn (liq) 84SHE/NIS
Dimethyl zinc
Heat Capacity 298.15 K, C_p=129.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=201.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 210.26 K, ΔH=1061 J·mol^{-1}
ΔS=5.05 J·mol^{-1}·K^{-1}
c,I/liq 230.13 K, ΔH=6830 J·mol^{-1}
ΔS=29.67 J·mol^{-1}·K^{-1}
Molecular Weight 95.4494
Wiswesser Line Notation 1-ZN-1
Evaluation A

C_2H_7N (liq) 39AST/EID
Dimethylamine
Heat Capacity 280.44 K, C_p=136.77 J·mol^{-1}·K^{-1}
Temperature range 14 to 280 K. Value for saturated liquid.
Entropy 280.03 K, S=173.85 J·mol^{-1}·K^{-1}
Saturated liquid at boiling point.
Phase Changes
c/liq 180.97 K, ΔH=5941 J·mol^{-1}
ΔS=32.83 J·mol^{-1}·K^{-1}
liq/g 280.03 K, ΔH=26485 J·mol^{-1}
ΔS=94.58 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 45.0840
Wiswesser Line Notation 1M1
Evaluation A

$C_2H_7NO_3S$ (c) 40HUF/FOX
2-Aminoethanesulfonic acid; Taurine
Heat Capacity 300.3 K, C_p=140.54 J·mol^{-1}·K^{-1}
Temperature range 90 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=154.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 44.18 J·mol^{-1}·K^{-1}.
Molecular Weight 125.1422
Wiswesser Line Notation Z2SWQ
Evaluation B(C_p),C(S)

$C_2H_8BF_4N$ (c) 92ISH/IWA
Dimethylammonium tetrafluoroborate
Phase Changes
c,III/c,I 283.5 K, ΔH=7500 J·mol^{-1}
c,I/liq 375 K, ΔH=3500 J·mol^{-1}
Molecular Weight 132.8955
Wiswesser Line Notation
Evaluation B

C_2H_8BrN (c) 90GEN/LUB
Ethylammonium bromide
Heat Capacity 300 K, C_p=106.6 J·mol^{-1}·K^{-1}
Temperature range 300 to 360 K. C_p(c)=343.6−1.69T+0.003T^2 J·mol^{-1}·K^{-1} (300 to 360 K).
C_p value calculated from equation.
Phase Changes
c,II/c,I 369.9 K, ΔH=12070 J·mol^{-1}
ΔS=32.63 J·mol^{-1}·K^{-1}
c,I/liq 439.5 K, ΔH=8520 J·mol^{-1}
ΔS=19.38 J·mol^{-1}·K^{-1}
Molecular Weight 125.9959
Wiswesser Line Notation Z2 &EH
Evaluation A

$C_2H_8N_2$ (liq) 51AST/JAN
N,N′-Dimethylhydrazine
Heat Capacity 298.15 K, C_p=171.04 J·mol^{-1}·K^{-1}
Temperature range 15 to 298 K.
Entropy 298.15 K, S=199.15 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 264.28 K, ΔH=13638 J·mol^{-1}
ΔS=51.60 J·mol^{-1}·K^{-1}
Molecular Weight 60.0986
Wiswesser Line Notation 1MM1
Evaluation A

$C_2H_8N_2$ (liq) 50HOU/MAS
1,2-Diaminoethane; Ethylenediamine
Heat Capacity 313 K, C_p=178.7 J·mol^{-1}·K^{-1}
Temperature range 313 to 333 K.
Molecular Weight 60.0986
Wiswesser Line Notation Z2Z
Evaluation B

$C_2H_8N_2$ (liq) 75MES/FIN
1,2-Diaminoethane; Ethylenediamine
Heat Capacity 298.15 K, C_p=172.59 J·mol^{-1}·K^{-1}
Temperature range 11 to 335 K.
Entropy 298.15 K, S=202.42 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 189.0 K, ΔH=487.4 J·mol^{-1}
ΔS=2.58 J·mol^{-1}·K^{-1}
c,I/liq 284.29 K, ΔH=22583.1 J·mol^{-1}
ΔS=79.44 J·mol^{-1}·K^{-1}
Molecular Weight 60.0986
Wiswesser Line Notation Z2Z
Evaluation A

$C_2H_8N_2$ (liq) 88BOB/KAM
1,2-Diaminoethan; Ethylenediamine
Heat Capacity 313 K, C_p=170 J·mol^{-1}·K^{-1}
Temperature range 313 to 413 K.
Molecular Weight 60.0986
Wiswesser Line Notation Z2Z
Evaluation D

$C_2H_8N_2$ (liq) 53AST/WOO
N,N-Dimethylhydrazine
Heat Capacity 298.15 K, C_p=164.05 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=200.25 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 215.95 K, ΔH=10072.6 J·mol^{-1}
ΔS=46.64 J·mol^{-1}·K^{-1}
liq/g 298.15 K, ΔH=35003 J·mol^{-1}
ΔS=117.4 J·mol^{-1}·K^{-1}
P=20.90 kPa
Molecular Weight 60.0896
Wiswesser Line Notation ZN1&1
Evaluation A

$C_2H_8N_2O_4$ (c) 39SAT/SOG
Ammonium oxalate
Heat Capacity 323 K, C_p=211.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 124.0962
Wiswesser Line Notation QVVQ &ZH2
Evaluation C

$C_2H_9BF_4N_2$ (c) 92ISH/TAK
1,1-Dimethylhydrazinium tetrafluoroborate
Phase Changes
c,III/c,II 265 K, ΔS=9.5 J·mol^{-1}·K^{-1}
c,II/c,I 268 K, ΔS=21 J·mol^{-1}·K^{-1}
c,I/liq 415 K, ΔS=11 J·mol^{-1}·K^{-1}
Molecular Weight 147.9101
Wiswesser Line Notation ZHN11 &BF4
Evaluation B

$C_2H_9N_2O_3$ (liq) 85ALL
Ethylammonium nitrate
Heat Capacity 298.15 K, C_p=90.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 109.1047
Wiswesser Line Notation Z2 &WNQ
Evaluation B

$C_2H_{10}Cl_2N_2Pt$ (c) 91PAL/
cis-Dichlorobis(methylamine)platinum
Heat Capacity 298.15 K, C_p=192.50 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=246.2 J·mol^{-1}·K^{-1}
Molecular Weight 328.1104
Wiswesser Line Notation Z1 2 .PT G2 -C
Evaluation A

$C_2H_{10}Cl_2N_2Pt$ (c) 91PAL/
trans-Dichlorobis(methylamine)platinum
Heat Capacity 298.15 K, C_p=188.22 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=249.5 J·mol^{-1}·K^{-1}
Molecular Weight 328.1104
Wiswesser Line Notation Z1 2 .PT G2 -T
Evaluation A

$C_2H_{11}B_2N$ (liq) 55FUR/I
N,N-Dimethylaminodiborane
Heat Capacity 285 K, C_p=160.8 J·mol^{-1}·K^{-1}
Temperature range 5 to 285 K.
Entropy 285 K, S=216.40 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 199.9 K, ΔH=7794 J·mol^{-1}
c,I/liq 218.4 K
Molecular Weight 70.7356
Wiswesser Line Notation B2 H5 N1&1
Evaluation A

$C_2H_{12}B_{10}$ (liq) 81GOR/
m-Carborane; 1,7-Carborane-12
Heat Capacity 298.15 K, C_p=229.2 J·mol^{-1}·K^{-1}
Temperature range 10 to 330 K.
Entropy 298.15 K, S=211.8 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 58.0 K, ΔH=41 J·mol^{-1}
ΔS=0.73 J·mol^{-1}·K^{-1}
c,II/c,I 165 K, ΔH=1903 J·mol^{-1}
ΔS=9.50 J·mol^{-1}·K^{-1}
c,I/liq 280.1 K, ΔH=4326 J·mol^{-1}
ΔS=14.8 J·mol^{-1}·K^{-1}
Molecular Weight 144.2168
Evaluation A

$C_2H_{12}Br_6N_2Te$ (c) 86ONO/
Bis(methylammonium) hexabromotellurate (IV)
Heat Capacity 298.15 K, C_p=314.70 J·mol^{-1}·K^{-1}
Temperature range 13 to 320 K.
Entropy 298.15 K, S=592.98 J·mol^{-1}·K^{-1}
Phase Changes
c,IV/c,III 129.0 K, ΔH=1677 J·mol^{-1}
ΔS=13.0 J·mol^{-1}·K^{-1}
c,III/c,II 163.9 K, ΔH=885 J·mol^{-1}
ΔS=5.4 J·mol^{-1}·K^{-1}
c,II/c,I 288.9 K, ΔH=4594 J·mol^{-1}
ΔS=15.9 J·mol^{-1}·K^{-1}
Molecular Weight 671.1542
Wiswesser Line Notation ZH&1 2 -TE- E6
Evaluation A
The phase transition at 129.0 K is a higher order transition.

$C_2H_{12}CdCl_4N_2$ (c) 81RAH/CLA

Tetrachlorobis-(methylammonium) cadmium II

Heat Capacity	298.15 K,	C_p=261.9 J·mol^{-1}·K^{-1}
Temperature range 2.3 to 301 K.		
Entropy	298.15 K,	S=410.9 J·mol^{-1}·K^{-1}
Phase Changes		
c,IV/c,III	164.2 K,	ΔH=1749 J·mol^{-1}
		ΔS=10.8 J·mol^{-1}·K^{-1}
c,III/c,II	282 K,	ΔH=66.5 J·mol^{-1}
		ΔS=0.25 J·mol^{-1}·K^{-1}
c,II/c,I	484 K,	ΔH=no data given. J·mol^{-1}

Molecular Weight 304.3455
Wiswesser Line Notation ZH&1 2 -CD- G4
Evaluation B

$C_2H_{12}Cl_4MnN_2$ (c) 75BOC/ARR

Tetrachlorobis-(methylammonium) manganese II

Phase Changes		
c,III/c,II	257 K,	ΔH=4.8 J·mol^{-1}
		ΔS=0.017 J·mol^{-1}·K^{-1}
c,II/c,I	393 K,	ΔH=3.6 J·mol^{-1}
		ΔS=0.007 J·mol^{-1}·K^{-1}

Molecular Weight 260.8802
Wiswesser Line Notation ZH&1 2 -MN- G4
Evaluation A

$C_2H_{12}Cl_4MnN_2$ (c) 82WHI/GRA

Tetrachlorobis-(methylammonium) manganese II

Heat Capacity	298.15 K,	C_p=263.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.		
Entropy	298.15 K,	S=402.9 J·mol^{-1}·K^{-1}
Phase Changes		
c,III/c,II	94.37 K,	ΔH=728 J·mol^{-1}
		ΔS=7.74 J·mol^{-1}·K^{-1}
c,II/c,I	257.02 K,	ΔH=117 J·mol^{-1}
		ΔS=0.452 J·mol^{-1}·K^{-1}

Molecular Weight 260.8802
Wiswesser Line Notation ZH&1 2 -MN- G4
Evaluation A

$C_2H_{12}Cl_6N_2Pt$ (c) 91KUM/MAT

Bis(methylammonium) hexachloroplatinate

Heat Capacity	298.15 K,	C_p=292.01 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.		
Entropy	298.15 K,	S=445.33 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/c,I	123.82 K,	ΔH=1490 J·mol^{-1}
		ΔS=14.5 J·mol^{-1}·K^{-1}

Molecular Weight 471.9382
Wiswesser Line Notation ZH&1 2 -PT- Cl6
Evaluation A

$C_2H_{12}Cl_6N_2Te$ (c) 88ONO/MAT

Bis(methylammonium) hexachlorotellurate

Heat Capacity	298.21 K,	C_p=314.9 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Unsmoothed experimental datum.		
Phase Changes		
c,VI/c,V	73.0 K,	ΔH=470 J·mol^{-1}
		ΔS=6.4 J·mol^{-1}·K^{-1}
c,V/c,IV	136.8 K,	ΔH=1810 J·mol^{-1}
		ΔS=14.9 J·mol^{-1}·K^{-1}
Lambda type transition.		
c,IV/c,III	155 K,	ΔH=390 J·mol^{-1}
		ΔS=2.5 J·mol^{-1}·K^{-1}
c,III/c,II	226.0 K,	ΔH=330 J·mol^{-1}
		ΔS=1.7 J·mol^{-1}·K^{-1}
c,II/c,I	439 K,	ΔH=4400 J·mol^{-1}
		ΔS=9.8 J·mol^{-1}·K^{-1}

Molecular Weight 376.4348
Wiswesser Line Notation ZH&1 2 -TE- G6
Evaluation B(C_p), A(Phase changes)

$C_2H_{12}I_6N_2Te$ (c) 86ONO/MAT

Bis(methylammonium) hexaiodotellurate

Heat Capacity	298.15 K,	C_p=307.05 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.		
Entropy	298.15 K,	S=639.71 J·mol^{-1}·K^{-1}
Phase Changes		
c,III/c,II	66.1 K,	ΔH=403 J·mol^{-1}
		ΔS=6.1 J·mol^{-1}·K^{-1}
c,II/c,I	115.6 K,	ΔH=2555 J·mol^{-1}
		ΔS=22.1 J·mol^{-1}·K^{-1}

Molecular Weight 718.1547
Wiswesser Line Notation ZH&1 2 -TE- I6
Evaluation A
The phase transition at 66.1 K is a higher order transition.

C_2N_2 (liq) 39RUE/GIA

Cyanogen

Heat Capacity	255 K,	C_p=105.73 J·mol^{-1}·K^{-1}
Temperature range 15 to 252 K.		
Entropy	252.0 K,	S=138.83 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	245.32 K,	ΔH=8109 J·mol^{-1}
		ΔS=33.05 J·mol^{-1}·K^{-1}
liq/g	252.0 K,	ΔH=23330 J·mol^{-1}
		ΔS=92.58 J·mol^{-1}·K^{-1}
		P=101.325 kPa

Molecular Weight 52.0354
Wiswesser Line Notation NCCN
Evaluation A

$C_2N_6O_{12}$ (c,I) 70KRI/LIC

Hexanitroethane

Heat Capacity	291 K,	C_p=327 J·mol^{-1}·K^{-1}
Temperature range 190 to 350 K.		
Phase Changes		
c,II/c,I	291 K,	ΔH=12400 J·mol^{-1}
		ΔS=42.6 J·mol^{-1}·K^{-1}

Temperature range 289 to 292 K; 291 K assumed.
Molecular Weight 300.0550
Wiswesser Line Notation WNXNWNWXNWNWNW
Evaluation C

$C_2Na_2O_4$ (c) 37CHE/CHE
Sodium oxalate
Heat Capacity 281 K, C_p=130 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K. Mean values, three temperatures.
Molecular Weight 133.9992
Wiswesser Line Notation OVVO .NA 2
Evaluation C

C_2O_4Pb (c) 60KAP/STR
Lead (II) oxalate
Heat Capacity 299.37 K, C_p=102.7 J·mol^{-1}·K^{-1}
Temperature range 66 to 300 K. Value is unsmoothed experimental datum.
Entropy 298.16 K, S=146.0 J·mol^{-1}·K^{-1}
Extrapolation below 66 K, 28.0 J·mol^{-1}·K^{-1}.
Molecular Weight 295.2196
Wiswesser Line Notation OVVO .PB
Evaluation B

$C_{2.2}H_{6.5}N_2O$ (c) 72GAN/PAR
Urea-1-dodecene adduct; 1-Dodecene-urea adduct
Heat Capacity 298.15 K, C_p=126.6 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Values for one mole of urea in adduct.
Entropy 298.15 K, S=141.3 J·mol^{-1}·K^{-1}
Does not include possible zero-point entropy.
Phase Changes
Anomalous region 225 to 235 K, ΔH=2 J·mol^{-1}(urea), ΔS=0.010 J·mol^{-1}·K^{-1}.
c,II/c,I 82.0 K, ΔH=426 J·mol^{-1}
ΔS=5.2 J·mol^{-1}·K^{-1}
Molecular Weight 76.9884
Wiswesser Line Notation ZVZ &11U1 0.1060
Evaluation B

$C_{2.2}H_{6.6}N_2O$ (c) 69COP/PAR
Urea-n-undecane adduct; n-Undecane-urea adduct
Heat Capacity 298.15 K, C_p=129.2 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Values for one mole urea in adduct.
Entropy 298.15 K, S=138.0 J·mol^{-1}·K^{-1}
Does not include possible zero-point entropy.
Phase Changes
Anomolous region 225 to 235 K, with ΔH=14 J·mol^{-1}(urea) and ΔS=0.061 J·mol^{-1}·K^{-1}.
c,II/c,I 122.4 K, ΔH=144.6 J·mol^{-1}
ΔS=1.18 J·mol^{-1}·K^{-1}
Molecular Weight 77.0892
Wiswesser Line Notation ZVZ &11H 0.1104
Evaluation B

$C_{2.3}H_{6.7}N_2O$ (c) 69COP/PAR
Urea-1-hexadecene adduct; 1-Hexadecene-urea adduct
Heat Capacity 298.15 K, C_p=129.6 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Values for one mole urea in adduct.
Entropy 298.15 K, S=141.2 J·mol^{-1}·K^{-1}
Does not include possible zero-point entropy.
Phase Changes
Anomolous region 225 to 235 K, with ΔH=23 J·mol^{-1}(urea) and ΔS=0.101 J·mol^{-1}·K^{-1}.
c,II/c,I 141.7 K, ΔH=140.2 J·mol^{-1}
ΔS=0.99 J·mol^{-1}·K^{-1}
Molecular Weight 78.3911
Wiswesser Line Notation ZVZ &15H 0.860
Evaluation B

$C_{2.3}H_{6.7}N_2O$ (c) 69COP/I
Urea-1-decene adduct; 1-Decene-urea adduct
Heat Capacity 298.15 K, C_p=133.7 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Values for one mole urea in addu
Entropy 298.15 K, S=145.4 J·mol^{-1}·K^{-1}
Does not include possible zero point entropy.
Phase Changes
Anomolous region 225 to 235 K, with ΔH=10 J·mol^{-1}(urea) ΔS=0.045 J·mol^{-1}·K^{-1}.
Molecular Weight 78.3911
Wiswesser Line Notation ZVZ &9U1 0.1370
Evaluation B

$C_{2.4}H_{6.8}N_2O$ (c) 72GAN/I
Urea-1-octadecene adduct; 1-Octadecene-urea adduct
Heat Capacity 298.15 K, C_p=128.1 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Values for one mole of urea in add
Entropy 298.15 K, S=142.0 J·mol^{-1}·K^{-1}
Does not include possible zero-point entropy.
Phase Changes
Anomolous region 225 to 235 K, ΔH=12 J·mol^{-1}(urea) ΔS=0.049 J·mol^{-1}·K^{-1}.
c,II/c,I 155.9 K, ΔH=1926 J·mol^{-1}
ΔS=12.4 J·mol^{-1}·K^{-1}
Molecular Weight 79.6930
Wiswesser Line Notation ZVZ &17U1 0.0785
Evaluation B

$C_{2.4}H_{6.8}N_2O$ (c) 69COP/I
Urea 1 eicosene adduct; 1-Eicosene-urea adduct
Heat Capacity 298.15 K, C_p=129.2 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Values for one mole urea in addu
Entropy 298.15 K, S=139.6 J·mol^{-1}·K^{-1}
Does not include zero-point entropy.
Phase Changes
Anomolous region 225 to 235 K, with ΔH=1 J·mol^{-1}(urea) ΔS=0.002 J·mol^{-1}·K^{-1}.
c,II/c,I 153.9 K, ΔH=100.0 J·mol^{-1}
ΔS=0.65 J·mol^{-1}·K^{-1}
Molecular Weight 79.6930
Wiswesser Line Notation ZVZ &19U1 0.0701
Evaluation B

$C_{2.4}H_{6.9}N_2O$ (c) 72GAN/
Urea-1-tetradecene adduct; 1-Tetradecene-urea adduct
Heat Capacity 298.15 K, C_p=129.2 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Values for one mole urea in addi
Entropy 298.15 K, S=145.1 J·mol^{-1}·K^{-1}
Does not include possible zero-point entropy.
Phase Changes
Anomalous region 225 to 235 K, with ΔH=15 J·mol^{-1} (urea) ΔS=0.067 J·mol^{-1}·K^{-1}.
c,II/c,I 256.6 K, ΔH=3634 J·mol^{-1}
ΔS=12.0 J·mol^{-1}·K^{-1}
Molecular Weight 80.0660
Wiswesser Line Notation ZVZ &13U1 0.1019
Evaluation B

$C_3CEN_3S_3\cdot 7H_2O$ (c) 91TAN/
Cerium isothiocyanate heptahydrate
Heat Capacity 298.15 K, C_p=537.62 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=611.16 J·mol^{-1}·K^{-1}
Molecular Weight 440.4595
Wiswesser Line Notation SCN-CE-NCS&NCS &QH 7
Evaluation A

C_3Cl_6 (c) 90SUH/MAN

Hexachlorocyclopropane

Phase Changes

301 K, ΔH=0.21 J·mol^{-1}

Lambda-type transition.

c,II/c,I 285 K,

ΔH=1.26 J·mol^{-1}

Anomalous transition plus lambda type transition.

c,I/liq 376 K,

ΔH=18600 J·mol^{-1}

ΔS=49 J·mol^{-1}·K^{-1}

Molecular Weight 248.7510

Wiswesser Line Notation L3TJ AG AG BG BG CG CG

Evaluation A

C_3F_6O (liq) 67PLA/PAC

Hexafluoropropanone; Hexafluoroacetone

Heat Capacity 245 K, C_p=181.29 J·mol^{-1}·K^{-1}

Temperature range 12 to 244 K.

Entropy 245.87 K, S=286.60 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 147.70 K, ΔH=8382.6 J·mol^{-1}

ΔS=56.75 J·mol^{-1}·K^{-1}

liq/g 245.87 K, ΔH=21615 J·mol^{-1}

ΔS=87.91 J·mol^{-1}·K^{-1}

P=101.325 kPa

Molecular Weight 166.0228

Wiswesser Line Notation FXFFVXFFF

Evaluation A

C_3F_8 (liq) 67PAC/PLA

Perfluoropropane; Octafluoropropane

Heat Capacity 235 K, C_p=181.38 J·mol^{-1}·K^{-1}

Temperature range 14 to 236 K.

Entropy 236.42 K, S=287.23 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 99.39 K, ΔH=3555.6 J·mol^{-1}

ΔS=35.77 J·mol^{-1}·K^{-1}

c,I/liq 125.45 K, ΔH=477.4 J·mol^{-1}

ΔS=3.81 J·mol^{-1}·K^{-1}

liq/g 236.42 K, ΔH=19761 J·mol^{-1}

ΔS=83.58 J·mol^{-1}·K^{-1}

101.325 kPa

Molecular Weight 188.0202

Wiswesser Line Notation FXFFXFFXFFF

Evaluation A

$C_3GdN_3S_3·6H_2O$ (c) 91TAN/MAT

Gadolinium isothiocyanate hexahydrate

Heat Capacity 298.15 K, C_p=459.98 J·mol^{-1}·K^{-1}

Temperature range 13 to 300 K.

Entropy 298.15 K, S=527.16 J·mol^{-1}·K^{-1}

Molecular Weight 439.5743

Wiswesser Line Notation SCN-GD-NCS&NCS &QH 6

Evaluation A

C_3HF_7 (liq) 92WIR/BRA

1,1,1,2,3,3,3-Heptafluoropropane: R227

Heat Capacity 303.15 K, C_p=137.3 J·mol^{-1}·K^{-1}

Temperature range 253 to 423 K. Extrapolation to p=0 kPa.

Molecular Weight 170.0297

Wiswesser Line Notation FXFFYFXFFF

Evaluation A

$C_3H_2ClF_5$ (liq) 74VOR/KOL

1-Chloro-1,1,3,3,3-pentafluoropropane

Heat Capacity 298.15 K, C_p=196.48 J·mol^{-1}·K^{-1}

Temperature range 12 to 300 K. Data in paper deposited at VINITI, No. 6783-73, 25 Sept. 1973.

Entropy 298.15 K, S=403.67 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 165.42 K, ΔH=10473 J·mol^{-1}

ΔS=63.31 J·mol^{-1}·K^{-1}

Molecular Weight 168.4938

Wiswesser Line Notation GXFF1XFFF

Evaluation A

$C_3H_2Cl_2O_3$ (liq) 76MAS/PET

4,5-Dichloro-1,3-dioxolan-2-one

Heat Capacity 298 K, C_p=195 J·mol^{-1}·K^{-1}

Temperature range 200 to 340 K. Data graphically only. Value estimated from graph.

Molecular Weight 156.9530

Wiswesser Line Notation T5OVOTJ DG EG

Evaluation D

$C_3H_2Cl_3F_3$ (liq) 71KOL/VOR

1,1,1-Trichloro-3,3,3-trifluoropropane

Heat Capacity 298.15 K, C_p=199.91 J·mol^{-1}·K^{-1}

Temperature range 12 to 300 K. Data in paper deposited at VINITI, No. 1760-70, 21 May 1970.

Entropy 298.15 K, S=311.42 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 232.69 K, ΔH=14067 J·mol^{-1}

ΔS=60.45 J·mol^{-1}·K^{-1}

Molecular Weight 201.4030

Wiswesser Line Notation GXGG1XFFF

Evaluation A

$C_3H_2N_2$ (c,I) 68GIR/WES

Malononitrile; Dicyanomethane

Heat Capacity 298.15 K, C_p=110.29 J·mol^{-1}·K^{-1}

Temperature range 5 to 320 K.

Entropy 298.15 K, S=130.96 J·mol^{-1}·K^{-1}

Entropy as calculated from data on undercooled, c,I from 5 K and from data on c,II, c,II/c,I transition, and c,I is the same.

Phase Changes

Transition between stable c,II and metastable c,I between 255 to 270 K; maximum in C_p at 260.3 with ΔH=1264 J·mol^{-1} and ΔS=4.86 J·mol^{-1}·K^{-1}. Metastable c,I can be undercooled to 5 K.

c,I/liq 304.99 K, ΔH=10795 J·mol^{-1}

ΔS=35.39 J·mol^{-1}·K^{-1}

Molecular Weight 66.0622

Wiswesser Line Notation NC1CN

Evaluation A

$C_3H_2N_2$ (c) 87WAS/OLE

Malononitrile; Dicyanomethane

Heat Capacity

Temperature range 150 to 320 K. Data given graphically.

Phase Changes

c,IV/c,II 140 K

Re-entrant phase transition; second order.

c,III/c,II

First order transition; slow.

c,I/c,I′ 303 K

First order transition.

c,III/c,II 260 K

Phase III is stable below 260 K.

c,II/c,I 295 K

Second order transition.

Molecular Weight 66.0622

Wiswesser Line Notation NC1CN

Evaluation A

$C_3H_3ClO_3$ (liq) 76MAS/PET
4-Chloro-1,3-dioxolan-2-one
Heat Capacity 298 K, C_p=238 J·mol^{-1}·K^{-1}
Temperature range 200 to 325 K. Data graphically only. Value estimated from graph.
Molecular Weight 122.5079
Wiswesser Line Notation T5OVOTJ DG
Evaluation D

$C_3H_3Cl_2F_3$ (liq) 72KOL/VOR
1,1,1-Trifluoro-3,3-dichloropropane
Heat Capacity 298.15 K, C_p=191.29 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=295.06 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 156.4 K, ΔH=−900.4 J·mol^{-1}
Metastable crystal transition. Non-equilibrium.
c,II/c,I 167.7 K, ΔH=200.8 J·mol^{-1}
ΔS=1.20 J·mol^{-1}·K^{-1}
c,I/liq 182.16 K, ΔH=10134 J·mol^{-1}
ΔS=55.63 J·mol^{-1}·K^{-1}
Molecular Weight 166.9579
Wiswesser Line Notation GYG1XFFF
Evaluation A

C_3H_3N (liq) 45DAV/WIE
Acrylonitrile; Cyanoethene; Vinyl cyanide
Heat Capacity 298 K, C_p=113 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 53.0634
Wiswesser Line Notation NC1U1
Evaluation D

C_3H_3N (liq) 71HAL/BAL
Acrylonitrile; Cyanoethene; Vinyl cyanide
Heat Capacity 297 K, C_p=106.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 53.0634
Wiswesser Line Notation NC1U1
Evaluation C

C_3H_3N (liq) 72FIN/MES
Acrylonitrile; Cyanoethene; Vinyl cyanide
Heat Capacity 298.15 K, C_p=108.78 J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Entropy 298.15 K, S=178.91 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 162.5 K, ΔH=1188.3 J·mol^{-1}
ΔS=7.31 J·mol^{-1}·K^{-1}
c,I/liq 189.63 K, ΔH=6230.0 J·mol^{-1}
ΔS=32.85 J·mol^{-1}·K^{-1}
Molecular Weight 53.0634
Wiswesser Line Notation NC1U1
Evaluation A

C_3H_3N (liq) 87MIR/SHA
Acrylonitrile; Cyanoethene; Vinyl cyanide
Heat Capacity 298.15 K, C_p=98.7 J·mol^{-1}·K^{-1}
Temperature range 213 to 333 K. Unsmoothed experimental datum given as 1.898 kJ/kg·K at 293 K. C_p(liq)=2.05105 +0.00465503T/K+1.34722×10^{-5}T^2/K^2 kJ/kg·K (213 to 333 K). Note, second coefficient should be negative.
Molecular Weight 53.0634
Wiswesser Line Notation NC1U1
Evaluation D

C_3H_3NO (liq) 93STE/
Isoxazole
Heat Capacity 298.15 K, C_p=108.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 69.0628
Wiswesser Line Notation T5NOJ
Evaluation A

C_3H_3NS (liq) 68GOU/
Thiazole
Heat Capacity 298.15 K, C_p=121.00 J·mol^{-1}·K^{-1}
Temperature range 5 to 340 K. Glass transition 145 to 175 K.
Entropy 298.15 K, S=169.95 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 239.48 K, ΔH=9590 J·mol^{-1}
ΔS=40.04 J·mol^{-1}·K^{-1}
Molecular Weight 85.1234
Wiswesser Line Notation T5N CSJ
Evaluation A

C_3H_3NS (liq) 69SOU/
Thiazole
Heat Capacity 298.15 K, C_p=121.00 J·mol^{-1}·K^{-1}
Temperature range 4 to 350 K.
Entropy 298.15 K, S=169.95 J·mol^{-1}·K^{-1}
Phase Changes
Anomalous region 145 to 175 K.
c/liq 239.53 K, ΔH=9539.7 J·mol^{-1}
ΔS=40.04 J·mol^{-1}·K^{-1}
Molecular Weight 85.1234
Wiswesser Line Notation T5N CSJ
Evaluation A

$C_3H_3N_3$ (c) 79BR
s-Triazine
Heat Capacity 298.15 K, C_p=95.6 J·mol^{-1}·K^{-1}
Temperature range 160 to 382 K.
Phase Changes
Transition between 130 and 177 K with ΔH=75 J·mol^{-1}.
c,I/liq 353.9 K, ΔH=14584 J·mol^{-1}
ΔS=41.21 J·mol^{-1}·K^{-1}
Molecular Weight 81.0768
Wiswesser Line Notation T6N CN ENJ
Evaluation B

$C_3H_3N_3$ (c) 88BON
s-Triazine
Heat Capacity 298.15 K, C_p=95.57 J·mol^{-1}·K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S=125.97 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 197.7 K, ΔH=74.0 J·mol^{-1}
First order treatment from 175 K
ΔH=127.4 J·mol^{-1}
First order treatment from 150 K
ΔH=362.8 J·mol^{-1}
Second order treatment
c,I/liq 353.44 K, ΔH=14560 J·mol^{-1}
Molecular Weight 81.0768
Wiswesser Line Notation T6N CN ENJ
Evaluation A

$C_3H_3N_3O_3$ (c) 83DEW/DEK
Cyanuric acid; Triazine triol
Heat Capacity 300 K, C_p=133.63 J·mol^{-1}·K^{-1}
Temperature range 90 to 340 K. C_p=20.63+0.3758 (T/K) J·mol^{-1}·K^{-1} (90 to 340 K).
Molecular Weight 129.0750
Wiswesser Line Notation T6N CN ENJ BQ DQ FQ
Evaluation B(C_p), A(Phase changes).

$C_3H_3N_3O_3$ (c) 92KOZ/KAB2
Cyanuric acid; Triazine triol
Heat Capacity 298.15 K, C_p=130.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=142.2 J·mol^{-1}·K^{-1}
Molecular Weight 129.0750
Wiswesser Line Notation T6N CN ENJ BQ DQ FQ
Evaluation A

$C_3H_4ClF_3$ (liq) 72KOL/VOR
1,1,1-Trifluoro-3-chloropropane
Heat Capacity 298.15 K, C_p=171.08 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=271.67 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 116.0 K, ΔH=−2533.0 J·mol^{-1}
Metastable crystal transition. Non-equilibrium.
c,II/c,I 169.8 K, ΔH=4489 J·mol^{-1}
ΔS=26.44 J·mol^{-1}·K^{-1}
c,I/liq 179.40 K, ΔH=5314 J·mol^{-1}
ΔS=29.62 J·mol^{-1}·K^{-1}
Molecular Weight 132.5128
Wiswesser Line Notation G2XFFF
Evaluation A

$C_3H_4ClF_3$ (liq) 74KOL/VOR
1,1,1-Trifluoro-3-chloropropane
Heat Capacity 298.15 K, C_p=171.08 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=271.67 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 116.0 K, ΔH=−2531 J·mol^{-1}
Maximum temperature of metastable phase. ΔH obtained from total heat 115 to 137 K, calculated to 116 K. Not reversible.
c,II/c,I 169.8 K, ΔH=4489 J·mol^{-1}
ΔS=26.44 J·mol^{-1}·K^{-1}
c,I/liq 179.32 K, ΔH=5050 J·mol^{-1}
ΔS=28.16 J·mol^{-1}·K^{-1}
Molecular Weight 132.5128
Wiswesser Line Notation G2XFFF
Evaluation A

$C_3H_4Cl_3NSi$ (c) 75KOS/SAM
β-Trichlorosilylpropionitrile
Heat Capacity 298.15 K, C_p=186.1 J·mol^{-1}·K^{-1}
Temperature range 13.4 to 322.5 K. Deposited in VINITI, No 586-75, 10 March 1975.
Entropy 298.15 K, S=246.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 307.90 K, ΔH=21242 J·mol^{-1}
ΔS=69.0 J·mol^{-1}·K^{-1}
Molecular Weight 188.5158
Wiswesser Line Notation NC2-SI-GGG
Evaluation A

$C_3H_4Cl_4$ (liq) 74KOL/VOR
1,1,1,3-Tetrachloropropane
Heat Capacity 298.15 K, C_p=196.40 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=284.30 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 219.9 K, ΔH=2205 J·mol^{-1}
ΔS=10.03 J·mol^{-1}·K^{-1}
c,I/liq 237.74 K, ΔH=10489 J·mol^{-1}
ΔS=44.12 J·mol^{-1}·K^{-1}
Molecular Weight 181.8766
Wiswesser Line Notation GXGG2G
Evaluation A

$C_3H_4N_2$ (c) 83DEW/DEK
Imidazole
Heat Capacity 300 K, C_p=89.78 J·mol^{-1}·K^{-1}
Temperature range 90 to 370 K.
Phase Changes
c/liq 362.69 K, ΔH=12821 J·mol^{-1}
ΔS=35.35 J·mol^{-1}·K^{-1}
Molecular Weight 68.0780
Wiswesser Line Notation T5M CNJ
Evaluation B(C_p), A(Phase changes).

$C_3H_4N_2$ (c) 83DEW/OFF
Imidazole
Heat Capacity 310 K, C_p=94.4 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c/liq 361.9 K, ΔH=12800 J·mol^{-1}
ΔS=35.37 J·mol^{-1}·K^{-1}
Molecular Weight 68.0780
Wiswesser Line Notation T5M CNJ
Evaluation B

$C_3H_4N_2$ (c) 87JIM/ROU
Imidazole
Heat Capacity 298.15 K, C_p=82.4 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.21 J·K^{-1}·g^{-1}.
Molecular Weight 68.0780
Wiswesser Line Notation T5M CNJ
Evaluation B

$C_3H_4N_2$ (c) 89HIL/MOU
Imidazole
Phase Changes
c/liq 363.7 K, ΔH=12500 J·mol^{-1}
Molecular Weight 68.0780
Wiswesser Line Notation T5M CNJ
Evaluation A

$C_3H_4N_2$ (c) 83DEW/OFF
Pyrazole
Heat Capacity 300 K, C_p=87.9 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c/liq 333.1 K, ΔH=13800 J·mol^{-1}
ΔS=41.43 J·mol^{-1}·K^{-1}
Molecular Weight 68.0780
Wiswesser Line Notation T5MNJ
Evaluation B

$C_3H_4N_2$ (c) 87JIM/ROU
Pyrazole
Heat Capacity 298.15 K, C_p=81.0 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.19 J·K^{-1}·g^{-1}.
Molecular Weight 68.0780
Wiswesser Line Notation T5MNJ
Evaluation B

$C_3H_4N_2$ (c) 89HIL/MOU
Pyrazole
Phase Changes
c/liq 343.2 K, ΔH=14200 J·mol^{-1}
Molecular Weight 68.0780
Wiswesser Line Notation T5MNJ
Evaluation A

$C_3H_4N_2O$ (c) 83DEW/OFF
Cyanoacetamide
Heat Capacity 300 K, C_p=111.1 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c,II/c,I 346.5 K, ΔH=1200 J·mol^{-1}
ΔS=3.46 J·mol^{-1}·K^{-1}
c,I/liq 387.3 K, ΔH=21700 J·mol^{-1}
ΔS=56.0 J·mol^{-1}·K^{-1}
Molecular Weight 84.0774
Wiswesser Line Notation ZV1CN
Evaluation B

$C_3H_4N_2OS$ (c) 82LEB/NOV
2-Imino-4-thiazolidinone; 2-Amino-4(5H)-thiazolone
Heat Capacity 277.8 K, C_p=106.0 J·mol^{-1}·K^{-1}
Temperature range 66 to 300 K.
Molecular Weight 102.1538
Wiswesser Line Notation T5MYSV EHJ BUM
Evaluation B

$C_3H_4O_2$ (liq) 83KAR/ABD2
Acrylic acid
Heat Capacity 300 K. C_p=145.70 J·mol^{-1}·K^{-1}
Temperature range 290 to 344 K. C_p given as 2021.8 J·kg^{-1}·K^{-1}.
Molecular Weight 72.0634
Wiswesser Line Notation QV1U1
Evaluation B

$C_3H_4O_2$ (liq) 85KAR/ABD2
Acrylic acid
Phase Changes
c/liq 285.7 K. ΔH=9509.7 J·mol^{-1}
ΔS=33.3 J·mol^{-1}·K^{-1}
Molecular Weight 72.0634
Wiswesser Line Notation QV1U1
Evaluation A

$C_3H_4O_2$ (liq) 85KAR/SAI
Acrylic acid
Heat Capacity 298.15 K. C_p=144.2 J·mol^{-1}·K^{-1}
Temperature range 90 to 350 K. C_p(c)=313.44+3.99T J/kg·K (103 to 252 K); C_p(liq)=695.42+4.38T J/kg·K (285.7 to 350 K). C_p data calculated from equation.
Phase Changes
c/liq 285.7 K
Molecular Weight 72.0634
Wiswesser Line Notation QV1U1
Evaluation B

$C_3H_4O_2$ (liq) 79YEV/L
β-Propiolactone
Heat Capacity 298.15 K, C_p=122.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K.
Entropy 298.15 K, S=175.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 239.86 K, ΔH=9410 J·mol^{-1}
ΔS=39.23 J·mol^{-1}·K^{-1}
Molecular Weight 72.0634
Wiswesser Line Notation T4OVTJ
Evaluation A

$C_3H_4O_2$ (liq) 83LEB/Y
β-Propiolactone
Heat Capacity 298.15 K, C_p=122.1 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 340 K.
Entropy 298.15 K, S=175.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 239.86 K, ΔH=9410 J·mol^{-1}
ΔS=39.23 J·mol^{-1}·K^{-1}
Molecular Weight 72.0634
Wiswesser Line Notation T4OVTJ
Evaluation A

$(C_3H_4O_2)_n$ (liq) 79YEV/L
Poly-β-propiolactone
Heat Capacity 298.15 K, C_p=134.8 J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K. Highly elastic polyn C_p(298.15)=89.74 J·mol^{-1}·K^{-1} for crystalline polymer.
Entropy 298.15 K, S=111.0 J·mol^{-1}·K^{-1}
Highly elastic polymer. S(298.15)=101.4 J·mol^{-1}·K^{-1} for crystall polymer.
Molecular Weight 72.0634
Wiswesser Line Notation /*OV2*/
Evaluation A
T(glass)=249 K.

$C_3H_4O_3$ (liq) 58I
Ethylene carbonate
Heat Capacity 323.15 K, C_p=133.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.0628
Wiswesser Line Notation T5OVOTJ
Evaluation C

$C_3H_4O_3$ (c) 73VAS/K
Ethylene carbonate
Heat Capacity 298.15 K, C_p=117.44 J·mol^{-1}·K^{-1}
Temperature range 52 to 310 K. Full data deposited in VINITI, 326-73, 21 June 1973.
Entropy 298.15 K, S=132.54 J·mol^{-1}·K^{-1}
Extrapolation below 52 K.
Phase Changes
c/liq 309.49 K, ΔH=13295 J·mol^{-1}
ΔS=42.96 J·mol^{-1}·K^{-1}
Molecular Weight 88.0628
Wiswesser Line Notation T5OVOTJ
Evaluation B

$C_3H_4O_3$ (c) 74VAS/KOR
Ethylene carbonate
Heat Capacity 298.15 K, C_p=117.44 J·mol^{-1}·K^{-1}
Temperature range 52 to 340 K. C_p(liq)=88.977+0.1586T J/mol·K (309 to 340 K).
Entropy 298.15 K, S=132.54 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 309.49 K, ΔH=13295 J·mol^{-1}
ΔS=42.96 J·mol^{-1}·K^{-1}
Molecular Weight 88.0628
Wiswesser Line Notation T5OVOTJ
Evaluation B

$C_3D_4O_4$ (c,II) 91FUK/MAT
Malonic acid-d_4
Heat Capacity 298.15 K, C_p=139.93 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=157.14 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 60.0 K, ΔH=23.86 J·mol^{-1}
ΔS=0.411 J·mol^{-1}·K^{-1}
c,II/c,I 348.0 K, ΔH=1810 J·mol^{-1}
ΔS=5.201 J·mol^{-1}·K^{-1}
Molecular Weight 108.0938
Wiswesser Line Notation QV1VQ &1/H-2 &3/H-2 2 &5/H-2
Evaluation A

$C_3H_4O_4$ (c) 88PET/TSY
Malonic acid
Phase Changes
c,II/c,I 351.2 K, ΔH=1600 J·mol^{-1}
ΔS=4.6 J·mol^{-1}·K^{-1}
Molecular Weight 104.0622
Wiswesser Line Notation QV1VQ
Evaluation A

$C_3H_4O_4$ (c,II) 91FUK/MAT
Malonic acid
Heat Capacity 298.15 K, C_p=127.63 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=149.00 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 47.3 K, ΔH=14.80 J·mol^{-1}
ΔS=0.313 J·mol^{-1}·K^{-1}
c,II/c,I 352.2 K, ΔH=1837 J·mol^{-1}
ΔS=5.217 J·mol^{-1}·K^{-1}
Molecular Weight 104.0622
Wiswesser Line Notation QV1VQ
Evaluation A

$C_3H_5D_3O_3$ (liq) 62RAB/NIK
1,2,3-Trihydroxypropane-d_3; 1,2,3-Propanetriol-d_3; Glycerol-d_3
Heat Capacity 298 K, C_p=231.00 J·mol^{-1}·K^{-1}
Temperature range 10 to 55 °C.
Molecular Weight 95.1130
Wiswesser Line Notation Q1YQ1Q &1/4/6/H-2 3
Evaluation B

$C_3H_5Br_3$ (liq) 48KUR
1,2,3-Tribromopropane
Heat Capacity 298 K, C_p=166.5 J·mol^{-1}·K^{-1}
Temperature range 17 to 218 °C. mean C_p, six temperatures.
Molecular Weight 280.7845
Wiswesser Line Notation E1YE1E
Evaluation D

C_3H_5Cl (liq) 1881REI
3-Chloropropene-1
Heat Capacity 298 K, C_p=125.1 J·mol^{-1}·K^{-1}
Temperature range 289 to 334 K.
Molecular Weight 76.5255
Wiswesser Line Notation G2U1
Evaluation D

C_3H_5ClO (liq) 1881REI
Propanoyl chloride; Propionyl chloride
Heat Capacity 298 K, C_p=147.3 J·mol^{-1}·K^{-1}
Temperature range 291 to 365 K.
Molecular Weight 92.5249
Wiswesser Line Notation GV2
Evaluation D

$C_3H_5Cl_3$ (liq) 41NEL/NEW
1,2,3-Trichloropropane
Heat Capacity 298 K, C_p=183.6 J·mol^{-1}·K^{-1}
Temperature range 0 to 60 °C. Equation only.
Molecular Weight 147.4315
Wiswesser Line Notation G1YG1G
Evaluation B

$C_3H_5Cl_3$ (liq) 48KUR
1,2,3-Trichloropropane
Heat Capacity 298 K, C_p=172.8 J·mol^{-1}·K^{-1}
Temperature range 17 to 155 °C, mean C_p, three temperatures.
Molecular Weight 147.4315
Wiswesser Line Notation G1YG1G
Evaluation D

$C_3H_5CsO_2$ (c) 75FER/SAN
Cesium propionate
Phase Changes
c,III/c,II 314 K, ΔH=1340 J·mol^{-1}
ΔS=4.3 J·mol^{-1}·K^{-1}
c,II/c,I 419 K, ΔH=1925 J·mol^{-1}
ΔS=4.6 J·mol^{-1}·K^{-1}
c,I/liq 580 K, ΔH=11715 J·mol^{-1}
ΔS=20.2 J·mol^{-1}·K^{-1}
Molecular Weight 205.9767
Wiswesser Line Notation OV2 .CS
Evaluation C

$C_3H_5KO_2$ (c) 75FER/SAN
Potassium propionate
Phase Changes
c,III/c,II 258 K, ΔH=330 J·mol^{-1}
ΔS=1.3 J·mol^{-1}·K^{-1}
c,II/c,I 352.5 K, ΔH=1715 J·mol^{-1}
ΔS=4.9 J·mol^{-1}·K^{-1}
c,I/liq 638.3 K, ΔH=20125 J·mol^{-1}
ΔS=31.5 J·mol^{-1}·K^{-1}
Molecular Weight 112.1696
Wiswesser Line Notation OV2 .KA
Evaluation C

$C_3H_5KO_2$ (c) 84FRA/WES
Potassium propionate
Heat Capacity 298.15 K, C_p=129.5 J·mol^{-1}·K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S=142.4 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 255 K, ΔH=515 J·mol^{-1}
ΔS=2.02 J·mol^{-1}·K^{-1}
c,II/c,I 372.5 K
c,I/liq 638.3 K
Molecular Weight 112.1696
Wiswesser Line Notation OV2 .KA
Evaluation A

$C_3H_5LiO_2$ (c) 75FER/SAN
Lithium propionate
Phase Changes
c,II/c,I 533 K. ΔH=3350 J·mol^{-1}
ΔS=6.3 J·mol^{-1}·K^{-1}
c,I/liq 606.5 K, ΔH=15860 J·mol^{-1}
ΔS=26.1 J·mol^{-1}·K^{-1}
Also metastable fusion at 584.6 K, ΔH=17824 J·mol^{-1}.
Molecular Weight 80.0123
Wiswesser Line Notation OV2 .LI
Evaluation C

$C_3H_5LiO_2$ (c) 84FRA/WES
Lithium propionate
Heat Capacity 298.15 K, C_p=143.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 600 K.
Entropy 298.15 K, S=175.9 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 514 K
c,I/liq 606.8 K
Molecular Weight 80.0123
Wiswesser Line Notation OV2 .LI
Evaluation A

$C_3H_5LiO_2$ (c) 85FRA/WES
Lithium propionate
Heat Capacity 298.15 K, C_p=130.29 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=143.17 J·mol^{-1}·K^{-1}
Molecular Weight 80.0123
Wiswesser Line Notation OV2 .LI
Evaluation A

C_3H_5N (liq) 07WAL
Propionitrile; Ethyl cyanide; Cyanoethane
Heat Capacity 290 K, C_p=117 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 55.0792
Wiswesser Line Notation NC2
Evaluation D

C_3H_5N (liq) 62WEB/I
Propionitrile; Ethyl cyanide; Cyanoethane
Heat Capacity 298.15 K, C_p=119.50 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=189.33 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 176.96 K, ΔH=1706.7 J·mol^{-1}
ΔS=9.64 J·mol^{-1}·K^{-1}
c,I/liq 180.37 K, ΔH=5030.0 J·mol^{-1}
ΔS=27.89 J·mol^{-1}·K^{-1}
liq/g 298.15 K, ΔH=36116 J·mol^{-1}
ΔS=121.1 J·mol^{-1}·K^{-1}
P=6.29 kPa
Molecular Weight 55.0792
Wiswesser Line Notation NC2
Evaluation A

C_3H_5N (liq) 71HAL/E
Propionitrile; Ethyl cyanide; Cyanoethane
Heat Capacity 297 K, C_p=112.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 55.0792
Wiswesser Line Notation NC2
Evaluation C

C_3H_5N (liq) 85GUS/N
Propionitrile; Ethyl cyanide; Cyanoethane
Heat Capacity 303.15 K, C_p=106.0 J·mol^{-1}·K^{-1}
Temperature range 303 to 363 K. p=0.1 MPa. Unsoothed experime
datum given as 1.9250 kJ/kg·K.
Molecular Weight 55.0792
Wiswesser Line Notation NC2
Evaluation B

C_3H_5N (liq) 87MIR/S
Propionitrile; Ethyl cyanide; Cyanoethane
Heat Capacity 298.15 K, C_p=105.3 J·mol^{-1}·K^{-1}
Temperature range 193 to 353 K. Unsmoothed experimental da
given as 1.845 kJ/kg·K at 293 K. C_p(liq)=1.9082+0.0027614
+9.3056×10^{-6}T^2/K^2 kJ/kg·K (193 to 353 K). Note, second t
should be negative.
Molecular Weight 55.0792
Wiswesser Line Notation NC2
Evaluation D

C_3H_5NO (c) 89STE/C
Acrylamide
Heat Capacity 298.15 K, C_p=110.58 J·mol^{-1}·K^{-1}
Temperature range 305 to 415 K. Csat/R(c)=0.0653T−6.17 (30
345 K); Csat/R(liq)=0.02546T+13.26 (365 to 415 K). Polymeriz
began at 415 K.
Phase Changes
c/liq 358 K, ΔH=15330 J·mol^{-1}
Molecular Weight 71.0786
Wiswesser Line Notation ZV1U1
Evaluation B

$(C_3H_5NO)_n$ (c) 75DAU/
Poly-L-alanine, α-helix
Heat Capacity
Temperature range 1 to 300 K. C_p data given graphically.
Entropy 273 K, S=101.7 J·mol^{-1}·K^{-1}
Molecular Weight 71.0786
Wiswesser Line Notation /*VYM*&1/ -L
Evaluation B

$(C_3H_5NO)_n$ (c) 75DAU/DEL
Poly-L-alanine, β-sheet
Heat Capacity
Temperature range 1 to 300 K. C_p data given graphically.
Entropy 273 K, $S=116.7\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 71.0786
Wiswesser Line Notation /*VYM*&1/ -L
Evaluation B

$(C_3H_5NO)_n$ (c) 91ROL
Poly-L-alanine
Heat Capacity 300 K, $C_p=93.47\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 220 to 390 K.
Molecular Weight 71.0786
Wiswesser Line Notation /*VYM*&1/ -L
Evaluation B

$(C_3H_5NO)_n$ (c) 91ROL/WUN
Poly-L-alanine
Heat Capacity 300 K, $C_p=93.47\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 230 to 390 K.
Molecular Weight 71.0786
Wiswesser Line Notation /*VYM*&1/ -L
Evaluation B

$(C_3H_5NO_2)_n$ (c) 91ROL
Poly-L-serine
Heat Capacity 300 K, $C_p=112.9\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 220 to 390 K.
Molecular Weight 87.0780
Wiswesser Line Notation /*VYM*&1Q/ -L
Evaluation B

$(C_3H_5NO_2)_n$ (c) 93ROL/XEN
Poly-L-serine
Heat Capacity 300 K, $C_p=112.9\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 220 to 390 K.
Molecular Weight 87.0780
Wiswesser Line Notation /*VYM*&1Q/ -L
Evaluation B

$C_3H_5NO_4$ (liq) 81LEB/RYA
Methyl ester of nitroacetic acid; Methyl nitroacetate
Heat Capacity $C_p=205.8\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 298 to 343 K. Data given over temperature range.
Molecular Weight 119.0768
Wiswesser Line Notation WN1VO1
Evaluation D

C_3H_5NS (liq) 36KUR/VOS
Ethyl isothiocyanate
Heat Capacity 290 K, $C_p=106.3\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 87.1392
Wiswesser Line Notation SCN2
Evaluation D

$C_3H_5NaO_2$ (c,III) 75FER/SAN
Sodium propanoate
Heat Capacity 340 K, $C_p=150.2\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 340 to 570 K.
Phase Changes
c,III/c,I 482 K, $\Delta H=7360\ J\cdot mol^{-1}$
$\Delta S=15.3\ J\cdot mol^{-1}\cdot K^{-1}$
Taken as sum of data for transitions at 470 and 494 K at average temperature.
c,I/liq 562.4 K, $\Delta H=13390\ J\cdot mol^{-1}$
$\Delta S=23.8\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 96.0611
Wiswesser Line Notation OV2 .NA
Evaluation B

$C_3H_5NaO_2$ (c) 83FRA/WES
Sodium propanoate
Heat Capacity 298.15 K, $C_p=134.4\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 9 to 580 K.
Entropy 298.15 K, $S=152.1\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c,III/c,II 467.00 K, $\Delta H=3209\ J\cdot mol^{-1}$
$\Delta S=6.87\ J\cdot mol^{-1}\cdot K^{-1}$
c,II/c,I 491.00 K, $\Delta H=4357\ J\cdot mol^{-1}$
$\Delta S=8.87\ J\cdot mol^{-1}\cdot K^{-1}$
c,I/liq 561.91 K, $\Delta H=13280.0\ J\cdot mol^{-1}$
$\Delta S=23.63\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 96.0611
Wiswesser Line Notation OV2 .NA
Evaluation A

$C_3H_5O_2Rb$ (c) 75FER/SAN
Rubidium propionate
Phase Changes
c,III/c,II 317 K, $\Delta H=1510\ J\cdot mol^{-1}$
$\Delta S=4.8\ J\cdot mol^{-1}\cdot K^{-1}$
c,II/c,I 564.3 K, $\Delta H=2970\ J\cdot mol^{-1}$
$\Delta S=5.3\ J\cdot mol^{-1}\cdot K^{-1}$
c,I/liq 623.1 K, $\Delta H=14560\ J\cdot mol^{-1}$
$\Delta S=23.4\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 158.5391
Wiswesser Line Notation OV2 .RB
Evaluation C

$C_3H_5O_2Tl$ (c) 76MEI/SEY
Thallium propionate
Phase Changes
c,II/c,I 365 K, $\Delta H=377\ J\cdot mol^{-1}$
$\Delta S=1.05\ J\cdot mol^{-1}\cdot K^{-1}$
c,I/liq 468 K, $\Delta H=9205\ J\cdot mol^{-1}$
$\Delta S=20.1\ J\cdot mol^{-1}\cdot K^{-1}$
Solid-mesophase.
Molecular Weight 277.4413
Wiswesser Line Notation OV2 .TL
Evaluation B

$C_3H_5O_2Tl$ (c) 84FER/LOP
Thallium propionate
Heat Capacity 320 K, $C_p=158\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 320 to 480 K.
Phase Changes
c,II/c,I 364.8 K, $\Delta H=316\ J\cdot mol^{-1}$
$\Delta S=0.83\ J\cdot mol^{-1}\cdot K^{-1}$
c,I/liq 468.0 K, $\Delta H=10476\ J\cdot mol^{-1}$
$\Delta S=22.5\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 277.4413
Wiswesser Line Notation OV2 .TL
Evaluation A

C_3H_6 (liq) 31HUF/PAR

Propylene; Propene

Heat Capacity 210.3 K, C_p=90.0 J·mol^{-1}·K^{-1}

Temperature range 69 to 210 K. Value is unsmoothed experimental datum.

Phase Changes

c/liq 88.2 K, ΔH=2933 J·mol^{-1}
ΔS=33.3 J·mol^{-1}·K^{-1}

Molecular Weight 42.0804

Wiswesser Line Notation 2U1

Evaluation B

C_3H_6 (liq) 39POW/GIA

Propylene; Propene

Heat Capacity 230 K, C_p=92.09 J·mol^{-1}·K^{-1}

Temperature range 14 to 225 K.

Phase Changes

c/liq 87.85 K, ΔH=3002 J·mol^{-1}
ΔS=34.18 J·mol^{-1}·K^{-1}

liq/g 225.35 K, ΔH=18418 J·mol^{-1}
ΔS=81.73 J·mol^{-1}·K^{-1}

Molecular Weight 42.0804

Wiswesser Line Notation 2U1

Evaluation B

C_3H_6 (liq) 50AUE/SAG

Propylene; Propene

Heat Capacity 300 K, C_p=98.9 J·mol^{-1}·K^{-1}

Temperature range 300 to 344 K. Datum at 80 °C is C_p at the bubble point, 0.5615 Btu(lb)$^{-1}$(°R)$^{-1}$.

Molecular Weight 42.0804

Wiswesser Line Notation 2U1

Evaluation A

C_3H_6 (liq) 83CHA/HAL

Propylene; Propene

Heat Capacity 298.15 K, C_p=102 J·mol^{-1}·K^{-1}

Temperature range 14 to 340 K.

Entropy 298.15 K, S=195.7 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 87.85 K, ΔH=3003 J·mol^{-1}
ΔS=34.18 J·mol^{-1}·K^{-1}

Molecular Weight 42.0804

Wiswesser Line Notation 2U1

Evaluation A

A reevaluation of the original measured data from: 31HUF/PAR, 39POW/GIA, 50AUE/SAG.

C_3H_6 (gls) 90TAK/OGU

Propylene; Propene

Phase Changes

c/gls 56.0 K

Molecular Weight 42.0804

Wiswesser Line Notation 2U1

Evaluation A

C_3H_6 (liq) 46RUE/

Cyclopropane

Heat Capacity 240 K, C_p=81.34 J·mol^{-1}·K^{-1}

Temperature range 14 to 240 K.

Entropy 240.34 K, S=142.63 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 145.57 K, ΔH=5443 J·mol^{-1}
ΔS=37.39 J·mol^{-1}·K^{-1}

liq/g 240.34 K, ΔH=20054 J·mol^{-1}
ΔS=83.44 J·mol^{-1}·K^{-1}
P=101.325 kPa

Molecular Weight 42.0804

Wiswesser Line Notation L3TJ

Evaluation A

$(C_3H_6)_n$ (gls) 62DAI/

Polypropylene, atactic

Heat Capacity 298.15 K, C_p=89.59 J·mol^{-1}·K^{-1}

Temperature range 20 to 310 K.

Entropy 298.15 K, S=78.99 J·mol^{-1}·K^{-1}

When extrapolated to 100% crystallinity, the entropy is 62.7 mol^{-1}·K^{-1}.

Phase Changes

c,I/gls 249 K

Molecular Weight 42.0804

Wiswesser Line Notation /*Y1&1*/

Evaluation A

$(C_3H_6)_n$ (gls) 62WIL/

Polypropylene, atactic

Heat Capacity 298.15 K, C_p=98.90 J·mol^{-1}·K^{-1}

Temperature range 217 to 477 K. C_p=0.510+0.00207t (−30 °C) cal·g^{-1}·deg^{-1}.C_p value calculated from equation.

Phase Changes

343 K, ΔH=373 J·mol^{-1}

Annealed sample.

428 K, ΔH=61 J·mol^{-1}

Annealed sample.

Molecular Weight 42.0804

Wiswesser Line Notation /*Y1&1*/

Evaluation A

T(glass)=−12 °C. The transition at 343 K is attributed to melti heterotactic sequences. The transition at 428 K is attributed isotactic or syndiotactic content.

$(C_3H_6)_n$ (gls) 63PAS/

Polypropylene, atactic

Heat Capacity 298.1 K, C_p=88.0 J·mol^{-1}·K^{-1}

Temperature range 87 to 484 K. Unsmoothed experimental datur

Phase Changes

c/gls 259 K

Molecular Weight 42.0804

Wiswesser Line Notation /*Y1&1*/

Evaluation B

2 to 3% crystallinity.

$(C_3H_6)_n$ (gls) 62DAI/

Polypropylene, isotatic

Heat Capacity 298.15 K, C_p=77.18 J·mol^{-1}·K^{-1}

Temperature range 20 to 310 K.

Entropy 298.15 K, S=72.05 J·mol^{-1}·K^{-1}

When extrapolated to 100% crystallinity, the entropy is 61. mol^{-1}·K^{-1}.

Phase Changes

c,I/gls 260 K

Molecular Weight 42.0804

Wiswesser Line Notation /*Y1&1*/

Evaluation A

$(C_3H_6)_n$ (gls) 62WIL/DOL
Polypropylene, isotactic
Heat Capacity 298.15 K, C_p=75.25 J·mol^{-1}·K^{-1}
Temperature range 253 to 484 K. C_p=0.3669+0.00242t (below 100 °C) cal·g^{-1}·deg^{-1}. C_p value calculated from equation.
Phase Changes
c/liq 449 K, ΔH=6162 J·mol^{-1}
Corrected to 100% crystallinity.
Molecular Weight 42.0804
Wiswesser Line Notation /*Y1&1*/
Evaluation A

$(C_3H_6)_n$ (gls) 63PAS/KEV2
Polypropylene, isotatic
Heat Capacity 299.8 K, C_p=72.4 J·mol^{-1}·K^{-1}
Temperature range 85 to 500 K. Unsmoothed experimental datum.
Phase Changes
c/gls 267 K, ΔH=7923 J·mol^{-1}
Molecular Weight 42.0804
Wiswesser Line Notation /*Y1&1*/
Evaluation B
64.9% crystallinity.

$(C_3H_6)_n$ (c) 68GEE/MEL
Polypropylene, syndiotatic
Heat Capacity 298.15 K, C_p=69.6 J·mol^{-1}·K^{-1}
Temperature range 180 to 460 K. Values per C_3H_6 unit.
Entropy 298.15 K, S=75.66 J·mol^{-1}·K^{-1}
Extrapolation below 180 K, 47.0 J·mol^{-1}·K^{-1}. Values per C_3H_6 unit.
Molecular Weight 42.0804
Wiswesser Line Notation /*Y1&1*/
Evaluation B(C_p),C(S)
Glassy transition at 270 K. Results corrected to 100% crystalline from 75%.

$(C_3H_6)_n$ (c) 84GRE/LAU
Polypropylene, isotatic, crystalline
Heat Capacity 298.15 K, C_p=68.99 J·mol^{-1}·K^{-1}
Temperature range 0 to 500 K.
Entropy 298.15 K, S=69.92 J·mol^{-1}·K^{-1}
Molecular Weight 42.0804
Wiswesser Line Notation /*Y1&1*/
Evaluation A
Glassy transitions range from 260 to 380 K for 51% crystallinity. T(glass) at 260, 272, and 325 K.

$(C_3H_6)_n$ (gls) 84GRE/LAU
Polypropylene, isotatic, amorphous
Heat Capacity 298.15 K, C_p=88.07 J·mol^{-1}·K^{-1}
Temperature range 0 to 500 K.
Entropy 298.15 K, S=80.79 J·mol^{-1}·K^{-1}
Molecular Weight 42.0804
Wiswesser Line Notation /*Y1&1*/
Evaluation A
Conformationally disordered crystal to monoclinic crystal at 380 K, ΔH=600 J·mol^{-1} (38% crystallinity).

$C_3H_6Br_2$ (liq) 48KUR
1,3-Dibromopropane
Heat Capacity 298 K, C_p=159.0 J·mol^{-1}·K^{-1}
Temperature range 16 to 160 °C, mean C_p three temperatures.
Molecular Weight 201.8884
Wiswesser Line Notation E3E
Evaluation D

$C_3H_6Br_2$ (c) 50CRO/SMY
1,3-Dibromopropane
Heat Capacity 245.7 K, C_p=156.1 J·mol^{-1}·K^{-1}
Temperature range 117 to 246 K. Value is unsmoothed experimental datum.
Phase Changes
c/liq 238.6 K, ΔH=14640 J·mol^{-1}
ΔS=61.4 J·mol^{-1}·K^{-1}
Molecular Weight 201.8884
Wiswesser Line Notation E3E
Evaluation C

$C_3H_6Br_2$ (liq) 92SVO/KUB2
1,3-Dibromopropane
Phase Changes
liq/g 439.4 K, ΔH=47890 J·mol^{-1}
Molecular Weight 201.8884
Wiswesser Line Notation E3E
Evaluation A

$C_3H_6Br_2$ (liq) 93SHE
1,3-Dibromopropane
Heat Capacity 298.15 K, C_p=163.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 201.8884
Wiswesser Line Notation E3E
Evaluation B

$C_3H_6Br_2$ (liq) 48KUR
1,2-Dibromopropane
Heat Capacity 298 K, C_p=172.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 133 °C, mean C_p three temperatures.
Molecular Weight 201.8884
Wiswesser Line Notation EY1&1E
Evaluation D

$C_3H_6ClNO_2$ (liq) 50CRO/SMY
2-Chloro-2-nitropropane
Phase Changes
c,II/c,I -213.8 K, ΔH=9540 J·mol^{-1}
ΔS=44.6 J·mol^{-1}·K^{-1}
c,I/liq 251.6 K, ΔH=1340 J·mol^{-1}
ΔS=5.3 J·mol^{-1}·K^{-1}
Molecular Weight 123.5389
Wiswesser Line Notation WNXG1&1
Evaluation C

$C_3H_6Cl_2$ (liq) 72MIL
2,2-Dichloropropane
Heat Capacity 270 K, C_p=151.4 J·mol^{-1}·K^{-1}
Temperature range 137 to 267 K.
Phase Changes
c,II/c,I 188 K, ΔH=5979 J·mol^{-1}
ΔS=31.8 J·mol^{-1}·K^{-1}
Temperature not certain; give explicitly as 184.8 K and in table as 188 K.
c,I/liq 239.25 K, ΔH=2341 J·mol^{-1}
ΔS=9.8 J·mol^{-1}·K^{-1}
Molecular Weight 112.9864
Wiswesser Line Notation GXG1&1
Evaluation B

$C_3H_6Cl_2$ (liq) 93HAL
1,3-Dichloropropane
Heat Capacity 298.15 K, C_p=157.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 112.9864
Wiswesser Line Notation G3G
Evaluation B

$C_3H_6Cl_2$ (liq) 48KUR
1,2-Dichloropropane; Propylene dichloride
Heat Capacity 298 K, C_p=154.4 J·mol^{-1}·K^{-1}
Temperature range 11 to 156 °C, mean C_p three temperatures.
Molecular Weight 112.9864
Wiswesser Line Notation GY1&1G
Evaluation D
Data may be poor. Highest reported temperature too far above listed boiling point.

$C_3H_6Cl_2Si$ (liq) 71GEI/DZH
Dichloromethylvinylsilane
Heat Capacity 298.15 K, C_p=177.9 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Deposited in VINITI, No 2722-71, 25 March 1971.
Entropy 298.15 K, S=381.3 J·mol^{-1}·K^{-1}
Molecular Weight 141.0719
Wiswesser Line Notation G-SI-G1&1U1
Evaluation A

$C_3H_6F_4N_2$ (liq) 70REE/SEE
1,2-Bis(difluoramino)propane
Heat Capacity 298.15 K, C_p=213 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 146.0874
Wiswesser Line Notation FNFY1&1NFF
Evaluation B

$C_3H_6I_2$ (liq) 93SHE
1,3-Diiodopropane
Heat Capacity 298.15 K, C_p=169.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 295.8894
Wiswesser Line Notation I3I
Evaluation B

$C_3H_6N_2O_2$ (c) 89IMA/TAK
Malonamide
Heat Capacity 298.15 K, C_p=124 J·mol^{-1}·K^{-1}
One temperature, estimated.
Phase Changes
c/g 298.15 K, ΔH=126400 J·mol^{-1}
ΔS=423.9 J·mol^{-1}·K^{-1}
Molecular Weight 102.0926
Wiswesser Line Notation ZV1VZ
Evaluation B

$C_3H_6N_2O_2$ (c) 89SAK/IMA
Malonamide
Phase Changes
c,II/c,I 393 K, ΔH=1900 J·mol^{-1}
c,I/liq 443 K, ΔH=35800 J·mol^{-1}
Molecular Weight 102.0926
Wiswesser Line Notation ZV1VZ
Evaluation A

$C_3H_6N_2O_4$ (c,I) 58BIL/N
2,2-Dinitropropane
Heat Capacity 298 K, C_p=206.3 J·mol^{-1}·K^{-1}
From PVT data −5 to 25 °C. Mean value.
Phase Changes
c,II/c,I 268 K, ΔH=12220 J·mol^{-1}
ΔS=45.6 J·mol^{-1}·K^{-1}
Calculated from Clausius-Clapeyron equation, from dp/dT and den measurements.
Molecular Weight 134.0914
Wiswesser Line Notation WNX1&1&NW
Evaluation C

$C_3H_6N_2O_4$ (c,I) 78GOD/R
2,2-Dinitropropane
Heat Capacity 300 K, C_p=205 J·mol^{-1}·K^{-1}
Temperature range 100 to 347 K. Data graphically only, v estimated.
Phase Changes
c,III/c,II 259.7 K, ΔH=1870 J·mol^{-1}
ΔS=7.20 J·mol^{-1}·K^{-1}
c,II/c,I 267.7 K, ΔH=11275 J·mol^{-1}
ΔS=42.12 J·mol^{-1}·K^{-1}
c,I/liq 324.5 K, ΔH=2635 J·mol^{-1}
ΔS=8.12 J·mol^{-1}·K^{-1}
Molecular Weight 134.0914
Wiswesser Line Notation WNX1&1&NW
Evaluation D(C_p), B(Phase changes)

$C_3H_6N_4O_4$ (c) 71I
1,3-Dinitro-1,3-diazacyclopentane
Phase Changes
c/liq 403 K, ΔH=25104 J·mol^{-1}
Molecular Weight 162.1048
Wiswesser Line Notation T5N CNTJ ANW CNW
Evaluation C

$C_3H_6N_6$ (c) 52STE/I
Melamine
Heat Capacity 299.95 K, C_p=156.11 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K. Value is unsmoothed experime datum.
Entropy 298.15 K, S=149.08 J·mol^{-1}·K^{-1}
Molecular Weight 126.1206
Wiswesser Line Notation T6N CN ENJ BZ DZ FZ
Evaluation A

$C_3H_6N_6O_3$ (c) 71I
1,3,5-Trinitroso-1,3,5-triazacyclohexane
Phase Changes
c,II/c,I 367 K, ΔH=17782 J·mol^{-1}
c,I/liq 376 K, ΔH=3766 J·mol^{-1}
Molecular Weight 174.1188
Wiswesser Line Notation T6N CN ENTJ ANO CNO ENO
Evaluation C′

$C_3H_6N_6O_6$ (c) 71
1,3,5-Trinitro-1,3,5-triazacyclohexane; Hexogen; RDX
Phase Changes
c/liq 478.5 K, ΔH=35648 J·mol^{-1}
Molecular Weight 222.1170
Wiswesser Line Notation T6N CN ENTJ ANW CNW ENW
Evaluation C

$C_3H_6N_6O_6$ (c) 73KRI/LIC
1,3,5-Trinitro-1,3,5-triazacyclohexane; Hexogen; RDX
Heat Capacity 298 K, C_p=248.9 J·mol^{-1}·K^{-1}
Temperature range 200 to 475 K. Equation only.
Molecular Weight 222.1170
Wiswesser Line Notation T6N CN ENTJ ANW CNW ENW
Evaluation C

$C_3H_6N_6O_6$ (c) 92MAK
1,3,5-Trinitro-1,3,5-triazacyclohexane; Hexogen; RDX
Phase Changes
c/liq 478.15 K, ΔH=37656 J·mol^{-1}
Molecular Weight 222.1170
Wiswesser Line Notation T6N CN ENTJ ANW CNW ENW
Evaluation B

C_3H_6O (liq) 1881REI
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298 K, C_p=133.9 J·mol^{-1}·K^{-1}
Temperature range 289 to 352 K.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation D

C_3H_6O (liq) 07WAL
Propanone; Acetone; Dimethyl ketone
Heat Capacity 291 K, C_p=126 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation D

C_3H_6O (liq) 16BRA
Propanone; Acetone; Dimethyl ketone
Heat Capacity 283 K, C_p=121.3 J·mol^{-1}·K^{-1}
Mean value, 0 to 20 °C.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation C

C_3H_6O (c) 25MAA/WAL
Propanone; Acetone; Dimethyl ketone
Heat Capacity 173 K, C_p=96 J·mol^{-1}·K^{-1}
Temperature range 93 to 173 K.
Phase Changes
c/liq 178.5 K, ΔH=4770 J·mol^{-1}
ΔS=26.7 J·mol^{-1}·K^{-1}
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation C

C_3H_6O (liq) 25PAR/KEL
Propanone; Acetone; Dimethyl ketone
Heat Capacity 289.4 K, C_p=124.7 J·mol^{-1}·K^{-1}
Temperature range 70 to 290 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=217.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 71.63 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 177.6 K, ΔH=5690 J·mol^{-1}
ΔS=32.03 J·mol^{-1}·K^{-1}
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B(C_p),C(S)

C_3H_6O (liq) 25WIL/DAN
Propanone; Acetone; Dimethyl ketone
Heat Capacity 293.2 K, C_p=125.9 J·mol^{-1}·K^{-1}
Temperature range 20 to 40 °C.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 28PAR/KEL
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298.4 K, C_p=123.8 J·mol^{-1}·K^{-1}
Temperature range 70 to 289 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=220.5 J·mol^{-1}·K^{-1}
Extrapolation below 70 K, 60.04 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 177.6 K, ΔH=5690 J·mol^{-1}
ΔS=32.0 J·mol^{-1}·K^{-1}
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B(C_p),C(S)

C_3H_6O (liq) 29KEL3
Propanone; Acetone; Dimethyl ketone
Heat Capacity 296.99 K, C_p=124.68 J·mol^{-1}·K^{-1}
Temperature range 16 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=200.4 J·mol^{-1}·K^{-1}
Phase Changes
Hump in C_p curve at about 126 K, with excess entropy of about 0.5 J·mol^{-1}·K^{-1}.
c/liq 176.62 K, ΔH=5715 J·mol^{-1}
ΔS=32.36 J·mol^{-1}·K^{-1}
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation A

C_3H_6O (liq) 29MIT/HAR
Propanone; Acetone; Dimethyl ketone
Heat Capacity 260 K, C_p=124.3 J·mol^{-1}·K^{-1}
Temperature range 200 to 260 K.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 29PAR/KEL
Propanone; Acetone; Dimethyl ketone
Entropy 298.1 K, S=200.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 54.0 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation C

C_3H_6O (liq) 32TRE
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298 K, C_p=124.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 33TRE/WAT
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298 K, C_p=124.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 39PHI
Propanone; Acetone; Dimethyl ketone
Heat Capacity 302.4 K, C_p=128.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation C

C_3H_6O (liq) 55STA/TUP
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298 K, C_p=128.24 J·mol^{-1}·K^{-1}
Temperature range 288 to 323 K.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 62LOW/MOE
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298.2 K, C_p=125.56 J·mol^{-1}·K^{-1}
Temperature range 253 to 308 K.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation A

C_3H_6O (liq) 67RAS/GAN
Propanone; Acetone; Dimethyl ketone
Heat Capacity 293 K, C_p=126.3 J·mol^{-1}·K^{-1}
Temperature range 293 to 333 K.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation C

C_3H_6O (liq) 71DES/BHA
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298 K, C_p=129.7 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 79SAL/PEA
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298.15 K, C_p=125.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 85COS/PAT
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298.15 K, C_p=123.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 85COS/P
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298.15 K, C_p=123.8 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 86ALP/
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298.15 K, C_p=126.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation A

C_3H_6O (liq) 89COS/
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298.15 K, C_p=123.80 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 89PET/
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298.15 K, C_p=126.6 J·mol^{-1}·K^{-1}
Temperature range 258.15, 278.15, 298.15, 318.15 K.
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 91MAL/W
Propanone; Acetone; Dimethyl ketone
Heat Capacity 298.15 K, C_p=125.45 J·mol^{-1}·K^{-1}
Temperature range 278 to 323 K. C_p(liq)=1.337+2.7752×10^{-3}(
kJ·kg^{-1}·K^{-1} (278.15 to 323.15 K).
Molecular Weight 58.0798
Wiswesser Line Notation 1V1
Evaluation B

C_3H_6O (liq) 1881
2-Propen-1-ol
Heat Capacity 298 K, C_p=138.9 J·mol^{-1}·K^{-1}
Temperature range 291 to 369 K.
Molecular Weight 58.0798
Wiswesser Line Notation Q2U1
Evaluation D

C_3H_6O (liq) 64
Propylene oxide; 2-Methyloxirane
Heat Capacity 298.15 K, C_p=120.37 J·mol^{-1}·K^{-1}
Temperature range 11 to 300 K.
Entropy 298.15 K, S=196.27 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 161.22 K, ΔH=6532.9 J·mol^{-1}
ΔS=40.52 J·mol^{-1}·K^{-1}
Molecular Weight 58.0798
Wiswesser Line Notation T3OTJ B1
Evaluation A

C_3H_6O (liq) 66BEA/CLE
Propylene oxide; 2-Methyloxirane
Heat Capacity 298.15 K, C_p=125.1 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 298.15 K, S=194.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 485 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 161.25 K, ΔH=6569 J·mol^{-1}
ΔS=40.74 J·mol^{-1}·K^{-1}
Molecular Weight 58.0798
Wiswesser Line Notation T3OTJ B1
Evaluation A(C_p),C(S)

C_3H_6O (liq) 82TAN/ZHO
Propylene oxide; 2-Methyloxirane
Heat Capacity 300 K, C_p=122.19 J·mol^{-1}·K^{-1}
Temperature range 170 to 325 K.
Molecular Weight 58.0798
Wiswesser Line Notation T3OTJ B1
Evaluation B

$C_3H_6O·17H_2O$ (c) 90YAM/KUR
Acetone clathrate hydrate
Heat Capacity
Temperature range 11 to 300 K. Data given graphically.
Phase Changes
c,I/c 46.6 K, ΔH=129 J·mol^{-1}
ΔS=2.48 J·mol^{-1}·K^{-1}
Per mole H_2O.
Molecular Weight 363.7977
Wiswesser Line Notation 1V1 &QH 17
Evaluation A
KOH-doped.

$C_3H_6O·17H_2O$ (c) 91KUR/YAM
Propanone clathrate hydrate; Acetone clathrate hydrate; Dimethyl ketone clathrate hydrate
Heat Capacity 160 K, C_p=468.36 J·mol^{-1}·K^{-1}
Temperature range 11 to 160 K.
Entropy 160 K, S=516.58 J·mol^{-1}·K^{-1}
Molecular Weight 364.3382
Wiswesser Line Notation 1V1 &QH 17
Evaluation A
T(glass)=90 K.

$C_3H_6O·17H_2O$ (c) 85HAN
Propylene oxide clathrate hydrate
Heat Capacity 260 K, C_p=718 J·mol^{-1}·K^{-1}
Temperature range 95 to 260 K.
Phase Changes
c/liq 268.6 K, ΔH=92700 J·mol^{-1}
ΔS=345.1 J·mol^{-1}·K^{-1}
Molecular Weight 364.3382
Wiswesser Line Notation T3OTJ B1 &QH 17
Evaluation A

C_3H_6O (liq) 76CON/GIN
Oxetane; Trimethylene oxide
Heat Capacity 298 K, C_p=99.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 58.0798
Wiswesser Line Notation T4OTJ
Evaluation B

$(C_3H_6O)_n$ (gls) 70YOS/SAK
Poly(oxacyclobutane)
Heat Capacity 302.13 K, C_p=125.9 J·mol^{-1}·K^{-1}
Temperature range 90 to 320 K. C_p at 302.13 K is unsmoothed experimental datum. Data also given graphically. C_p reported as 2.170 J·g^{-1}·K^{-1} at 302.13 K for annealed sample. C_p given for quenched sample from 95 to 205 K.
Phase Changes
c,I/gls 195 K
c,I/liq 305 K, ΔH=9439 J·mol^{-1}
ΔS=30.96 J·mol^{-1}·K^{-1}
Melting region extended from 200 to 300 K.
Molecular Weight 58.0798
Wiswesser Line Notation /*T4OTJ*/
Evaluation B

C_3H_6O (liq) 1881REI
Propanal; Propaldehyde
Heat Capacity 298 K, C_p=134.7 J·mol^{-1}·K^{-1}
Temperature range 288 to 328 K.
Molecular Weight 58.0798
Wiswesser Line Notation VH2
Evaluation D

C_3H_6O (liq) 84VAS/PET
Propanal; Propaldehyde
Heat Capacity 298.15 K, C_p=159.1 J·mol^{-1}·K^{-1}
Temperature range 15 to 335 K.
Entropy 298.15 K, S=212.90 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 171.32 K, ΔH=8590 J·mol^{-1}
Molecular Weight 58.0798
Wiswesser Line Notation VH2
Evaluation A

C_3H_6O (liq) 77KOR/VAS
Propanal; Propaldehyde
Heat Capacity 298.15 K, C_p=159.1 J·mol^{-1}·K^{-1}
Temperature range 15 to 335 K.
Entropy 298.15 K, S=212.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 171.32 K, ΔH=8590 J·mol^{-1}
liq/g 321.08 K, ΔH=28320 J·mol^{-1}
Molecular Weight 58.0798
Wiswesser Line Notation VH2
Evaluation A
Anomalies in the liquid phase over the temperature range 265 to 315 K.

$(C_3H_6O)_n$ (c) 92LEB/VAS
Polypropanal
Heat Capacity 298.15 K, C_p=105.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 360 K.
Entropy 298.15 K, S=127.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 347 K, ΔH=4990 J·mol^{-1}
ΔS=5.4 J·mol^{-1}·K^{-1}
Molecular Weight 58.0798
Wiswesser Line Notation /*OY*2/
Evaluation A
T(glass)=240 K.

$(C_3H_6O_2)_n$ (c) 69CLE/MEL4
Poly-1,3-dioxolane
Heat Capacity 298.15 K, C_p=113.1 J·mol^{-1}·K^{-1}
Temperature range 80 to 390 K. Extrapolated data.
Entropy 298.15 K, S=112.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 209 K
Glass transition.
c,I/liq 325 K, ΔH=16698 J·mol^{-1}
ΔS=5.14 J·mol^{-1}·K^{-1}
Molecular Weight 74.0792
Wiswesser Line Notation /*1O1O1*/
Evaluation B

$C_3H_6O_2$ (liq) 71HAL/BAL
Methyl ethanoate; Methyl acetate
Heat Capacity 297 K, C_p=123.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation 1VO1
Evaluation C

$C_3H_6O_2$ (liq) 85COS/PAT
Methyl ethanoate; Methyl acetate
Heat Capacity 298.15 K, C_p=140.56 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 74.0792
Wiswesser Line Notation 1VO1
Evaluation B

$C_3H_6O_2$ (liq) 85COS/PAT2
Methyl ethanoate; Methyl acetate
Heat Capacity 298.15 K, C_p=140.6 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 74.0792
Wiswesser Line Notation 1VO1
Evaluation B

$C_3H_6O_2$ (liq) 88PIN/BRA
Methyl ethanoate; Methyl acetate
Heat Capacity 298.15 K, C_p=141.34 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation 1VO1
Evaluation B

$C_3H_6O_2$ (liq) 92OKA/OGU
Methyl ethanoate; Methyl acetate
Heat Capacity 288.58 K, C_p=140.2 J·mol^{-1}·K^{-1}
Temperature range 13 to 290 K. Unsmoothed experimental datum.
Phase Changes
Anom1 36 K
Anom2 155 K
c/liq 174.897 K, ΔH=7486 J·mol^{-1}
Molecular Weight 74.0792
Wiswesser Line Notation 1VO1
Evaluation B
The slight peak at 155 K is probably due to eutectic melting of the cystal with an unidentified impurity.

$C_3H_6O_2$ (liq) 02L
Propionic acid; Propanoic acid
Heat Capacity 350 K, C_p=172 J·mol^{-1}·K^{-1}
Mean value 20 to 136 °C.
Molecular Weight 74.0792
Wiswesser Line Notation QV2
Evaluation D

$C_3H_6O_2$ (liq) 34RAD/
Propionic acid; Propanoic acid
Heat Capacity 289 K, C_p=159.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation QV2
Evaluation C

$C_3H_6O_2$ (liq) 71KON/W
Propionic acid; Propanoic acid
Heat Capacity 298.15 K, C_p=151 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation QV2
Evaluation B

$C_3H_6O_2$ (liq) 78WOY/I
Propionic acid; Propanoic acid
Heat Capacity 333.15 K, C_p=154.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation QV2
Evaluation B

$C_3H_6O_2$ (liq) 82BIR/
Propionic acid; Propanoic acid
Heat Capacity 298.15 K, C_p=158.6 J·mol^{-1}·K^{-1}
Temperature range 270 to 370 K. Equation only. C_p=129.7−0.1 T+0.0007486 T^2 J·mol^{-1}·K^{-1}.
Molecular Weight 74.0792
Wiswesser Line Notation QV2
Evaluation C

$C_3H_6O_2$ (liq) 82MAR/A
Propionic acid; Propanoic acid
Heat Capacity 298.15 K, C_p=152.8 J·mol^{-1}·K^{-1}
Temperature range 13 to 450 K. Data also given by equation.
Entropy 298.15 K, S=191.0 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 252.65 K, ΔH=10660 J·mol^{-1}
ΔS=42.19 J·mol^{-1}·K^{-1}
Molecular Weight 74.0792
Wiswesser Line Notation QV2
Evaluation A

$C_3H_6O_2$ (liq) 69CLE/M
1,3-Dioxolane
Heat Capacity
Temperature range 80 to 390 K.
Entropy 298.15 K, S=280.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 142.4 K, ΔH=2677 J·mol^{-1}
ΔS=18.8 J·mol^{-1}·K^{-1}
c,I/liq 175.93 K, ΔH=6567 J·mol^{-1}
ΔS=37.3 J·mol^{-1}·K^{-1}
Molecular Weight 74.0792
Wiswesser Line Notation T5O COTJ
Evaluation B

$C_3H_6O_2$ (liq) 76CON/GIN
1,3-Dioxolane
Heat Capacity 298 K, C_p=118.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation T5O COTJ
Evaluation B

$C_3H_6O_2$ (liq) 81ING/CAS
1,3-Dioxolane
Heat Capacity 298.15 K, C_p=120.84 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation T5O COTJ
Evaluation B

$C_3H_6O_2$·17H_2O (liq) 85HAN
1,3-Dioxolane clathrate hydrate
Heat Capacity 260 K, C_p=731 J·mol^{-1}·K^{-1}
Temperature range 95 to 260 K.
Phase Changes
c/liq 270.5 K, ΔH=99100 J·mol^{-1}
ΔS=366.4 J·mol^{-1}·K^{-1}
Molecular Weight 380.3376
Wiswesser Line Notation T5O COTJ &QH 17
Evaluation A

$C_3H_6O_2$ (liq) 33KOL/UDO
Ethyl methanoate; Ethyl formate
Heat Capacity 294.7 K, C_p=148.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation VHO2
Evaluation C

$C_3H_6O_2$ (liq) 34KOL/UDO2
Ethyl methanoate; Ethyl formate
Heat Capacity 294.7 K, C_p=148.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation VHO2
Evaluation C

$C_3H_6O_2$ (liq) 36KUR/VOS
Ethyl methanoate; Ethyl formate
Heat Capacity 290 K, C_p=158.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation VHO2
Evaluation D

$C_3H_6O_2$ (liq) 79FUC
Ethyl methanoate; Ethyl formate
Heat Capacity 298.15 K, C_p=144.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.0792
Wiswesser Line Notation VHO2
Evaluation B

$C_3H_6O_2S$ (liq) 35HUF/ELL
3-Thiolpropanoic acid; β-Thiolactic acid
Heat Capacity 299.8 K, C_p=202.5 J·mol^{-1}·K^{-1}
Temperature range 85 to 310 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=228.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 49.71 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 291.9 K, ΔH=16974 J·mol^{-1}
ΔS=58.2 J·mol^{-1}·K^{-1}
Molecular Weight 106.1392
Wiswesser Line Notation SH2VQ
Evaluation B(C_p),C(S)

$(C_3H_6O_2S)_n$ (c) 62DAI/EVA6
Propene polysulphone
Heat Capacity 298.15 K, C_p=134.22 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 298.15 K, S=J·mol^{-1}·K^{-1}
Molecular Weight 106.1392
Wiswesser Line Notation
Evaluation A

$C_3H_6O_3$ (liq) 83SAN/CIO
Methylene glycol monoacetate
Heat Capacity 298.15 K, C_p=214 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K. C_p°(kJ·kg^{-1}·K^{-1})=0.033053 T−7.401
Molecular Weight 87.0549
Wiswesser Line Notation Q1OV1
Evaluation D

$C_3H_6O_3$ (liq) 36PAR/THO
2-Hydroxypropanoic acid (DL); Lactic acid (DL)
Heat Capacity 298.1 K, C_p=210.4 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K. Unsmoothed experimenal datum.
Entropy 298.1 K, S=192.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 48.16 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 289.9 K, ΔH=11340 J·mol^{-1}
ΔS=39.12 J·mol^{-1}·K^{-1}
Molecular Weight 90.0786
Wiswesser Line Notation QY1&VQ -DL
Evaluation B(C_p),C(S)

$C_3H_6O_3$ (c) 40HUF/ELL
2-Hydroxypropanoic acid (D); Lactic acid (D)
Heat Capacity 298.2 K, C_p=127.65 J·mol^{-1}·K^{-1}
Temperature range 84 to 312 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=143.51 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 43.64 J·mol^{-1}·K^{-1}.
Molecular Weight 90.0786
Wiswesser Line Notation QY1&VQ -D
Evaluation A(C_p), C(S)

$C_3H_6O_3$ (c) 40HUF/ELL
2-Hydroxypropanoic acid (L); Lactic acid (L)
Heat Capacity 297.9 K, C_p=128.57 J·mol^{-1}·K^{-1}
Temperature range 84 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=142.26 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 42.93 J·mol^{-1}·K^{-1}.
Molecular Weight 90.0786
Wiswesser Line Notation QY1&VQ -L
Evaluation A(C_p), C(S)

$C_3H_6O_3$ (liq) 44YOS
2-Hydroxypropanoic acid (DL); Lactic acid (DL)
Phase Changes
c/liq 290 K, $\Delta H = 11344$ J·mol^{-1}
$\Delta S = 39.1$ J·mol^{-1}·K^{-1}
Molecular Weight 90.0786
Wiswesser Line Notation QY1&VQ -DL
Evaluation B

$C_3H_6O_3$ (c) 68CLE/MEL
1,3,5-Trioxane
Heat Capacity 298.15 K, $C_p = 111.4$ J·mol^{-1}·K^{-1}
Temperature range 80 to 310 K.
Entropy 298.15 K, $S = 133.0$ J·mol^{-1}·K^{-1}
Molecular Weight 90.0786
Wiswesser Line Notation T6O CO EOTJ
Evaluation B

$C_3H_6O_3$ (c) 88BOM/MIL
1,3,5-Trioxane
Heat Capacity 298.15 K, $C_p = 113.08$ J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, $S = 142.89$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 333.44 K, $\Delta H = 15105$ J·mol^{-1}
Molecular Weight 90.0786
Wiswesser Line Notation T6O CO EOTJ
Evaluation A

C_3H_6S (liq) 53SCO/FIN
Thiacyclobutane
Heat Capacity 294.37 K, $C_p = 112.59$ J·mol^{-1}·K^{-1}
Temperature range 12 to 321 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S = 184.93$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 176.7 K, $\Delta H = 668.6$ J·mol^{-1}
$\Delta S = 3.78$ J·mol^{-1}·K^{-1}
c,I/liq 199.91 K, $\Delta H = 8248.3$ J·mol^{-1}
$\Delta S = 41.26$ J·mol^{-1}·K^{-1}
Molecular Weight 74.1404
Wiswesser Line Notation T4STJ
Evaluation A

C_3H_7Br (liq) 1881REI
1-Bromopropane; n-Propyl bromide
Heat Capacity 298 K, $C_p = 130.5$ J·mol^{-1}·K^{-1}
Temperature range 289 to 364 K.
Molecular Weight 122.9923
Wiswesser Line Notation E3
Evaluation D

C_3H_7Br (liq) 48KUR
1-Bromopropane; n-Propyl bromide
Heat Capacity 298 K, $C_p = 140.2$ J·mol^{-1}·K^{-1}
Temperature range −30 to 67 °C, mean C_p three temperatures.
Molecular Weight 122.9923
Wiswesser Line Notation E3
Evaluation D

C_3H_7Br (liq) 93S
1-Bromopropane; n-Propyl bromide
Heat Capacity 298.15 K, $C_p = 134.6$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 122.9923
Wiswesser Line Notation E3
Evaluation B

C_3H_7Br (liq) 1881F
2-Bromopropane; Isopropyl bromide
Heat Capacity 298 K, $C_p = 132.2$ J·mol^{-1}·K^{-1}
Temperature range 287 to 344 K.
Molecular Weight 122.9923
Wiswesser Line Notation EY1&1
Evaluation D

C_3H_7Br (liq) 50KUS/Cl
2-Bromopropane; Isopropyl bromide
Heat Capacity 209.6 K, $C_p = 126.8$ J·mol^{-1}·K^{-1}
Temperature range 117 to 209 K. Value is unsmoothed experimer datum.
Phase Changes
c/liq 184.1 K, $\Delta H = 6530$ J·mol^{-1}
$\Delta S = 35.5$ J·mol^{-1}·K^{-1}
Molecular Weight 122.9923
Wiswesser Line Notation EY1&1
Evaluation B

C_3H_7Br (liq) 93S
2-Bromopropane; Isopropyl bromide
Heat Capacity 298.15 K, $C_p = 135.6$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 122.9923
Wiswesser Line Notation EY1&1
Evaluation B

C_3H_7Cl (liq) 1881I
1-Chloropropane; n-Propyl chloride
Heat Capacity 298 K, $C_p = 131.4$ J·mol^{-1}·K^{-1}
Temperature range 288 to 333 K.
Molecular Weight 78.5413
Wiswesser Line Notation G3
Evaluation D

C_3H_7Cl (liq) 48E
1-Chloropropane; n-Propyl chloride
Heat Capacity 297 K, $C_p = 130.5$ J·mol^{-1}·K^{-1}
Temperature range 200 to 297 K. (4 pts) from unpublis measurements of A. Landsberg.
Molecular Weight 78.5413
Wiswesser Line Notation G3
Evaluation C

C_3H_7Cl (liq) 48K
1-Chloropropane; n-Propyl chloride
Heat Capacity 298 K, $C_p = 132.2$ J·mol^{-1}·K^{-1}
Temperature range −39 to 43 °C, mean C_p, two temperatures.
Molecular Weight 78.5413
Wiswesser Line Notation G3
Evaluation D

C_3H_7I (liq) 1881REI
1-Iodopropane; n-Propyl iodide
Heat Capacity 298 K, C_p=126.8 J·mol^{-1}·K^{-1}
Temperature range 293 to 383 K.
Molecular Weight 169.9928
Wiswesser Line Notation I3
Evaluation D

C_3H_7I (liq) 93SHE
1-Iodopropane; n-Propyl iodide
Heat Capacity 298.15 K, C_p=136.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 169.9928
Wiswesser Line Notation I3
Evaluation B

C_3H_7I (liq) 93SHE
2-Iodopropane; Isopropyl iodide
Heat Capacity 298.15 K, C_p=137.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 169.9928
Wiswesser Line Notation IY1&1
Evaluation B

C_3H_7N (liq) 81FIN/MES
Cyclopropylamine
Heat Capacity 298.15 K, C_p=147.11 J·mol^{-1}·K^{-1}
Temperature range 12 to 315 K. Equation also given in temperature range 242 to 315 K.
Entropy 298.15 K, S=187.69 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 237.76 K, ΔH=13183.4 J·mol^{-1}
ΔS=55.45 J·mol^{-1}·K^{-1}
Molecular Weight 57.0950
Wiswesser Line Notation L3TJ AZ
Evaluation A

C_3H_7NO (liq) 61GEL
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298 K, C_p=156.69 J·mol^{-1}·K^{-1}
Temperature range 273 to 323 K.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation C

C_3H_7NO (liq) 74VIS/SOM
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p=152.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation A

C_3H_7NO (liq) 76BON/CER
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p=146 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 77DEV/PER2
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p=148 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 77DEV/PER3
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p=150.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 77VIS/PER
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298 K, C_p=148 J·mol^{-1}·K^{-1}
One temperature only.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 78KAR/RAB2
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Phase Changes
c/liq 212.85 K, ΔH=8950 J·mol^{-1}
ΔS=41.8 J·mol^{-1}·K^{-1}
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation A

C_3H_7NO (liq) 78MAR/CIO
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298 K, C_p=120.5 J·mol^{-1}·K^{-1}
Temperature range 298 to 427 K. Mean value over range.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation D

C_3H_7NO (liq) 79DEV/SOM
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p=150.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 79VIS/SOM
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p=150.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 82VOR/YAK
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p=150.5 J·mol^{-1}·K^{-1}
Temperature range 297.15 to 299.15 K. C_p given as 2.059 J·K^{-1}·g^{-1}.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 84ZEG/SOM
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p=148.36 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 89PET/PES
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p=150.0 J·mol^{-1}·K^{-1}
Temperature range 258.15, 278.15, 298.15, 318.15 K.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 89KUL/KRE
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 308 K, C_p=149.28 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 92KOL/KUL
N,N-Dimethylformamide; N,N-Dimethylmethanimide; DMF
Heat Capacity 298.15 K, C_p=148.16 J·mol^{-1}·K^{-1}
Temperature range 283 to 323 K.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 93GRO/ROU
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p=146.05 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

$C_3H_7NO_2$ (c) 77SAB/LAF
Sarcosine; N-Methylglycine
Heat Capacity 298.15 K, C_p=128.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 89.0938
Wiswesser Line Notation QV1M1
Evaluation B

$C_3H_7NO_2$ (c) 83SKO/SAB
3-Aminopropanoic acid; β-Alanine
Heat Capacity 298 K, C_p=116.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 89.0938
Wiswesser Line Notation Z2VQ
Evaluation B

$C_3H_7NO_2$ (c) 89KUL/K
3-Aminopropanoic acid; β-Alanine
Heat Capacity 298 K, C_p=109.3 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 89.0938
Wiswesser Line Notation Z2VQ
Evaluation C

$C_3H_7NO_2$ (c) 90BAD/K
3-Aminopropanoic acid; β-Alanine
Heat Capacity 298 K, C_p=109 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 89.0938
Wiswesser Line Notation Z2VQ
Evaluation D

$C_3H_7NO_2$ (c) 76BER/B
Ethyl carbamate; Urethane
Phase Changes
c/liq 321.7 K, ΔH=20900 J·mol^{-1}
ΔS=64.8 J·mol^{-1}·K^{-1}
Molecular Weight 89.0938
Wiswesser Line Notation ZVO2
Evaluation A

$C_3H_7NO_2$ (c) 83DEW/D
Ethyl carbamate; Urethane
Heat Capacity 300 K, C_p=156.43 J·mol^{-1}·K^{-1}
Temperature range 90 to 330 K.
Phase Changes
c/liq 321.41 K, ΔH=16794 J·mol^{-1}
ΔS=52.25 J·mol^{-1}·K^{-1}
Molecular Weight 89.0938
Wiswesser Line Notation ZVO2
Evaluation B(C_p), A(Phase changes).

$C_3H_7NO_2$ (c) 32HUF/B
2-Aminopropanoic acid(D); Alanine(D)
Heat Capacity 296.8 K, C_p=120.8 J·mol^{-1}·K^{-1}
Temperature range 84 to 297 K. Value is unsmoothed experimer datum.
Entropy 298.1 K, S=132.2 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 37.15 J·mol^{-1}·K^{-1}.
Molecular Weight 89.0938
Wiswesser Line Notation ZY1&VQ -D
Evaluation B(C_p),C(S)

$C_3H_7NO_2$ (c) 37HUF/E
2-Aminopropanoic acid(DL); Alanine(DL)
Heat Capacity 297.5 K, C_p=121.71 J·mol^{-1}·K^{-1}
Temperature range 85 to 298 K. Value is unsmoothed experime datum.
Entropy 298.15 K, S=132.2 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 36.99 J·mol^{-1}·K^{-1}.
Molecular Weight 89.0938
Wiswesser Line Notation ZY1&VQ -DL
Evaluation B(C_p),C(S)

$C_3H_7NO_2$ (c) 75SPI/W
2-Aminopropanoic acid(DL); Alanine(DL)
Heat Capacity 298.15 K, C_p=121.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 89.0938
Wiswesser Line Notation ZY1&VQ -DL
aluation B

$C_3H_7NO_2$ (c) 89KUL/KOZ
2-Aminopropanoic acid(DL); Alanine(DL)
Heat Capacity 298 K, C_p=113.8 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 89.0938
Wiswesser Line Notation ZY1&VQ -DL
Evaluation C

$C_3H_7NO_2$ (c) 90BAD/KUL
2-Aminopropanoic acid(DL); Alanine(DL)
Heat Capacity 298 K, C_p=114 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 89.0938
Wiswesser Line Notation ZY1&VQ -DL
Evaluation D

$C_3H_7NO_2$ (c) 60HUT/COL
2-Aminopropanoic acid(L); Alanine(L)
Heat Capacity 298.15 K, C_p=122.26 J·mol^{-1}·K^{-1}
Temperature range 11 to 305 K.
Entropy 298.15 K, S=129.21 J·mol^{-1}·K^{-1}
Molecular Weight 89.0938
Wiswesser Line Notation ZY1&VQ -L
Evaluation A

$C_3H_7NO_2$ (c) 75DAU/DEL
2-Aminopropanoic acid(L); Alanine(L)
Heat Capacity
Temperature range 1 to 300 K. C_p data given graphically.
Entropy 273 K, S=118.8 J·mol^{-1}·K^{-1}
Molecular Weight 89.0938
Wiswesser Line Notation ZY1&VQ -L
Evaluation B

$C_3H_7NO_2$ (c) 89KUL/KOZ
2-Aminopropanoic acid(L); Alanine(L)
Heat Capacity 298 K, C_p=115.2 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 89.0938
Wiswesser Line Notation ZY1&VQ -L
Evaluation C

$C_3H_7NO_2$ (c) 90BAD/KUL
2-Aminopropanoic acid(L); Alanine(L)
Heat Capacity 298 K, C_p=115 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 89.0938
Wiswesser Line Notation ZY1&VQ -L
Evaluation D

$C_3H_7NO_2S$ (c) 35HUF/ELL
Cysteine(L)
Heat Capacity 297.6 K, C_p=162.3 J·mol^{-1}·K^{-1}
Temperature range 85 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=169.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 48.99 J·mol^{-1}·K^{-1}.
Molecular Weight 121.1538
Wiswesser Line Notation SH1YZVQ -L
Evaluation B(C_p),C(S)

$C_3H_7NO_3$ (c) 64HUT/COL2
2-Amino-3-hydroxypropanoic acid(L); Serine(L)
Heat Capacity 298.15 K, C_p=135.56 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S=149.16 J·mol^{-1}·K^{-1}
Molecular Weight 105.0932
Wiswesser Line Notation QVYZ1Q -L
Evaluation A

$C_3H_7NO_3$ (c) 75SPI/WAD
2-Amino-3-hydroxypropanoic acid(DL); Serine(DL)
Heat Capacity 298.15 K, C_p=132.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 105.0932
Wiswesser Line Notation QVYZ1Q -DL
Evaluation B

$C_3H_7NO_3$ (c) 78SAB/LAF
2-Amino-3-hydroxypropanoic acid(L); Serine(L)
Heat Capacity 298.15 K, C_p=138.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 105.0932
Wiswesser Line Notation QVYZ1Q -L
Evaluation B

$C_3H_7NO_3$ (liq) 88BUN
Isopropyl nitrate
Heat Capacity 350 K, C_p=200.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 105.0932
Wiswesser Line Notation WNOY1&1
Evaluation B

$C_3H_7NO_3$ (liq) 88LUS/RUB
Isopropyl nitrate
Heat Capacity 298.15 K, C_p=191.1 J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K.
Entropy 298.15 K, S=263.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 190.81 K, ΔH=10010 J·mol^{-1}
ΔS=52.43 J·mol^{-1}·K^{-1}
Molecular Weight 105.0932
Wiswesser Line Notation WNOY1&1
Evaluation A

C_3H_8 (liq) 38KEM/EGA
Propane
Heat Capacity 230 K, C_p=98.28 J·mol^{-1}·K^{-1}
Temperature range 15 to 230 K.
Entropy 231.04 K, S=171.0 J·mol^{-1}·K^{-1}
Debye extrapolation, 0 to 15 K.
Phase Changes
c,I/liq 85.45 K, ΔH=3524 J·mol^{-1}
ΔS=41.24 J·mol^{-1}·K^{-1}
liq/g 231.04 K, ΔH=18774 J·mol^{-1}
ΔS=81.26 J·mol^{-1}·K^{-1}
Molecular Weight 44.0962
Wiswesser Line Notation 3H
Evaluation A

C_3H_8 (liq) 78GOO
Propane
Heat Capacity 300 K, C_p=119.6 J·mol^{-1}·K^{-1}
Temperature range 81 to 289 K. C_p data reported for an extended data set; unsmoothed experimental datum.
Molecular Weight 44.0962
Wiswesser Line Notation 3H
Evaluation A

C_3H_8 (liq) 82VAS
Propane
Heat Capacity 230 K, C_p=98.36 J·mol^{-1}·K^{-1}
Temperature range 90 to 230 K. C_p given as 2.2305 J·g·K^{-1}.
Molecular Weight 44.0962
Wiswesser Line Notation 3H
Evaluation A
Sample purity, 99.95 mol%.

C_3H_8 (gls) 90TAK/OGU
Propane
Phase Changes
c/gls 45.5 K
Molecular Weight 44.0962
Wiswesser Line Notation 3H
Evaluation A

$C_3H_8N_2O$ (c) 87DEL/FER
1,3-Dimethylurea
Phase Changes
c/liq 379.5 K, ΔH=13620 J·mol^{-1}
ΔS=35.9 J·mol^{-1}·K^{-1}
Molecular Weight 88.1090
Wiswesser Line Notation 1MVM1
Evaluation A

$C_3H_8N_2O$ (c) 87DEL/FER
Ethylurea; Monoethylurea
Phase Changes
c/liq 367.8 K, ΔH=13940 J·mol^{-1}
ΔS=37.9 J·mol^{-1}·K^{-1}
Molecular Weight 88.1090
Wiswesser Line Notation ZVM2
Evaluation A

$C_3H_8N_2O$ (c) 87DEL/FER
1,1-Dimethylurea
Phase Changes
c/liq 454.0 K, ΔH=29610 J·mol^{-1}
ΔS=65.2 J·mol^{-1}·K^{-1}
Molecular Weight 88.1090
Wiswesser Line Notation ZVN1&1
Evaluation A

$C_3H_8N_2O_3$ (c) 81SHE/KAM
Dimethanolurea
Heat Capacity 300 K, C_p=157.7 J·mol^{-1}·K^{-1}
Temperature range 4 to 300 K.
Entropy 300 K, S=173.6 J·mol^{-1}·K^{-1}
Molecular Weight 120.1078
Wiswesser Line Notation Q1MVM1Q
Evaluation A

C_3H_8O (liq) 188
1-Propanol; n-Propyl alcohol
Heat Capacity 298 K, C_p=144.8 J·mol^{-1}·K^{-1}
Temperature range 289 to 363 K.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation D

C_3H_8O (liq) 20GIB/
1-Propanol; n-Propyl alcohol
Heat Capacity 274.6 K, C_p=131.3 J·mol^{-1}·K^{-1}
Temperature range 77 to 274.6 K. Unsmoothed experimental datu
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 26PAR/
1-Propanol; n-Propyl alcohol
Heat Capacity 275.0 K, C_p=133.5 J·mol^{-1}·K^{-1}
Temperature range 86 to 275 K. Value is unsmoothed experim datum.
Entropy 298.1 K, S=214.2 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 64.85 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 147.0 K, ΔH=5192 J·mol^{-1}
ΔS=35.3 J·mol^{-1}·K^{-1}
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B(C_p),C(S)

C_3H_8O (liq) 27PAR/
1-Propanol; n-Propyl alcohol
Heat Capacity 275.4 K, C_p=133.5 J·mol^{-1}·K^{-1}
Temperature range 86 to 275 K. Value is unsmoothed experim datum.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 29MIT/
1-Propanol; n-Propyl alcohol
Heat Capacity 270 K, C_p=136.0 J·mol^{-1}·K^{-1}
Temperature range 170 to 270 K.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 29PAR
1-Propanol; n-Propyl alcohol
Heat Capacity 298.1 K, C_p=192.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 43.5 J·mol^{-1}·K^{-1}.
Revision of previous data.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation C

C_3H_8O (liq) 3
1-Propanol; n-Propyl alcohol
Heat Capacity 301.2 K, C_p=164.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation C

C_3H_8O (liq) 41ZHD
1-Propanol; n-Propyl alcohol
Heat Capacity 298.1 K, C_p=145.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 46 °C.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation C

C_3H_8O (liq) 51EUC/EIG
1-Propanol; n-Propyl alcohol
Heat Capacity 303 K, C_p=140.21 J·mol^{-1}·K^{-1}
Temperature range 303 to 393 K.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation A

C_3H_8O (liq) 60SWI/ZIE
1-Propanol; n-Propyl alcohol
Heat Capacity 320 K, C_p=155.6 J·mol^{-1}·K^{-1}
Mean value 21 to 74 °C.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation C

C_3H_8O (gls) 68COU/LEE
1-Propanol; n-Propyl alcohol
Heat Capacity 150 K, C_p=106.3 J·mol^{-1}·K^{-1}
Temperature range 10 to 150 K.
Entropy 150 K, S=112.7 J·mol^{-1}·K^{-1}
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation A

C_3H_8O (liq) 68COU/LEE
1-Propanol; n-Propyl alcohol
Heat Capacity 298.15 K, C_p=143.8 J·mol^{-1}·K^{-1}
Temperature range 11 to 350 K.
Entropy 298.15 K, S=192.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 148.75 K, ΔH=5372 J·mol^{-1}
ΔS=36.11 J·mol^{-1}·K^{-1}
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation A

C_3H_8O (liq) 68REC
1-Propanol; n-Propyl alcohol
Heat Capacity 298 K, C_p=146.1 J·mol^{-1}·K^{-1}
Temperature range 24 to 40 °C, equation only.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation C

C_3H_8O (liq) 70PAZ/PAZ
1-Propanol; n-Propyl alcohol
Heat Capacity 313.2 K, C_p=158.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 76FOR/BEN
1-Propanol; n-Propyl alcohol
Heat Capacity 298.15 K, C_p=143.87 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 76FOR/BEN2
1-Propanol; n-Propyl alcohol
Heat Capacity 298.15 K, C_p=144.062 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B
Data from 76FOR/BEN.

C_3H_8O (liq) 77MUR/SUB
1-Propanol; n-Propyl alcohol
Heat Capacity 298.15 K, C_p=149.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 77VES/SVO
1-Propanol; n-Propyl alcohol
Heat Capacity 298.15 K, C_p=143.78 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 79GRI/YAN
1-Propanol; n-Propyl alcohol
Heat Capacity 303.4 K, C_p=147.9 J·mol^{-1}·K^{-1}
Temperature range 303 to 463 K. p=0.98 bar.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 79GRI/YAN
2-Propanol; Isopropyl alcohol
Heat Capacity 311.6 K, C_p=165.6 J·mol^{-1}·K^{-1}
Temperature range 311 to 453 K. p=0.98 bar.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation B

C_3H_8O (liq) 79VES/ZAB
1-Propanol; n-Propyl alcohol
Heat Capacity 298.15 K, C_p=143.77 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 80KAL/JED
1-Propanol; n-Propyl alcohol
Heat Capacity 298.216 K, C_p=146.34 J·mol^{-1}·K^{-1}
Temperature range 185 to 300 K. Unsmoothed experimental datum.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 81ARU/BAG
1-Propanol; n-Propyl alcohol
Heat Capacity 293.15 K, C_p=141.8 J·mol^{-1}·K^{-1}
Temperature range 293 to 353 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.360 kJ/kg·K. C_p given from 293.25 to 533.15 K for pressure range 10 to 60 MPa.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 82BEN/DAR
1-Propanol; n-Propyl alcohol
Heat Capacity 288.15 K, C_p=138.40 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 82VIL/CAS
1-Propanol; n-Propyl alcohol
Heat Capacity 298.15 K, C_p=146.88 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 84ZEG/SOM
1-Propanol; n-Propyl alcohol
Heat Capacity 298.15 K, C_p=144.44 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 86KOR/KUK
1-Propanol; n-Propyl alcohol
Heat Capacity 298 K, C_p=144.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 86TAN/TOY
1-Propanol; n-Propyl alcohol
Heat Capacity 298.15 K, C_p=143.96 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation A

C_3H_8O (liq) 24WIL/DAN
2-Propanol; Isopropyl alcohol
Heat Capacity 303 K, C_p=169.9 J·mol^{-1}·K^{-1}
Temperature range 303 to 323 K. Equation only.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation C

C_3H_8O (liq) 25PAR/
2-Propanol; Isopropyl alcohol
Heat Capacity 293.1 K, C_p=152.3 J·mol^{-1}·K^{-1}
Temperature range 71 to 293 K. Value is unsmoothed experim datum.
Entropy 298.1 K, S=190.8 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 53.22 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 184.6 K, ΔH=5297 J·mol^{-1}
ΔS=28.7 J·mol^{-1}·K^{-1}
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation B(C_p),C(S)

C_3H_8O (liq) 28PAR/
2-Propanol; Isopropyl alcohol
Heat Capacity 293.1 K, C_p=151.0 J·mol^{-1}·K^{-1}
Temperature range 71 to 293 K. Value is unsmoothed experim datum.
Entropy 298.1 K, S=192.9 J·mol^{-1}·K^{-1}
Extrapolation below 70 K, 43.56 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 184.6 K, ΔH=5301 J·mol^{-1}
ΔS=28.72 J·mol^{-1}·K^{-1}
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation B(C_p),C(S)

C_3H_8O (liq) 29K
2-Propanol; Isopropyl alcohol
Heat Capacity 292.84 K, C_p=149.75 J·mol^{-1}·K^{-1}
Temperature range 16 to 298 K. Value is unsmoothed experim datum.
Entropy 298.15 K, S=179.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 184.67 K, ΔH=5372 J·mol^{-1}
ΔS=29.09 J·mol^{-1}·K^{-1}
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation A

C_3H_8O (liq) 29PAR/
2-Propanol; Isopropyl alcohol
Heat Capacity 298.1 K, C_p=180.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 42.68 J·mol^{-1}·K^{-1}.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation C

C_3H_8O (liq) 33TRE/
2-Propanol; Isopropyl alcohol
Heat Capacity 298 K, C_p=163.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation B

C_3H_8O (liq) 3
2-Propanol; Isopropyl alcohol
Heat Capacity 303.2 K, C_p=172.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation C

C_3H_8O (liq) 45ZHD
2-Propanol; Isopropyl alcohol
Heat Capacity 298.04 K, C_p=159.99 J·mol^{-1}·K^{-1}
Temperature range 7 to 41 °C. Value is unsmoothed experimental datum.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation C

C_3H_8O (liq) 48GIN/COR
2-Propanol; Isopropyl alcohol
Heat Capacity 298 K, C_p=154.0 J·mol^{-1}·K^{-1}
Temperature range 0 to 200 °C.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation B

C_3H_8O (liq) 58SWI/ZIE2
2-Propanol; Isopropyl alcohol
Heat Capacity 324 K, C_p=180.3 J·mol^{-1}·K^{-1}
Mean value 21 to 81 °C.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation C

C_3H_8O (liq) 62KAT
2-Propanol; Isopropyl alcohol
Heat Capacity 298.2 K, C_p=162.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 60 °C.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation B

C_3H_8O (liq) 63AND/COU2
2-Propanol; Isopropyl alcohol
Heat Capacity 298.15 K, C_p=154.43 J·mol^{-1}·K^{-1}
Temperature range 10 to 330 K.
Entropy 298.15 K, S=180.58 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 185.20 K, ΔH=5410 J·mol^{-1}
ΔS=29.21 J·mol^{-1}·K^{-1}
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation A

C_3H_8O (liq) 79BRO/ZIE
2-Propanol; Isopropyl alcohol
Heat Capacity 298.15 K, C_p=154.75 J·mol^{-1}·K^{-1}
Temperature range 185 to 304 K. Results as equation only.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation B

C_3H_8O (liq) 80ROU/ROB
2-Propanol; Isopropyl alcohol
Heat Capacity 298.15 K, C_p=161.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation QY1&1
Evaluation B

$C_3H_8O_2$ (liq) 1881REI
Methylal; 2,4-Dioxapentane; Formaldehyde, dimethylacetal; Dimethoxymethane
Heat Capacity 298 K, C_p=163.6 J·mol^{-1}·K^{-1}
Temperature range 289 to 323 K.
Molecular Weight 76.0950
Wiswesser Line Notation 1O1O1
Evaluation D

$C_3H_8O_2$ (liq) 64MCE/KIL
Methylal; 2,4-Dioxapentane; Formaldehyde, dimethylacetal; Dimethoxymethane
Heat Capacity 298.15 K, C_p=161.42 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=244.01 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 168.01 K, ΔH=8331.6 J·mol^{-1}
ΔS=49.59 J·mol^{-1}·K^{-1}
liq/g 298.15 K, ΔH=28886 J·mol^{-1}
ΔS=96.9 J·mol^{-1}·K^{-1}
P=53.14 kPa
Molecular Weight 76.0950
Wiswesser Line Notation 1O1O1
Evaluation A

$C_3H_8O_2$ (liq) 73KUS/SUU
3-Oxa-1-butanol; 2-Methoxyethanol
Heat Capacity 298.15 K, C_p=174.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 76.0950
Wiswesser Line Notation Q2O1
Evaluation B

$C_3H_8O_2$ (liq) 78ROU/PER
3-Oxa-1-butanol; 2-Methoxyethanol
Heat Capacity 298.15 K, C_p=176.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 76.0950
Wiswesser Line Notation Q2O1
Evaluation C

$C_3H_8O_2$ (liq) 91SVO/ZAB
3-Oxa-1-butanol; 2-Methoxyethanol
Heat Capacity 298.15 K, C_p=175.38 J·mol^{-1}·K^{-1}
Temperature range 298 to 330 K. C_p(liq)=84.235+0.3057(T/K) J·mol^{-1}·K^{-1}. C_p value calculated from equation.
Molecular Weight 76.0950
Wiswesser Line Notation Q2O1
Evaluation B

$C_3H_8O_2$ (liq) 27PAR/HUF
Propylene glycol; 1,2 Propanediol; 1,2-Dihydroxypropane
Heat Capacity 276.7 K, C_p=180.3 J·mol^{-1}·K^{-1}
Temperature range 91 to 277 K. Value is unsmoothed experimental datum.
Molecular Weight 76.0950
Wiswesser Line Notation QY1&1Q
Evaluation B

$C_3H_8O_2$ (liq) 72KAW/OTA
Propylene glycol; 1,2-Propanediol; 1,2-Dihydroxypropane
Heat Capacity 303 K, C_p=177.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 76.0950
Wiswesser Line Notation QY1&1Q
Evaluation B

$C_3H_8O_2$ (liq) 82ZAR
Propylene glycol; 1,2-Propanediol; 1,2-Dihydroxypropane
Heat Capacity 298 K, C_p=189.9 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 76.0950
Wiswesser Line Notation QY1&1Q
Evaluation B

$C_3H_8O_3$ (liq) 03MAG
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 298 K, C_p=221.9 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.576 cal·g^{-1}·K^{-1}.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation D

$C_3H_8O_3$ (liq) 22SIM
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 289.7 K, C_p=225.9 J·mol^{-1}·K^{-1}
Temperature range 19 to 294 K. Value is unsmoothed experimental datum. C_p also measured for glass.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation C
Contained 1.3% water. Mp 17 °C.

$C_3H_8O_3$ (liq) 23GIB/GIA
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 299.4 K, C_p=223.4 J·mol^{-1}·K^{-1}
Temperature range 70.2 to 299.4 K. Value is unsmoothed experimental datum. C_p also measured for glass.
Phase Changes
c/liq 291.0 K, ΔH=18285 J·mol^{-1}
ΔS=62.8 J·mol^{-1}·K^{-1}
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation B

$C_3H_8O_3$ (liq) 29PAR/KEL
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 298.1 K, C_p=207.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 41.4 J·mol^{-1}·K^{-1}.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation C

$C_3H_8O_3$ (c) 31VOL/MAR
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 279–284 K, C_p=150 J·mol^{-1}·K^{-1}
Temperature range 279 to 284 K. C_p measured for the solid phase is an average value over the temperature range.
Phase Changes
c/liq 291.75 K, ΔH=18476 J·mol^{-1}
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation C

$C_3H_8O_3$ (liq) 36ERN/W
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 298 K, C_p=213.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation C

$C_3H_8O_3$ (c) 37AHL/BI
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 86.92 K, C_p=49.79 J·mol^{-1}·K^{-1}
Temperature range 3 to 87 K. Value is unsmoothed experimental datu
Entropy 90 K, S=37.87 J·mol^{-1}·K^{-1}
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation A

$C_3H_8O_3$ (gls) 37AHL/BI
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 85.12 K, C_p=50.21 J·mol^{-1}·K^{-1}
Temperature range 2.3 to 95 K. Value is unsmoothed experimen datum.
Entropy 90 K, S=42.34 J·mol^{-1}·K^{-1}
Value $S-S_0$; zero point entropy calculated as 19.41 J·mol^{-1}·K^{-1}.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation A

$C_3H_8O_3$ (liq) 44Y(
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Phase Changes
c/liq 292 K, ΔH=18303 J·mol^{-1}
ΔS=62.7 J·mol^{-1}·K^{-1}
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation B

$C_3H_8O_3$ (liq) 62OM
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 293.15 K, C_p=221.18 J·mol^{-1}·K^{-1}
Temperature range 273 to 523 K. A reexamination of the literatu C_p(liq)=32.9+0.0761T −0.0000269T^2(T in K) cal·mol^{-1}·°C^{-1} (0 250 °C).
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation A

$C_3H_8O_3$ (liq) 62RAB/N
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 298 K, C_p=218.5 J·mol^{-1}·K^{-1}
Temperature range 10 to 55 °C.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation B

$C_3H_8O_3$ (liq) 70PAZ/F
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 301.2 K, C_p=221.7 J·mol^{-1}·K^{-1}
Temperature range 28, 40 °C.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation B

$C_3H_8O_3$ (liq) 77MUR/SUB
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 298.15 K, C_p=221.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation B

$C_3H_8O_3$ (liq) 81ATA/ELS
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 293.15 K, C_p=219.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation B

$C_3H_8O_3$ (liq) 82CHE/GE
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 313.15 K, C_p=229.3 J·mol^{-1}·K^{-1}
Temperature range 20 to 60 K. C_p given as 2.49 kJ·kg^{-1}·C^{-1} at 40 °C. C_p at 25 °C estimated from graph to be ca. 2.43 kJ·kg^{-1}·C^{-1} or 223 J·mol^{-1}·K^{-1}.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation B

$C_3H_8O_3$ (liq) 88BAS/NIL
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 298.15 K, C_p=218.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation A

C_3H_8S (liq) 51SCO/FIN
Thiabutane; Ethyl methyl sulfide
Heat Capacity 298.15 K, C_p=144.64 J·mol^{-1}·K^{-1}
Temperature range 14 to 298 K.
Entropy 298.15 K, S=239.07 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 167.23 K, ΔH=9761 J·mol^{-1}
ΔS=58.37 J·mol^{-1}·K^{-1}
liq/g 301.66 K, ΔH=31644 J·mol^{-1}
ΔS=104.90 J·mol^{-1}·K^{-1}
P=24.75 kPa
Molecular Weight 76.1562
Wiswesser Line Notation 2S1
Evaluation A

C_3H_8S (liq) 56PEN/SCO
1-Propanethiol; n-Propyl mercaptan
Heat Capacity 298.15 K, C_p=144.56 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=242.50 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 142.10 K, ΔH=3971.0 J·mol^{-1}
ΔS=27.95 J·mol^{-1}·K^{-1}
c,I/liq 160.00 K, ΔH=5476.9 J·mol^{-1}
ΔS=34.23 J·mol^{-1}·K^{-1}
Molecular Weight 76.1562
Wiswesser Line Notation SH3
Evaluation A

C_3H_8S (liq) 54MCC/FIN2
2-Propanethiol; Isopropyl mercaptan
Heat Capacity 298.15 K, C_p=145.35 J·mol^{-1}·K^{-1}
Temperature range 12 to 322 K.
Entropy 298.15 K, S=233.55 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 112.5 K, ΔH=52.84 J·mol^{-1}
ΔS=0.47 J·mol^{-1}·K^{-1}
c,I/liq 142.64 K, ΔH=5736 J·mol^{-1}
ΔS=40.21 J·mol^{-1}·K^{-1}
liq/g 325.72 K, ΔH=27910 J·mol^{-1}
ΔS=85.69 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 76.1562
Wiswesser Line Notation SHY1&1
Evaluation A

$(C_3H_8Si)_n$ (liq) 78LEB/RAB3
Polydimethylsilamethylene
Heat Capacity 298.15 K, C_p=137.6 J·mol^{-1}·K^{-1}
Temperature range 60 to 330 K. Rubber like elastic state.
Entropy 298.15 K, S=157.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 266 K, ΔH=8000 J·mol^{-1}
ΔS=30 J·mol^{-1}·K^{-1}
Molecular Weight 72.1817
Wiswesser Line Notation /*-SI-1&1&1*/
Evaluation A
T(glass)=178 K.

C_3H_9Al (liq) 61MCC
Trimethylaluminum
Heat Capacity 298.15 K, C_p=155.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 380 K.
Entropy 298.15 K, S=209.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 288.43 K, ΔH=8790.6 J·mol^{-1}
ΔS=30.48 J·mol^{-1}·K^{-1}
Molecular Weight 72.0856
Wiswesser Line Notation 1-AL-1&1
Evaluation A

C_3H_9Al (liq) 63MCC/MES
Trimethylaluminum
Heat Capacity 298.15 K, C_p=155.60 J·mol^{-1}·K^{-1}
Temperature range 10 to 380 K.
Entropy 298.15 K, S=209.41 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 288.43 K, ΔH=8790.6 J·mol^{-1}
ΔS=30.48 J·mol^{-1}·K^{-1}
Molecular Weight 72.0856
Wiswesser Line Notation 1-AL-1&1
Evaluation A

C_3H_9As (liq) 88NIS/SHE
Trimethylarsine
Heat Capacity 298.15 K, C_p=154.0 J·mol^{-1}·K^{-1}
Temperature range 13 to 310 K.
Entropy 298.15 K, S=251.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 186.60 K, ΔH=8962 J·mol^{-1}
ΔS=48.03 J·mol^{-1}·K^{-1}
Molecular Weight 120.0257
Wiswesser Line Notation 1-AS-1&1
Evaluation A

C_3H_9B (liq) 54FUR/PAR
Trimethylborane
Heat Capacity 210 K, $C_p = 116.79\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 15 to 220 K.
Entropy 210 K, $S = 198.95\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 113.21 K, $\Delta H = 3250\ J \cdot mol^{-1}$
$\Delta S = 28.71\ J \cdot mol^{-1} \cdot K^{-1}$
liq/g 199.91 K, $\Delta H = 23089\ J \cdot mol^{-1}$
$\Delta S = 115.5\ J \cdot mol^{-1} \cdot K^{-1}$
P=6.20 kPa
Molecular Weight 55.9141
Wiswesser Line Notation 1B1&1
Evaluation A

$C_3H_9BO_3$ (liq) 59HAN/HUG
Trimethyl borate
Heat Capacity 298.15 K, $C_p = 189.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 273 to 453 K. C_p(liq)=0.75534 t 0.0012419t Btu/lb·°C (0 to 180 °C). C_p value calculated from equation.
Molecular Weight 103.9042
Wiswesser Line Notation
Evaluation A

C_3H_9ClSi (liq) 71SAM/KOS
Chlorotrimethylsilane
Heat Capacity 298.15 K, $C_p = 187.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 12.38 to 303.05 K. C_p(liq) $= 18.19046 + 0.077664T + 309052T^{-2}$ $cal \cdot mol^{-1} \cdot deg^{-1}$. Value is calculated from equation. Deposited in VINITI, No 2501-71, 18 January 1971.
Entropy 298.15 K, $S = 275.1\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 185.1 K, $\Delta H = 695\ J \cdot mol^{-1}$
$\Delta S = 3.75\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 217.97 K, $\Delta H = 9682\ J \cdot mol^{-1}$
$\Delta S = 44.39\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 108.6426
Wiswesser Line Notation G-SI-1&1&1
Evaluation B
Debeye temperature=115.8 K.

C_3H_9Ga (liq) 73MAS/NOV
Trimethylgallium
Heat Capacity 298.15 K, $C_p = 178.87\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 60 to 300 K.
Phase Changes
c/liq 257.9 K, $\Delta H = 11046\ J \cdot mol^{-1}$
$\Delta S = 42.83\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 114.8241
Wiswesser Line Notation 1-GA-1&1
Evaluation B

C_3H_9Ga (liq) 88LEB/SMI
Trimethylgallium
Heat Capacity 298.15 K, $C_p = 188.0\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 0 to 330 K.
Entropy 298.15 K, $S = 252.1\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 244.5 K, $\Delta H = 333\ J \cdot mol^{-1}$
$\Delta S = 1.36\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 257.81 K, $\Delta H = 10602\ J \cdot mol^{-1}$
$\Delta S = 41.1\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 114.8241
Wiswesser Line Notation 1-GA-1&1
Evaluation A

C_3H_9In (c) 91URY/R
Trimethylindium
Heat Capacity
Temperature range 230 to 250 K and 355 to 408 K.
Phase Changes
c/liq 358.7 K, $\Delta H = 14300\ J \cdot mol^{-1}$
Molecular Weight 159.9241
Wiswesser Line Notation 1-IN-1&1
Evaluation B
Anomaly in the temperature range 230 to 250 K.

C_3H_9N (liq) 44AST/S
Trimethylamine
Heat Capacity 280 K, $C_p = 132.55\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 12 to 280 K.
Entropy 276.03 K, $S = 197.82\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 156.08 K, $\Delta H = 6544\ J \cdot mol^{-1}$
$\Delta S = 41.93\ J \cdot mol^{-1} \cdot K^{-1}$
liq/g 276.03 K, $\Delta H = 22937\ J \cdot mol^{-1}$
$\Delta S = 83.10\ J \cdot mol^{-1} \cdot K^{-1}$
P=101.325 kPa
Molecular Weight 59.1108
Wiswesser Line Notation 1N1&1
Evaluation A

C_3H_9N (liq) 67SMI/GC
1-Aminopropane; n-Propylamine
Heat Capacity 298.15 K, $C_p = 162.3\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 59.1108
Wiswesser Line Notation Z3
Evaluation B

C_3H_9N (liq) 71KON/W
1-Aminopropane; n-Propylamine
Heat Capacity 298.15 K, $C_p = 160\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 59.1108
Wiswesser Line Notation Z3
Evaluation B

C_3H_9N (liq) 71VAS/
1-Aminopropane; n-Propylamine
Heat Capacity 298.15 K, $C_p = 166.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 60 to 300 K. Details deposited VINITI, 2530-71, 30 Jan 1971.
Entropy 298.15 K, $S = 228.2\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 60 K, 26.7 $J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 188.36 K, $\Delta H = 10625\ J \cdot mol^{-1}$
$\Delta S = 56.4\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 59.1108
Wiswesser Line Notation Z3
Evaluation A(C_p),B(S)

C_3H_9N (liq) 72FIN/I
1-Aminopropane; n-Propylamine
Heat Capacity 298.15 K, $C_p = 162.51\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 12 to 350 K.
Entropy 298.15 K, $S = 227.44\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 188.36 K, $\Delta H = 10974.2\ J \cdot mol^{-1}$
$\Delta S = 58.26\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 59.1108
Wiswesser Line Notation Z3
Evaluation A

C_3H_9N (liq) 50HOU/MAS
2-Aminopropane; Isopropylamine
Heat Capacity 313 K, C_p=164.0 J·mol^{-1}·K^{-1}
Temperature range 313 to 343 K.
Molecular Weight 59.1108
Wiswesser Line Notation ZY1&1
Evaluation B

C_3H_9N (liq) 67SMI/GOO2
2-Aminopropane; Isopropylamine
Heat Capacity 298.15 K, C_p=165.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.1108
Wiswesser Line Notation ZY1&1
Evaluation B

C_3H_9N (liq) 71KON/WAD
2-Aminopropane; Isopropylamine
Heat Capacity 298.15 K, C_p=164 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.1108
Wiswesser Line Notation ZY1&1
Evaluation B

C_3H_9N (liq) 72FIN/MES
2-Aminopropane; Isopropylamine
Heat Capacity 298.15 K, C_p=163.85 J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Entropy 298.15 K, S=218.32 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 177.99 K, ΔH=7324.5 J·mol^{-1}
ΔS=41.15 J·mol^{-1}·K^{-1}
Molecular Weight 59.1108
Wiswesser Line Notation ZY1&1
Evaluation A

$C_3H_{10}BrN$ (c) 90GEN/LUB
n-Propylammonium bromide
Heat Capacity 300 K, C_p=131.21 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K. C_p(c)=59.4+0.212T+9.12×10^{-5} T^2 J·mol^{-1}·K^{-1} (300 to 450 K). C_p value calculated from equation.
Phase Changes
c/liq 464.6 K, ΔH=13340 J·mol^{-1}
ΔS=28.72 J·mol^{-1}·K^{-1}
Molecular Weight 140.0227
Wiswesser Line Notation Z3 &EH
Evaluation A

$C_3H_{10}CdCl_3N$ (c) 92HOU/DUN
Trimethylammonium trichlorocadmate
Phase Changes
c,IV/c,III 333 K, ΔH=150 J·mol^{-1}
ΔS=0.45 J·mol^{-1}·K^{-1}
c,III/c,II 365 K, ΔH=420 J·mol^{-1}
ΔS=1.15 J·mol^{-1}·K^{-1}
c,II/c,I 408 K, ΔH=35 J·mol^{-1}
ΔS=0.086 J·mol^{-1}·K^{-1}
Molecular Weight 278.8877
Wiswesser Line Notation 1N1&1 &GH .CD G2
Evaluation A
Only the transition at 333 K is reversible. It shows considerable thermal hysteresis.

$C_3H_{10}N_2$ (liq) 55AST/ZOL
Trimethylhydrazine
Heat Capacity 292.15 K, C_p=185.94 J·mol^{-1}·K^{-1}
Temperature range 12 to 294 K.
Entropy 292.15 K, S=231.96 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 201.24 K, ΔH=9485 J·mol^{-1}
ΔS=47.13 J·mol^{-1}·K^{-1}
liq/g 292.15 K, ΔH=33259 J·mol^{-1}
ΔS=113.84 J·mol^{-1}·K^{-1}
P=19.83 kPa
Molecular Weight 74.1254
Wiswesser Line Notation 1N1&M1
Evaluation A
Corrected for 2 mole % unsym-dimethylhydrazine.

$C_3H_{10}N_2$ (liq) 75MES/FIN
1,2-Diaminopropane; 1,2-Propanediamine
Heat Capacity 298.15 K, C_p=205.64 J·mol^{-1}·K^{-1}
Temperature range 11 to 368 K.
Entropy 298.15 K, S=247.27 J·mol^{-1}·K^{-1}
Includes 5.77 J·mol^{-1}·K^{-1} for mixing of D and L isomers.
Phase Changes
c,II/c,I 222.0 K, ΔH=67.4 J·mol^{-1}
ΔS=0.304 J·mol^{-1}·K^{-1}
c,I/liq 236.53 K, ΔH=18422.6 J·mol^{-1}
ΔS=77.89 J·mol^{-1}·K^{-1}
Molecular Weight 74.1254
Wiswesser Line Notation ZY1&1Z
Evaluation A

$C_3H_{10}N_2O_3$ (c) 88SCH/EIS
Isopropylamine nitrate
Phase Changes
c/liq 346.6 K, ΔH=15876 J·mol^{-1}
Molecular Weight 122.1236
Wiswesser Line Notation ZY1&1 &WNQ
Evaluation A

$C_3H_{12}BN$ (c,III) 70FIN/TOD
Trimethylamineborane
Heat Capacity 298.15 K, C_p=173.76 J·mol^{-1}·K^{-1}
Temperature range 12 to 390 K.
Entropy 298.15 K, S=169.58 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 350.1 K, ΔH=2535 J·mol^{-1}
ΔS=7.24 J·mol^{-1}·K^{-1}
c,II/c,I 360.4 K, ΔH=594 J·mol^{-1}
ΔS=16.48 J·mol^{-1}·K^{-1}
c,I/liq 368.70 K, ΔH=4947.2 J·mol^{-1}
ΔS=13.42 J·mol^{-1}·K^{-1}
Molecular Weight 72.9445
Wiswesser Line Notation 1N1&1 &BHHH
Evaluation A

$C_3H_{12}CdCl_4N_2$ (c) 88ABE/CHH
Propyldiammonium cadmium tetrachloride
Heat Capacity 298.15 K, C_p=275.54 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=351.94 J·mol^{-1}·K^{-1}
Molecular Weight 330.3632
Wiswesser Line Notation Z3Z &GH 2 .CD G2
Evaluation A
Magnetic transition around 50 K.

$C_3H_{12}Cl_4MnN_2$ (c) 85CHH/BOC
Propyldiammonium manganese tetrachloride
Heat Capacity 298.15 K, C_p=298.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S=357.4 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 307.6 K, ΔH=710 J·mol^{-1}
ΔS=2.4 J·mol^{-1}·K^{-1}
DSC study yields $\Delta\Delta H$=725 J·mol^{-1}·K^{-1} at 305 K.
c,II/c,I 336 K, ΔH=640 J·mol^{-1}
ΔS=1.90 J·mol^{-1}·K^{-1}
From DSC study.
Molecular Weight 272.8912
Wiswesser Line Notation Z3Z &GH 2 .MN G2
Evaluation A
A magnetic transition is observed in the temperature range 45 to 65 K.

$C_3H_{12}N_6O_3$ (c) 40HUF/ELL
Guanidine carbonate
Heat Capacity 298.1 K, C_p=258.86 J·mol^{-1}·K^{-1}
Temperature range 86 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=295.35 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 93.35 J·mol^{-1}·K^{-1}
Molecular Weight 121.0956
Wiswesser Line Notation ZYZUM 2 &QVQ
Evaluation A(C_p), C(S)

$C_3H_{12}N_6S_3\cdot CCl_4$ (c) 90SEK/MAT
Thiourea carbon tetrachloride inclusion compound
Heat Capacity 298.15 K, C_p=384.2 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=546.6 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 41.3 K, ΔH=149 J·mol^{-1}
ΔS=3.7 J·mol^{-1}·K^{-1}
c,II/c,I 67.17 K, ΔH=241 J·mol^{-1}
ΔS=3.9 J·mol^{-1}·K^{-1}
Molecular Weight 382.1710
Wiswesser Line Notation ZYZUS 3 GXGGG
Evaluation A

$C_3H_{16}B_3N$ (c) 59LEV/WES
Trimethylamine-triborane
Heat Capacity 298.15 K, C_p=217.48 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S=228.43 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 209.6 K, ΔH=3528.8 J·mol^{-1}
ΔS=16.74 J·mol^{-1}·K^{-1}
Lambda-type transition.
Molecular Weight 98.5961
Wiswesser Line Notation 1N1&1 &B3H7
Evaluation A

$C_3H_{18}Bi_2Cl_9N_3$ (c) 92BEL/MOK
Tris(methylammonium)nonachlorodibismuthate
Phase Changes
c,III/c,II 247 K, ΔH=854 J·mol^{-1}
ΔS=3.46 J·mol^{-1}·K^{-1}
c,II/c,I 349 K
Molecular Weight 833.2331
Wiswesser Line Notation ZH&1 3 -BI- 2 Q 9
Evaluation A

$C_3LaN_3S_3\cdot 7H_2O$ (c) 91TAN/I
Lanthanum isothiocyanate heptahydrate
Heat Capacity 298.15 K, C_p=537.07 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=606.17 J·mol^{-1}·K^{-1}
Molecular Weight 439.2430
Wiswesser Line Notation SCN-LA-NCS&NCS &QH 7
Evaluation A

$C_3N_3NdS_3\cdot 7H_2O$ (c) 91TAN/I
Neodymium isothiocyanate heptahydrate
Heat Capacity 298.15 K, C_p=551.74 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=608.13 J·mol^{-1}·K^{-1}
Molecular Weight 444.5795
Wiswesser Line Notation SCN-ND-NCS&NCS &QH 7
Evaluation A

$C_3N_3PrS_3\cdot 7H_2O$ (c) 91TAN/I
Praseodymium isothiocyanate heptahydrate
Heat Capacity 298.15 K, C_p=540.80 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=613.41 J·mol^{-1}·K^{-1}
Molecular Weight 441.2472
Wiswesser Line Notation SCN-PR-NCS&NCS &QH 7
Evaluation A

$C_3N_3S_3Sm\cdot 6H_2O$ (c) 91TAN/I
Samarium isothiocyanate hexahydrate
Heat Capacity 298.15 K, C_p=465.92 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=543.11 J·mol^{-1}·K^{-1}
Molecular Weight 432.7243
Wiswesser Line Notation SCN-SM-NCS&NCS &QH 6
Evaluation A

$C_3N_3S_3Yb\cdot 6H_2O$ (c) 91TAN/
Ytterbium isothiocyanate hexahydrate
Heat Capacity 298.15 K, C_p=456.14 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=521.86 J·mol^{-1}·K^{-1}
Molecular Weight 455.3643
Wiswesser Line Notation SCN-YB-NCS&NCS &QH 6
Evaluation A

$C_3N_3S_3Y\cdot 6H_2O$ (c) 91TAN/
Yttrium isothiocyanate hexahydrate
Heat Capacity 298.15 K, C_p=454.25 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=511.57 J·mol^{-1}·K^{-1}
Molecular Weight 371.2302
Wiswesser Line Notation SCN-Y-NCS&NCS &QH 6
Evaluation A

$C_4Br_2Cl_2F_6$ (liq) 88SVC
1,4-Dibromo-2,3-dichlorohexafluorobutane
Heat Capacity 298.16 K, C_p=298.5 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K. C_p (J·mol^{-1}·K^{-1})=215.6+0.278 (T/K) (298 to 318 K).
Molecular Weight 392.7484
Wiswesser Line Notation FXFEXGFXGFXFFE
Evaluation A

C_4F_8 (liq) 54FUR/MCC

Freon C318; Octafluorocyclobutane

Heat Capacity 268.52 K, C_p=209.77 J·mol^{-1}·K^{-1}

Temperature range 17 to 270 K. Value is unsmoothed experimental datum.

Entropy 261.25 K, S=291.1 J·mol^{-1}·K^{-1}

Phase Changes

Solid state transitions at 141.3 K, 174.6 K, 214.84 K, and 216.99 K. No enthalpies of transition reported, entropy changes calculated from integration of total heat input and temperature measurements. Anomalous heat capacity region about 97 K.

c,I/liq 232.96 K, ΔH=2768.2 J·mol^{-1}
ΔS=11.89 J·mol^{-1}·K^{-1}

liq/g 261.25 K, ΔH=23721 J·mol^{-1}
ΔS=90.80 J·mol^{-1}·K^{-1}
P=78.78

Molecular Weight 200.0312

Wiswesser Line Notation L4TJ AF AF BF BF CF CF DF DF

Evaluation A

C_4F_8 (liq) 82PON

Freon C318; Octafluorocyclobutane

Heat Capacity 296.41 K, C_p=222.4 J·mol^{-1}·K^{-1}

Temperature range 240 to 340 K. Value is unsmoothed experimental datum: C_p given as 1.112 J·g^{-1}·K^{-1}.

Molecular Weight 200.0312

Wiswesser Line Notation L4TJ AF AF BF BF CF CF DF DF

Evaluation B

C_4F_{10} (liq) 83CAM/DIA

n-Perfluorobutane

Heat Capacity 293 K, C_p=127.2 J·mol^{-1}·K^{-1}

Calculated value from Sargent, J.W. *et al.*, Amer. Soc. Test Mater. Spect. Tech. Bull. 346:51, 1964.

Molecular Weight 238.0280

Wiswesser Line Notation FXFFXFFXFFXFFF

Evaluation C

$C_4H_2N_2O_4$ (c) 35STI/HUF

Alloxan

Heat Capacity 297.2 K, C_p=153.01 J·mol^{-1}·K^{-1}

Temperature range 85 to 297 K. Value is unsmoothed experimental datum.

Entropy 298.15 K, S=153.0 J·mol^{-1}·K^{-1}

Extrapolation below 90 K, 55.02 J·mol^{-1}·K^{-1}

Molecular Weight 142.0708

Wiswesser Line Notation T6MVMVVVJ

Evaluation B(C_p),C(S)

$C_4H_2O_3$ (c) 52SPE/TAM

Maleic anhydride

Phase Changes

c/liq 325 K, ΔH=12930 J·mol^{-1}
ΔS=39.8 J·mol^{-1}·K^{-1}

Molecular Weight 98.0580

Wiswesser Line Notation T5VOVJ

Evaluation C

$C_4H_2O_3$ (c) 57MAS

Maleic anhydride

Phase Changes

c/liq 326.00 K, ΔH=13648 J·mol^{-1}

Molecular Weight 98.0580

Wiswesser Line Notation T5VOVJ

Evaluation A

$C_4H_2O_3$ (c) 78MAR/CIO2

Maleic anhydride

Heat Capacity 298.15 K, C_p=67.4 J·mol^{-1}·K^{-1}

Temperature range 298 to 480 K.

Phase Changes

c/liq 325.64 K, ΔH=12260 J·mol^{-1}
ΔS=37.6 J·mol^{-1}·K^{-1}

Molecular Weight 98.0580

Wiswesser Line Notation T5VOVJ

Evaluation D

$C_4H_2O_3$ (c) 83DEW/DEK

Maleic anhydride

Heat Capacity 300 K, C_p=119.9 J·mol^{-1}·K^{-1}

Temperature range 90 to 350 K. Linearly extrapolated.

Phase Changes

c/liq 325.72 K, ΔH=13550 J·mol^{-1}
ΔS=41.6 J·mol^{-1}·K^{-1}

Molecular Weight 98.0580

Wiswesser Line Notation T5VOVJ

Evaluation B(C_p), A(Phase changes).

$C_4H_2O_3$ (c) 83DEW/OFF

Maleic anhydride

Heat Capacity 310 K, C_p=123.2 J·mol^{-1}·K^{-1}

Temperature range 300 to 450 K.

Phase Changes

c/liq 325.3 K, ΔH=13600 J·mol^{-1}
ΔS=41.8 J·mol^{-1}·K^{-1}

Molecular Weight 98.0580

Wiswesser Line Notation T5VOVJ

Evaluation B

$C_4H_2O_4$ (c,II) 79BAR/HEL

Squaric acid

Heat Capacity 300 K, C_p=121 J·mol^{-1}·K^{-1}

Temperature range 300 to 420 K. Data graphically only.

Phase Changes

c,II/c,I 373.57 K, ΔH=347 J·mol^{-1}
ΔS=0.93 J·mol^{-1}·K^{-1}

Molecular Weight 114.0574

Wiswesser Line Notation L4VVJ CQ DQ

Evaluation B

$C_4H_2O_4$ (c) 83DEW/OFF

Squaric acid

Heat Capacity 315 K, C_p=121.6 J·mol^{-1}·K^{-1}

Temperature range 300 to 450 K.

Phase Changes

c,II/c,I 372.2 K, ΔH=300 J·mol^{-1}
ΔS=0.8 J·mol^{-1}·K^{-1}

Molecular Weight 114.0574

Wiswesser Line Notation L4VVJ CQ DQ

Evaluation B

C_4H_3BrS (liq) 92GON/SZW

2-Bromothiophene

Phase Changes

c,III/liq 196.2 K, ΔH=6290 J·mol^{-1}
ΔS=32.1 J·mol^{-1}·K^{-1}

c,II/liq 200.3 K, ΔH=6500 J·mol^{-1}
ΔS=32.5 J·mol^{-1}·K^{-1}

c,I/liq 203.9 K, ΔH=7580 J·mol^{-1}
ΔS=37.2 J·mol^{-1}·K^{-1}

Molecular Weight 163.0317

Wiswesser Line Notation T5SJ BE

Evaluation A

C_4H_3BrS (liq) 93FUJ/OGU
2-Bromothiophene
Heat Capacity 298.15 K, C_p=144.0 J·mol^{-1}·K^{-1}
Temperature range 4 to 300 K.
Entropy 298.15 K, S=219.7 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 55.3 K, ΔH=13.9 J·mol^{-1}
ΔS=0.251 J·mol^{-1}·K^{-1}
c,I/liq 205.30 K, ΔH=7903 J·mol^{-1}
ΔS=38.43 J·mol^{-1}·K^{-1}
Molecular Weight 163.0317
Wiswesser Line Notation T5SJ BE
Evaluation A
T(glass)=120 K.

C_4H_3ClS (liq) 93FUJ/OGU2
2-Chlorothiophene
Heat Capacity 298.15 K, C_p=139.43 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=209.11 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 201.30 K, ΔH=8966 J·mol^{-1}
ΔS=44.54 J·mol^{-1}·K^{-1}
Molecular Weight 118.5807
Wiswesser Line Notation T5SJ BG
Evaluation A
T(glass)=164, 186 K.

$C_4H_3Cl_3OS$ (liq) 80SHA/LYU
Methyl trichlorothioacrylate
Heat Capacity 298.15 K, C_p=244.9 J·mol^{-1}·K^{-1}
Temperature range 15 to 330 K.
Entropy 298.15 K, S=324.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 286.25 K, ΔH=20370 J·mol^{-1}
ΔS=71.2 J·mol^{-1}·K^{-1}
Molecular Weight 205.4861
Wiswesser Line Notation GYGUYGVS1
Evaluation A

C_4H_3Cu (c) 82BYK/LEB
Copper vinylacetylenide
Heat Capacity 298.15 K, C_p=109.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=132.6 J·mol^{-1}·K^{-1}
Molecular Weight 114.6137
Wiswesser Line Notation -CU-1UU2U1
Evaluation A

$C_4H_3F_5O_3$ (liq) 84GOL/KOL
α-(Trifluoromethoxy)-α,α-difluoromethyl acetate
Phase Changes
c/liq 167.4 K, ΔH=8510 J·mol^{-1}
ΔS=50.8 J·mol^{-1}·K^{-1}
Molecular Weight 194.0579
Wiswesser Line Notation FXFFOXFFVO1
Evaluation A

$C_4H_3O_4K$ (c) 88FUK/MAT
Potassium hydrogen cis-butenedioate; Potassium hydrogen maleate
Heat Capacity 298.15 K, C_p=159.26 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=195.94 J·mol^{-1}·K^{-1}
Molecular Weight 154.1636
Wiswesser Line Notation QV1U1VO & K -C
Evaluation A

$C_4H_3O_4K$ (c) 88FUK/M
Potassium hydrogen trans-butenedioate; Potassium hydrogen fumarat
Heat Capacity 298.15 K, C_p=156.44 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=185.98 J·mol^{-1}·K^{-1}
Molecular Weight 154.1636
Wiswesser Line Notation QV1U1VO & K -T
Evaluation A

$C_4H_4KNaO_6\cdot4H_2O$ (c) 38HIC/H
Sodium potassium tartrate tetrahydrate; Rochelle salt; Potassium sod tartrate tetrahydrate
Heat Capacity 300 K, C_p=389.1 J·mol^{-1}·K^{-1}
Temperature range 15 to 340 K.
Phase Changes
c,II/c,I 328.78 K, ΔH=42752 J·mol^{-1}
ΔS=130.0 J·mol^{-1}·K^{-1}
Molecular Weight 282.2209
Wiswesser Line Notation OVYQYQVO .K .NA &QH4
Evaluation B

$C_4H_4KNaO_6\cdot4H_2O$ (c) 38
Sodium potassium tartrate tetrahydrate; Rochelle salt; Potassium sod tartrate tetrahydrate
Heat Capacity 298.15 K, C_p=385.9 J·mol^{-1}·K^{-1}
Temperature range 243 to 303 K. C_p(c)=1.290+0.0031t/°C J/g (24 303 K), large single cystals. C_p(298.15 K)=387.8 J/mo C_p=1.289+0.0034t/°C J/g (243 to 303 K), crystalline powder.
Molecular Weight 282.2209
Wiswesser Line Notation OVYQYQVO .K .NA &QH4
Evaluation B

$C_4H_4KNaO_6\cdot4H_2O$ (c) 78TAT/M
Sodium potassium tartrate tetrahydrate; Rochelle salt; Potassium soc tartrate tetrahydrate
Heat Capacity 298.15 K, C_p=386.13 J·mol^{-1}·K^{-1}
Temperature range 190 to 308 K.
Molecular Weight 282.2209
Wiswesser Line Notation OVYQYQVO .K .NA &QH4
Evaluation A

$C_4H_4KNaO_6\cdot4H_2O$ (c) 93DEY/S
Sodium potassium tartrate tetrahydrate; Rochelle salt; Potassium soc tartrate tetrahydrate
Phase Changes
c,IV/c,III 212 K
c,III/c,II 256 K
c,II/c,I 297 K
Molecular Weight 282.2209
Wiswesser Line Notation OVYQYQVO .K .NA &QH4
Evaluation A
Anomalous transitions observed at three temperatures with po directions of heat capacity peaks.

$(C_4H_4NNaO_3)_n$ (c) 91
Poly-L-aspartic acid, sodium salt
Heat Capacity 300 K, C_p=150.8 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 137.0703
Wiswesser Line Notation /*V1YVO &-NA- &M*/ -L
Evaluation B

$(C_4H_4NNaO_3)_n$ (c) 93ROL/XEN
Poly-L-aspartic acid, sodium salt
Heat Capacity 300 K, C_p=150.8 J·mol^{-1}·K^{-1}
Temperature range 230 to 390 K.
Molecular Weight 137.0703
Wiswesser Line Notation /*V1YVO &-NA- &M*/ -L
Evaluation B

$C_4H_4N_2$ (c,I) 63WUL/WES
Succinonitrile: 1.4-Butanedinitrile
Heat Capacity 298.15 K, C_p=145.60 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=191.59 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 233.3 K, ΔH=6199.4 J·mol^{-1}
ΔS=26.57 J·mol^{-1}·K^{-1}
c,I/liq 331.16 K, ΔH=3703.3 J·mol^{-1}
ΔS=11.18 J·mol^{-1}·K^{-1}
Molecular Weight 80.0890
Wiswesser Line Notation NC2CN
Evaluation A

$C_4H_4N_2$ (c) 87RAI/SIN
Succinonitrile; 1,4-Butanedinitrile
Phase Changes
c/liq 334 K, ΔH=3704 J·mol^{-1}
ΔS=11.1 J·mol^{-1}·K^{-1}
Molecular Weight 80.0890
Wiswesser Line Notation NC2CN
Evaluation B

$C_4H_4N_2$ (c,III) 79BOY/COM
Pyrazine
Heat Capacity 298 K, C_p=180 J·mol^{-1}·K^{-1}
Temperature range 295 to 312 K. Data graphically only.
Phase Changes
c,III/c,II 300.6 K, ΔH=969 J·mol^{-1}
ΔS=3.22 J·mol^{-1}·K^{-1}
c,II/c,I 310 K, ΔH=60 J·mol^{-1}
ΔS=0.2 J·mol^{-1}·K^{-1}
Molecular Weight 80.0890
Wiswesser Line Notation T6N DNJ
Evaluation C(C_p), B(Phase changes)

$C_4H_4N_2O_2$ (c) 78KIL4
Uracil
Heat Capacity 298 K, C_p=120.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 112.0878
Wiswesser Line Notation T6MVMVJ
Evaluation B

$C_4H_4N_2O_3$ (c) 85KOS/ISM
Barbituric acid
Heat Capacity 298.15 K, C_p=141.1 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 298.15 K, S=157.6 J·mol^{-1}·K^{-1}
Extrapolated below 90 K.
Molecular Weight 128.0872
Wiswesser Line Notation T6VMVMV FHJ
Evaluation B(C_p), C(S)

$C_4H_4N_2O_3$ (c) 90SOL/KAB
Barbituric acid
Heat Capacity 298.15 K, C_p=141.1 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K. C_p(c)=25.67+0.3361T+3.382 ×10-4T2−5.64×10-7T3 J· mol^{-1}·K^{-1} (200 to 450 K).
Entropy 298.15 K, S=157.3 J·mol^{-1}·K^{-1}
Molecular Weight 128.0872
Wiswesser Line Notation T6VMVMV FHJ
Evaluation A

$C_4H_4Na_2O_4$ (c) 55STR/GAN
Sodium succinate
Heat Capacity 300.43 K, C_p=172.5 J·mol^{-1}·K^{-1}
Temperature range 69.77 to 300.43 K. Unsmoothed experimental datum.
Entropy 298 K, S=211.7 J·mol^{-1}·K^{-1}
Molecular Weight 162.0527
Wiswesser Line Notation OV2VO &-NA-2
Evaluation B

C_4H_4O (liq) 52GUT/SCO
Furan
Heat Capacity 298.15 K, C_p=114.56 J·mol^{-1}·K^{-1}
Temperature range 11 to 300 K.
Entropy 298.15 K, S=176.65 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 150.0 K, ΔH=2046.8 J·mol^{-1}
ΔS=13.65 J·mol^{-1}·K^{-1}
c,I/liq 187.55 K, ΔH=3802.4 J·mol^{-1}
ΔS=20.27 J·mol^{-1}·K^{-1}
liq/g 298.15 K, ΔH=27451 J·mol^{-1}
ΔS=92.07 J·mol^{-1}·K^{-1}
P=79.934 kPa
Molecular Weight 68.0750
Wiswesser Line Notation T5OJ
Evaluation A

$C_4H_4O_4$ (c) 30PAR/HUF2
cis-2-Butenedioic acid; Maleic acid
Heat Capacity 294.4 K, C_p=135.6 J·mol^{-1}·K^{-1}
Temperature range 91 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=159.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 50.63 J·mol^{-1}·K^{-1}.
Molecular Weight 116.0732
Wiswesser Line Notation QV1U1VQ -C
Evaluation B(C_p),C(S)

$C_4H_4O_4$ (c) 30PAR/HUF2
trans-2-Butenedioic acid; Fumaric acid
Heat Capacity 297.1 K, C_p=141.8 J·mol^{-1}·K^{-1}
Temperature range 91 to 297.1 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=166.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 51.51 J·mol^{-1}·K^{-1}.
Molecular Weight 116.0732
Wiswesser Line Notation QV1U1VQ -T
Evaluation B(C_p),C(S)

$C_4H_4O_4$ (c,II) 77LEB/EVS2
Glycolide; 1,4-Dioxane-2,5-dione
Heat Capacity 298.15 K, C_p=133.3 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 550 K.
Entropy 298.15 K, S=157.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 312.1 K, ΔH=1840 J·mol^{-1}
ΔS=5.90 J·mol^{-1}·K^{-1}
c,I/liq 356.2 K, ΔH=14800 J·mol^{-1}
ΔS=41.5 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OV DOVTJ
Evaluation A

$C_4H_4O_4$ (c,II) 78EVS/BEL
Glycolide; 1,4-Dioxane-2,5-dione
Heat Capacity 298.15 K, C_p=133.2 J·mol^{-1}·K^{-1}
Temperature range 14 to 350 K. Complete data deposited in VINITI, No. 2144-77, 2 June 1977.
Entropy 298.15 K, S=157.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 312.1 K, ΔH=1810 J·mol^{-1}
ΔS=5.80 J·mol^{-1}·K^{-1}
c,I/liq 356.2 K, ΔH=14800 J·mol^{-1}
ΔS=41.5 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OV DOVTJ
Evaluation B

$C_4H_4O_4$ (c,II) 78LEB/YEV
Glycolide; 1,4-Dioxane-2,5-dione
Heat Capacity 298.15 K, C_p=133.3 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 550 K.
Entropy 298.15 K, S=157.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 312.1 K, ΔH=1810 J·mol^{-1}
ΔS=5.80 J·mol^{-1}·K^{-1}
c,I/liq 356.2 K, ΔH=14800 J·mol^{-1}
ΔS=41.5 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OV DOVTJ
Evaluation A
Data also given for metastable crystalline phase, c,I′ at 298.15 K: C_p=137.0 J·mol^{-1}·K^{-1} and S °=163.1 J·mol^{-1}·K^{-1}.

$C_4H_4O_4$ (c,II) 88LEB/KUL
Glycolide; 1,4-Dioxane-2,5-dione
Heat Capacity 298.15 K, C_p=133.28 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 400 K.
Entropy 298.15 K, S=157.23 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 312.1 K, ΔH=1840.0 J·mol^{-1}
ΔS=5.90 J·mol^{-1}·K^{-1}
c,I/liq 356.2 K, ΔH=14800 J·mol^{-1}
ΔS=41.49 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OV DOVTJ
Evaluation A

$C_4H_4O_4$ (c) 82LEB/KUL
Ethylene oxalate
Heat Capacity 298.15 K, C_p=141.9 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=149.7 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OVVOTJ
Evaluation A

$C_4H_4O_4$ (c) 82LEB/K
Ethylene oxalate
Heat Capacity 298.15 K, C_p=141.9 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=158.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 415 K, ΔH=13400 J·mol^{-1}
ΔS=32.29 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OVVOTJ
Evaluation A

$(C_4H_4O_4)_n$ (c) 77LEB/E
Polyglycolide
Heat Capacity 298.15 K, C_p=130.3 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 550 K.
Entropy 298.15 K, S=150.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 501 K, ΔH=23500 J·mol^{-1}
ΔS=47 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation /*V1OV1O*/
Evaluation A
T(glass)=318 K.

$(C_4H_4O_4)_n$ (gls) 78LEB/
Polyglycolide
Heat Capacity 298.15 K, C_p=136.7 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 550 K.
Entropy 298.15 K, S=151.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 501 K, ΔH=23500 J·mol^{-1}
ΔS=47 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation /*V1OV1O*/
Evaluation A
T(glass)=318 K.

$(C_4H_4O_4)_n$ (gls) 82LEB/F
Polyethylene oxalate
Heat Capacity 298.15 K, C_p=129.1 J·mol^{-1}·K^{-1}
Temperature range 8 to 360 K.
Entropy 298.15 K, S=163.5 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation /*VVO2O*/
Evaluation A
T(glass)=306 K.

C_4H_4S (liq) 34JAC
Thiophene
Heat Capacity 289.3 K, C_p=123.22 J·mol^{-1}·K^{-}
Temperature range 93 to 294 K. Data for solid, 90 to 237 K, not (table omitted, apparently). Value is unsmoothed experimental d
Entropy 298.1 K, S=176.6 J·mol^{-1}·K^{-1}
Details of extrapolation below 90 K not given. Scatter in data fo introduce uncertainty. Value good to about 4 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 171.1 K, ΔH=1209 J·mol^{-1}
ΔS=7.1 J·mol^{-1}·K^{-1}
c,I/liq 233.7 K, ΔH=4966 J·mol^{-1}
ΔS=21.3 J mol^{-1} K^{-1}
Molecular Weight 84.1356
Wiswesser Line Notation T5SJ
Evaluation B(C_p),C(S)

C_4H_4S (liq) 49WAD/KNO
Thiophene
Heat Capacity 297.45 K, C_p=123.85 J·mol^{-1}·K^{-1}
Temperature range 11 to 336 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=181.17 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 171.6 K, ΔH=637.6 J·mol^{-1}
ΔS=3.72 J·mol^{-1}·K^{-1}
Anomalous heat capacity 100 to 150 K. Apparently two second order transitions at about 112, 138 K, with small energies involved.
c,I/liq 234.95 K, ΔH=5086.1 J·mol^{-1}
ΔS=21.65 J·mol^{-1}·K^{-1}
Molecular Weight 84.1356
Wiswesser Line Notation T5SJ
Evaluation A

C_4H_4S (c) 82AND/DWO
Thiophene
Heat Capacity
Temperature range 50 to 200 K. Data graphically only in the region of the phase transitions.
Phase Changes
c,V/c,IV 111.3 K
c,IV/c,III 136.8 K
c,III/c,II 170.5 K
c,II/c,I 174.5 K
Molecular Weight 84.1356
Wiswesser Line Notation T5SJ
Evaluation A

C_4H_4S (c) 84FIG/SZW
Thiophene
Heat Capacity
Temperature range 14 to 300 K. Data given graphically only.
Phase Changes
c,V′/c,IV′ 90.76 K
Metastable transition.
c,IV′/c,III′ 139.2 K
Metastable transition.
c,V/c,IV 112.35 K
c,IV/c,III 138.5 K
c,III/c,II 170.70 K
c,II/c,I 175.03 K
c,I/liq 235.03 K
Molecular Weight 84.1356
Wiswesser Line Notation T5SJ
Evaluation A

C_4H_4S (liq) 85FIG/SZW
Thiophene
Heat Capacity 298.14 K, C_p=122.40 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=181.2 J·mol^{-1}·K^{-1}
Phase Changes
c,V/c,III 44–170 K, ΔH=428 J·mol^{-1}
ΔS=4.0 J·mol^{-1}·K^{-1}
c,III/c,II 170.70 K, ΔH=809.7 J·mol^{-1}
ΔS=4.74 J·mol^{-1}·K^{-1}
c,II′/c,I 37–216 K, ΔH=1836 J·mol^{-1}
ΔS=15.0 J·mol^{-1}·K^{-1}
c,II″/c,II′/c,II/c,I
c,I/liq 235.02 K, ΔH=5040 J·mol^{-1}
ΔS=21.43 J·mol^{-1}·K^{-1}
Molecular Weight 84.1356
Wiswesser Line Notation T5SJ
Evaluation A

C_4H_4Se (liq) 91DWO/SZW
Selenophene
Phase Changes
c,III/c,II 122.7 K, ΔH=304 J·mol^{-1}
ΔS=2.48 J·mol^{-1}·K^{-1}
c,II/c,I 192.8 K, ΔH=1106 J·mol^{-1}
ΔS=5.73 J·mol^{-1}·K^{-1}
c,I/liq 240.2 K, ΔH=4584 J·mol^{-1}
ΔS=19.1 J·mol^{-1}·K^{-1}
c,I3/c,I2 125.54 K, ΔH=702 J·mol^{-1}
ΔS=5.59 J·mol^{-1}·K^{-1}
Metastable phase.
c,I2/c,I1 155.4 K, ΔH=1003 J·mol^{-1}
ΔS=6.45 J·mol^{-1}·K^{-1}
Metastable phase.
Molecular Weight 131.0356
Wiswesser Line Notation T5-SE-J
Evaluation A

$C_4H_5ClHgN_3$ (c) 91ZAN/CHA
Ethylammonium dicyanochloromercurate (II)
Phase Changes
c,II/c,I 252 K, ΔH=2650 J·mol^{-1}
Molecular Weight 331.1466
Wiswesser Line Notation 2ZH .HG CN 2 G
Evaluation A

$C_4H_5ClO_2$ (c) 28SKA/SAX
cis-3-Chloro-2-butenoic acid; β-Chloroisocrotonic acid
Heat Capacity 298 K, C_p=140.2 J·mol^{-1}·K^{-1}
Temperature range 295 to 394 K. Equations only.
Phase Changes
c/liq 333.7 K, ΔH=13810 J·mol^{-1}
ΔS=41.1 J·mol^{-1}·K^{-1}
Molecular Weight 120.5353
Wiswesser Line Notation QV1UYG1 -C
Evaluation C

$C_4H_5ClO_2$ (c) 28SKA/SAX
trans-3-Chloro-2-butenoic acid; β-Chlorocrotonic acid
Heat Capacity 298 K, C_p=159.8 J·mol^{-1}·K^{-1}
Temperature range 295 to 394 K. Equations only.
Phase Changes
c/liq 366.8 K, ΔH=20710 J·mol^{-1}
ΔS=56.5 J·mol^{-1}·K^{-1}
Molecular Weight 120.5353
Wiswesser Line Notation QV1UYG1 -T
Evaluation C

$C_4H_5ClO_3$ (liq) 76MAS/PET
4-Chloromethyl-1,3-dioxolan-2-one
Heat Capacity 298 K, C_p=248 J·mol^{-1}·K^{-1}
Temperature range 200 to 320 K. Data graphically only. Value estimated from graph.
Molecular Weight 136.5347
Wiswesser Line Notation T5OVOTJ D1G
Evaluation D

$C_4H_5Cl_3O$ (liq) 1881REI
2,2,3-Trichlorobutanal; Butylchloral
Heat Capacity 298 K, C_p=241.8 J·mol^{-1}·K^{-1}
Temperature range 291 to 457 K.
Molecular Weight 175.4419
Wiswesser Line Notation VHXGGYG1
Evaluation D

$C_4H_5Cl_3O_2$ (liq) 1881REI
Ethyltrichloroacetate
Heat Capacity 298 K, C_p=230.1 J·mol^{-1}·K^{-1}
Temperature range 289 to 457 K.
Molecular Weight 191.4413
Wiswesser Line Notation GXGGVO2
Evaluation D

C_4H_5N (liq) 71HAL/BAL
Cyclopropyl cyanide; Cyanocyclopropane
Heat Capacity 297 K, C_p=115.4 J mol^{-1} K^{-1}
One temperature.
Molecular Weight 67.0902
Wiswesser Line Notation L3TJ ACN
Evaluation C

C_4H_5N (liq) 87MIR/SHA
2-Methylpropenenitrile; Methacrylonitrile
Heat Capacity 298.15 K, C_p=126.3 J·mol^{-1}·K^{-1}
Temperature range 253 to 353 K. Unsmoothed experimental datum given as 1.863 kJ/kg·K at 293 K. C_p(liq)=2.2117 +0.0056352T/K +1.52×10^{-5}T^2/K^2 kJ/kg·K (253 to 353 K). Note, second coefficient should be negative.
Molecular Weight 67.0902
Wiswesser Line Notation NCY1&U1
Evaluation C

C_4H_5N (liq) 67SCO/BER
Pyrrole
Heat Capacity 298.15 K, C_p=127.74 J·mol^{-1}·K^{-1}
Temperature range 11 to 365 K.
Entropy 298.15 K, S=156.44 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 249.74 K, ΔH=7907.8 J·mol^{-1}
ΔS=31.66 J·mol^{-1}·K^{-1}
Molecular Weight 67.0902
Wiswesser Line Notation T5MJ
Evaluation A

C_4H_5NO (liq) 79DZH/KAR
β-Cyanopropionaldehyde
Heat Capacity 300 K, C_p=195.9 J·mol^{-1}·K^{-1}
Temperature range 55 to 300 K.
Phase Changes
c,II/c,I 140 K
c,I/liq 230 K
Molecular Weight 83.0896
Wiswesser Line Notation VH2CN
Evaluation C

C_4H_5NO (liq) 81MUS/GAN
α-Cyanopropionaldehyde
Heat Capacity 300 K, C_p=169.5 J·mol^{-1}·K^{-1}
Temperature range 220 to 370 K. C_p given as 2040 J·kg^{-1}·deg^{-1}.
Molecular Weight 83.0896
Wiswesser Line Notation VHY1&CN
Evaluation C

$C_4H_5NO_2$ (c) 41SAT/SOG4
Succinimide
Heat Capacity 323 K, C_p=131.4 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 99.0890
Wiswesser Line Notation T6VMVTJ
Evaluation C
Same data in 40SAT/SOG5.

$C_4H_5NO_2$ (c) 89STE/C
Succinimide
Heat Capacity 298.15 K, C_p=123.88 J·mol^{-1}·K^{-1}
Temperature range 305 to 495 K. Csat/R(c)=0.0438T+1.87 (30
355 K); Csat/R(liq)=0.0265T+13.38 (405 to 495 K).
Phase Changes
c/liq 400 K, ΔH=17000 J·mol^{-1}
Molecular Weight 99.0890
Wiswesser Line Notation T6VMVTJ
Evaluation B

C_4H_5NS (liq) 36KUR/
Allyl isothiocyanate
Heat Capacity 290 K, C_p=156.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 99.1502
Wiswesser Line Notation *SCN2U1*
Evaluation D

C_4H_5NS (liq) 68GOU/
2-Methylthiazole
Heat Capacity 298.15 K, C_p=150.67 J·mol^{-1}·K^{-1}
Temperature range 5 to 340 K.
Entropy 298.15 K, S=211.88 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 248.42 K, ΔH=12163 J·mol^{-1}
ΔS=48.96 J·mol^{-1}·K^{-1}
c,II/liq 246.5 K, ΔH=11347 J·mol^{-1}
ΔS=46.03 J·mol^{-1}·K^{-1}
Metastable crystal form.
Molecular Weight 99.1502
Wiswesser Line Notation T5N CSJ B1
Evaluation A

C_4H_5NS (liq) 68GOU/V
2-Methylthiazole
Heat Capacity 298.15 K, C_p=150.67 J·mol^{-1}·K^{-1}
Temperature range 15 to 298 K.
Entropy 298.15 K, S=211.88 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 248.43 K, ΔH=12162.5 J·mol^{-1}
ΔS=48.96 J·mol^{-1}·K^{-1}
c,II/liq 246.53 K, ΔH=11349.9 J·mol^{-1}
ΔS=46.04 J·mol^{-1}·K^{-1}
Molecular Weight 99.1502
Wiswesser Line Notation T5N CSJ B1
Evaluation A

C_4H_5NS (liq) 69SOU/
2-Methylthiazole
Heat Capacity 298.15 K, C_p=150.7 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=211.9 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 248.43 K, ΔH=12159 J·mol^{-1}
ΔS=48.94 J·mol^{-1}·K^{-1}
c,II/liq 246.5 K, ΔH=11351 J·mol^{-1}
ΔS=46.05 J·mol^{-1}·K^{-1}
Metastable crystals.
Molecular Weight 99.1502
Wiswesser Line Notation T5N CSJ B1
Evaluation A

$C_4H_5N_3O$ (c) 78KIL3
Cytosine
Heat Capacity 298 K, C_p=132.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 111.1030
Wiswesser Line Notation T6MVNJ DZ
Evaluation B

C_4H_6 (liq) 45SCO/MEY
1,3-Butadiene
Heat Capacity 298.15 K, C_p=123.65 J·mol^{-1}·K^{-1}
Temperature range 15 to 303 K.
Entropy 298.15 K, S=199.00 J·mol^{-1}·K^{-1}
At vapor pressure of 2105 Torr.
Phase Changes
c/liq 164.24 K, ΔH=7983.9 J·mol^{-1}
ΔS=48.61 J·mol^{-1}·K^{-1}
liq/g 273.15 K, ΔH=81.41 J·mol^{-1}
ΔS=280.64 J·mol^{-1}·K^{-1}
P=119.95 kPa
Molecular Weight 54.0914
Wiswesser Line Notation 1U2U1
Evaluation A

C_4H_6 (liq) 47AST/SZA
1,2-Butadiene
Heat Capacity 290 K, C_p=122.80 J·mol^{-1}·K^{-1}
Temperature range 14 to 282 K.
Entropy 290 K, S=206.19 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 136.92 K, ΔH=6961.3 J·mol^{-1}
ΔS=50.84 J·mol^{-1}·K^{-1}
liq/g 273.24 K, ΔH=24623 J·mol^{-1}
ΔS=90.11 J·mol^{-1}·K^{-1}
P=66.41 kPa
Molecular Weight 54.0914
Wiswesser Line Notation 2UCU1
Evaluation A
Values of S and C_p for liquid for saturation vapor pressure.

C_4H_6 (liq) 40OSB/GAR
2-Butyne; Dimethylacetylene
Phase Changes
c/liq 240.93 K, ΔH=9232.8 J·mol^{-1}
ΔS=38.33 J·mol^{-1}·K^{-1}
liq/g 291.00 K, ΔH=26945 J·mol^{-1}
ΔS=92.59 J·mol^{-1}·K^{-1}
Molecular Weight 54.0914
Wiswesser Line Notation 2UU2
Evaluation A

C_4H_6 (liq) 41YOS/OSB
2-Butyne; Dimethylacetylene
Heat Capacity 290 K, C_p=124.14 J·mol^{-1}·K^{-1}
Temperature range 15 to 290 K.
Entropy 298.15 K, S=195.10 J·mol^{-1}·K^{-1}
Extrapolated from 291.0 K. Anomalous heat capacity between 145 and 160 K. ΔS obtained from total energy divided by average temperature.
Phase Changes
c/liq 240.92 K, ΔH=9234.9 J·mol^{-1}
ΔS=38.348 J·mol^{-1}·K^{-1}
liq/g 291.0 K, ΔH=26945 J·mol^{-1}
ΔS=92.59 J·mol^{-1}·K^{-1}
P=71.46 kPa
Molecular Weight 54.0914
Wiswesser Line Notation 2UU2
Evaluation A

C_4H_6 (liq) 50AST/MAS
1-Butyne
Heat Capacity 280 K, C_p=132.42 J·mol^{-1}·K^{-1}
Temperature range 13 to 280 K.
Entropy 281.23 K, S=197.48 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 147.43 K, ΔH=6029.1 J·mol^{-1}
ΔS=40.89 J·mol^{-1}·K^{-1}
liq/g 281.23 K, ΔH=24522 J·mol^{-1}
ΔS=87.20 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 54.0914
Wiswesser Line Notation 3UU1
Evaluation A

$(C_4H_6)_n$ (liq) 53FUR/MCC2
1,4-Polybutadiene, MS-1045
Heat Capacity 300 K, C_p=106.56 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Molecular Weight 54.0914
Wiswesser Line Notation /*2U2*/
Evaluation A
T(glass)=195 K.

$(C_4H_6)_n$ (liq) 53FUR/MCC2
1,4-Polybutadiene, GL-657
Heat Capacity 298.15 K, C_p=105.64 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=110.35 J·mol^{-1}·K^{-1}
Molecular Weight 54.0914
Wiswesser Line Notation /*2U2*/
Evaluation A
T(glass)=187 K.

$(C_4H_6)_n$ (liq) 62DAI/EVA5
cis-1,4-Polybutadiene
Heat Capacity 298.15 K, C_p=100.9 J·mol^{-1}·K^{-1}
Temperature range 20 to 310 K.
Entropy 298.15 K, S=115.6 J·mol^{-1}·K^{-1}
Phase Changes
c,I/gls 165 K
c,I/liq 262 K, ΔH=3953 J·mol^{-1}
ΔS=15.1 J·mol^{-1}·K^{-1}
Molecular Weight 54.0914
Wiswesser Line Notation /*2U2*/ -C
Evaluation B

$(C_4H_6)_n$ (liq) 86GRE/AYC
cis-1,4-Polybutadiene
Heat Capacity 298.2 K, C_p=105.7 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.2 K, S=126.68 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 171–172 K
Glass transition.
c,I/liq 284 K
Molecular Weight 54.0914
Wiswesser Line Notation /*2U2*/ -C
Evaluation A

$(C_4H_6)_n$ (c) 62DAI/EVA5
trans-1,4-Polybutadiene
Heat Capacity 298.15 K, C_p=130.8 J·mol^{-1}·K^{-1}
Temperature range 20 to 345 K.
Phase Changes
c,II/c,I 317 K, ΔH=3456 J·mol^{-1}
ΔS=10.8 J·mol^{-1}·K^{-1}
Solid-solid transition is a linear to helical crystal structure.
Molecular Weight 54.0914
Wiswesser Line Notation /*2U2*/ -T
Evaluation B

$(C_4H_6)_n$ (c) 86GRE/AYC
trans-1,4-Polybutadiene
Heat Capacity 298.2 K, C_p=87.59 J·mol^{-1}·K^{-1}
Temperature range 10 to 500 K.
Entropy 298.2 K, S=91.23 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 356 K, ΔH=7980 J·mol^{-1}
ΔS=21.9 J·mol^{-1}·K^{-1}
Fully ordered/conformationally disordered transition.
c,I/liq 437 K
Molecular Weight 54.0914
Wiswesser Line Notation /*2U2*/ -T
Evaluation A

$C_4H_6Cl_2O_2$ (liq) 1881REI
Ethyl dichloroacetate
Heat Capacity 298 K, C_p=209.6 J·mol^{-1}·K^{-1}
Temperature range 291 to 434 K.
Molecular Weight 156.9962
Wiswesser Line Notation GYGVO2
Evaluation D

$C_4H_6MgO_4$ (gls) 71ONO/KIM
Magnesium acetate
Heat Capacity 310.02 K, C_p=20.452 J·mol^{-1}·K^{-1}
Temperature range 310 to 500 K. Unsmoothed experimental datum.
Data also given for crystalline state from 348 to 501 K.
Molecular Weight 142.3942
Wiswesser Line Notation OV1 2 .MG
Evaluation B
T(glass)=470 K.

$C_4H_6MgO_4 \cdot 4H_2O$ (c) 84MEI/GRO
Magnesium diethanoate tetrahydrate; Magnesium diacetate tetrahydrate
Heat Capacity 298.15 K, C_p=321.0 J·mol^{-1}·K^{-1}
Temperature range 270 to 400 K.
Phase Changes
c/aq 336 K, ΔH=35800 J·mol^{-1}
ΔS=106.5 J·mol^{-1}·K^{-1}
Transition of tetrahydrate to less hydrated salt, presumably the monohydrate.
Molecular Weight 214.4548
Wiswesser Line Notation OV2 2 .MG &QH 4
Evaluation B

$C_4H_6N_2$ (c) 92JIM/ROU
2-Methylimidazole
Heat Capacity 298.15 K, C_p=105.09 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 82.1048
Wiswesser Line Notation T5N CMJ B1
Evaluation A

$C_4H_6N_2O$ (c) 73HAM/A
3-Amino-5-methylisoxazole
Heat Capacity 287.15 K, C_p=146.4 J·mol^{-1}·K^{-1}
One value.
Molecular Weight 98.1042
Wiswesser Line Notation T5NOJ C1 EZ
Evaluation C

$C_4H_6N_2O_2$ (c) 81LEB/I
2,5-Dioxopiperazine
Heat Capacity 298.15 K, C_p=133.9 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=145.6 J·mol^{-1}·K^{-1}
Molecular Weight 114.1036
Wiswesser Line Notation T6MV DMVTJ
Evaluation A

$C_4H_6N_2O_2$ (c) 82LEB/I
2,5-Dioxopiperazine
Heat Capacity 298.15 K, C_p=134.0 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=145.5 J·mol^{-1}·K^{-1}
Molecular Weight 114.1036
Wiswesser Line Notation T6MV DMVTJ
Evaluation A

$(C_4H_6N_2O_2)_n$ (c) 911
Poly-L-asparagine
Heat Capacity 300 K, C_p=139.0 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 114.1036
Wiswesser Line Notation /*V1YVZ&M*/ -L
Evaluation B

$(C_4H_6N_2O_2)_n$ (c) 93ROL/
Poly-L-asparagine
Heat Capacity 300 K, C_p=139.0 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 114.1036
Wiswesser Line Notation /*V1YVZ&M*/ -L
Evaluation B

$C_4H_6N_4O_3$ (c) 35STI/
Allantoin
Heat Capacity 296.6 K, C_p=179.95 J·mol^{-1}·K^{-1}
Temperature range 84 to 297 K. Value is unsmoothed experim datum.
Entropy 298.15 K, S=195.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 59.33 J·mol^{-1}·K^{-1}.
Molecular Weight 158.1164
Wiswesser Line Notation T5MVMV EHJ EMVZ
Evaluation B(C_p),C(S)

C_4H_6O (liq) 89STE/
2,3-Dihydrofuran
Heat Capacity 298.15 K, C_p=122.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 70.0908
Wiswesser Line Notation T5O BH CHJ
Evaluation B

C_4H_6O (liq) 84BAG/BAE
2-Butenal; Crotonaldehyde
Heat Capacity 298.35 K, C_p=148.6 J·mol^{-1}·K^{-1}
Temperature range 273 to 343 K. C_p(liq)=−0.23229+0.14081T −2.1×10^{-5}T^2 kJ/kg·K (273 to 343 K).
Molecular Weight 70.0908
Wiswesser Line Notation VH1U2
Evaluation B

$C_4H_6O \cdot 17H_2O$ (liq) 85HAN
2,5-Dihydrofuran clathrate hydrate
Heat Capacity 260 K, C_p=726 J·mol^{-1}·K^{-1}
Temperature range 95 to 260 K.
Phase Changes
c,I/liq 272.0 K, ΔH=92900 J·mol^{-1}
ΔS=341.5 J·mol^{-1}·K^{-1}
Molecular Weight 70.0908
Wiswesser Line Notation T5O BH EHJ &QH 17
Evaluation A
Actual composition is a mixed hydrate: 0.978 DHF−0.022 THF−17 H2O.

C_4H_6O (liq) 88BAG/GUR
2-Butenal; Crotonaldehyde
Heat Capacity 298.35 K, C_p=148.6 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 70.0908
Wiswesser Line Notation VH1U2
Evaluation B

$C_4H_6O_2$ (liq) 71HAL/BAL
Methyl propenoate; Methyl acrylate
Heat Capacity 297 K, C_p=133.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.0902
Wiswesser Line Notation 1U1VO1
Evaluation C

$C_4H_6O_2$ (liq) 79FUC
Methyl propenoate; Methyl acrylate
Heat Capacity 298.15 K, C_p=161.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.0902
Wiswesser Line Notation 1U1VO1
Evaluation B

$C_4H_6O_2$ (liq) 84VAS/PET
Methyl propenoate; Methyl acrylate
Heat Capacity 300 K, C_p=158.8 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, S=239.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 196.21 K
Molecular Weight 86.0902
Wiswesser Line Notation 1U1VO1
Evaluation A

$C_4H_6O_2$ (liq) 85KAR/ABD2
Methyl propenoate; Methyl acrylate
Phase Changes
c/liq 197.5 K, ΔH=9729 J·mol^{-1}
ΔS=49.26 J·mol^{-1}·K^{-1}
Molecular Weight 86.0902
Wiswesser Line Notation 1U1VO1
Evaluation A

$C_4H_6O_2$ (liq) 85KAR/SAI
Methyl propenoate; Methyl acrylate
Heat Capacity 298.15 K, C_p=172.3 J·mol^{-1}·K^{-1}
Temperature range 90 to 290 K. C_p(c)=285.21+5.32T J/kg·K (103 to 175 K; C_p(liq)=1568.62+1.45T (197.5 to 290 K). C_p data calculated from equation.
Phase Changes
c/liq 197.5 K
Molecular Weight 86.0902
Wiswesser Line Notation 1U1VO1
Evaluation B

$C_4H_6O_2$ (liq) 59BEN/THO
Ethenyl ethanoate; Vinyl acetate
Heat Capacity 298 K, C_p=169.5 J·mol^{-1}·K^{-1}
Mean value 23 to 50 °C.
Molecular Weight 86.0902
Wiswesser Line Notation 1VO1U1
Evaluation C

$(C_4H_6O_2)_n$ (gls) 80YEV/LEB
Poly-γ-butyrolactone
Heat Capacity 298.15 K, C_p=155.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 345 K. C_p is for the high-elastic state. C_p(c, 300 K)=117.9 J/mole·K.
Entropy 298.15 K, S=167.6 J·mol^{-1}·K^{-1}
S is for the high-elastic state. S(c, 300 K)=133.4 J/mole·K.
Phase Changes
c/liq 337.5 K, ΔH=13200 J·mol^{-1}
ΔS=39.4 J·mol^{-1}·K^{-1}
100% crystallinity.
Molecular Weight 86.0902
Wiswesser Line Notation /*MV32*/
Evaluation A

$C_4H_6O_2$ (liq) 79FUC
γ-Butyrolactone
Heat Capacity 298.15 K, C_p=141.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.0902
Wiswesser Line Notation T5OVTJ
Evaluation B

$C_4H_6O_2$ (liq) 80YEV/LEB
γ-Butyrolactone
Heat Capacity 298.15 K, C_p=141.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=197.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 229.78 K, ΔH=9570 J·mol^{-1}
ΔS=41.56 J·mol^{-1}·K^{-1}
Molecular Weight 86.0902
Wiswesser Line Notation T5OVTJ
Evaluation A

$C_4H_6O_2$ (liq) 83LEB/YEV
γ-Butyrolactone
Heat Capacity 298.15 K, C_p=141.3 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 340 K.
Entropy 298.15 K, S=197.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 229.78 K, ΔH=9570 J·mol^{-1}
ΔS=41.56 J·mol^{-1}·K^{-1}
Molecular Weight 86.0902
Wiswesser Line Notation T5OVTJ
Evaluation A

$C_4H_6O_2$ (liq) 88ISM/GAB
γ-Butyrolactone
Heat Capacity 298.15 K, C_p=140.9 J·mol^{-1}·K^{-1}
Temperature range 290 to 410 K. C_p(liq)=101.0829 +763.3375×10^{-4}T+1.918968×10^{-4}T^2 J/mol·K (290 to 410 K).
Entropy 298.15 K, S=201.28 J·mol^{-1}·K^{-1}
Molecular Weight 86.0902
Wiswesser Line Notation T5OVTJ
Evaluation B

$C_4H_6O_2$ (liq) 89STE/CHI3
γ-Butyrolactone
Heat Capacity 298.15 K, C_p=140.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.0902
Wiswesser Line Notation T5OVTJ
Evaluation B
C_p given as C_p/R=33.8, R=8.31441. This value appears to be in error by a factor of two.

$C_4H_6O_2$ (liq) 84VAS/PET
Methacrylic acid; α-Methyl acrylic acid
Heat Capacity 300 K, C_p=161.1 J·mol^{-1}·K^{-1}
Temperature range 25 to 300 K.
Entropy 300 K, S=186.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 289.36 K
Molecular Weight 86.0902
Wiswesser Line Notation QVY1&U1
Evaluation A

$C_4H_6O_2$ (liq) 85KAR/ABD
Methacrylic acid; α-Methyl acrylic acid
Heat Capacity 298.15 K, C_p=159.7 J·mol^{-1}·K^{-1}
Temperature range 287 to 350 K. Equation only. C_p (J·kg^{-1}·K^{-1})=−551.8+8.0712 T. C_p data calculated from equation.
Phase Changes
c/liq 287.5 K
Molecular Weight 86.0902
Wiswesser Line Notation QVY1&U1
Evaluation B

$C_4H_6O_2$ (liq) 85KAR/ABD2
Methacrylic acid; α-Methyl acrylic acid
Phase Changes
c/liq 287.5 K, ΔH=8062.5 J·mol^{-1}
ΔS=28.04 J·mol^{-1}·K^{-1}
Molecular Weight 86.0902
Wiswesser Line Notation QVY1&U1
Evaluation A

$C_4H_6O_2$ (liq) 85KAR/SAI
Methacrylic acid; α-Methyl acrylic acid
Heat Capacity 298.15 K, C_p=159.7 J·mol^{-1}·K^{-1}
Temperature range 90 to 350 K. C_p(c)=244.98+4.92T J/kg·K (95 to 287.5 K); C_p(liq)=−551.47+8.07T J/kg·K (287.5 to 350 K). C_p data calculated from equation.
Phase Changes
c/liq 287.5 K
Molecular Weight 86.0902
Wiswesser Line Notation QVY1&U1
Evaluation B

$(C_4H_6O_2)_n$ (c) 67PAV/R
Polymethacrylic acid
Heat Capacity 298 K, C_p=92.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 463 K. C_p=0.233+9.00×10^{-4}T cal·g·(20 to 130 °C). Value calculated from equation.
Molecular Weight 86.0902
Wiswesser Line Notation /*1X*1&VQ/
Evaluation B
T(glass)=433 K.

$C_4H_6O_3$ (liq) 39I
Ethanoic anhydride; Acetic anhydride
Heat Capacity 303.2 K, C_p=168.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.0896
Wiswesser Line Notation 1VOV1
Evaluation C

$C_4H_6O_3$ (liq) 58I
Propylene carbonate
Heat Capacity 323.15 K, C_p=184.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.0896
Wiswesser Line Notation T5OVOTJ D1
Evaluation C

$C_4H_6O_3$ (liq) 74VAS/K
Propylene carbonate; 4-Methyl-1,3-dioxolan-2-one
Heat Capacity 298.15 K, C_p=167.60 J·mol^{-1}·K^{-1}
Temperature range 80 to 310 K. C_p(c)=2.9899+91.0386(T/100) −35.8262(T/100)^2+7.2335(T/100)^3 J/mol·K (55 to 224.5 K).
Entropy 298.15 K, S=219.17 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 224.85 K, ΔH=9617 J·mol^{-1}
Molecular Weight 102.0896
Wiswesser Line Notation T5OVOTJ D1
Evaluation B

$C_4H_6O_3$ (liq) 76MAS/I
Propylene carbonate; 4-Methyl-1,3-dioxolan-2-one
Heat Capacity 298 K, C_p=175 J·mol^{-1}·K^{-1}
Temperature range 200 to 325 K. Data graphically only. V estimated from graph.
Molecular Weight 102.0896
Wiswesser Line Notation T5OVOTJ D1
Evaluation D

$C_4H_6O_3$ (liq) 76VAS/I
Propylene carbonate; 4-Methyl-1,3-dioxolan-2-one
Heat Capacity 298.15 K, C_p=167.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 415 K.
Entropy 298.15 K, S=218.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 224.85 K, ΔH=9617 J·mol^{-1}
ΔS=42.8 J·mol^{-1}·K^{-1}
Molecular Weight 102.0896
Wiswesser Line Notation T5OVOTJ D1
Evaluation B

$C_4H_6O_3$ (liq) 84VAS/PET

Propylene carbonate; 4-Methyl-1,3-dioxolan-2-one

Heat Capacity 298.15 K, C_p=167.4 J·mol^{-1}·K^{-1}

Temperature range 5 to 415 K.

Entropy 298.15 K, S=218.6 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 224.85 K, ΔH=9620 J·mol^{-1}

ΔS=42.8 J·mol^{-1}·K^{-1}

Molecular Weight 102.0896

Wiswesser Line Notation T5OVOTJ D1

Evaluation A

$C_4H_6O_4$ (c,I) 30PAR/HUF2

1,4-Butanedioic acid; Succinic acid

Heat Capacity 289.8 K, C_p=149.8 J·mol^{-1}·K^{-1}

Temperature range 93 to 290 K. Value is unsmoothed experimental datum.

Entropy 298.15 K, S=175.7 J·mol^{-1}·K^{-1}

Extrapolation below 90 K, 55.10 J·mol^{-1}·K^{-1}.

Phase Changes

c,II/c,I 272 K, ΔH=172 J·mol^{-1}

ΔS=0.63 J·mol^{-1}·K^{-1}

Molecular Weight 118.0890

Wiswesser Line Notation QV2VQ

Evaluation B(C_p),C(S)

$C_4H_6O_4$ (c) 39SAT/SOG

1,4-Butanedioic acid; Succinic acid

Heat Capacity 323 K, C_p=164.0 J·mol^{-1}·K^{-1}

Temperature range 0 to 100 °C. Mean value.

Molecular Weight 118.0890

Wiswesser Line Notation QV2VQ

Evaluation C

$C_4H_6O_4$ (c) 70VAN/WES2

1,4-Butanedioic acid; Succinic acid

Heat Capacity 298.15 K, C_p=152.93 J·mol^{-1}·K^{-1}

Temperature range 5 to 328 K.

Entropy 298.15 K, S=167.32 J·mol^{-1}·K^{-1}

Molecular Weight 118.0890

Wiswesser Line Notation QV2VQ

Evaluation A

$C_4H_6O_4$ (c) 74CIN/BER

1,4-Butanedioic acid; Succinic acid

Phase Changes

c/liq 457.0 K, ΔH=32945 J·mol^{-1}

ΔS=72.09 J·mol^{-1}·K^{-1}

Molecular Weight 118.0890

Wiswesser Line Notation QV2VQ

Evaluation B

$C_4H_6O_4$ (c) 88PET/TSY

1,4-Butanedioic acid; Succinic acid

Phase Changes

c,II/c,I 389.7 K

Molecular Weight 118.0890

Wiswesser Line Notation QV2VQ

Evaluation A

$C_4H_6O_4Zn$ (c) 84SPI/PRO

Zinc acetate

Heat Capacity 298 K, C_p=153.6 J·mol^{-1}·K^{-1}

Temperature range 243 to 293 K. Value calculated from equation: C_p(kJ·mol^{-1}·K^{-1})=3.44×10^{-2}+4×10^{-4}T(K).

Molecular Weight 183.4690

Wiswesser Line Notation OV1 2 .ZN

Evaluation C

$C_4H_6O_4Zn·2H_2O$ (c) 84SPI/PRO

Zinc acetate dihydrate

Heat Capacity 298 K, C_p=212.8 J·mol^{-1}·K^{-1}

Temperature range 243 to 293 K. Value calculated from equation: C_p(kJ·mol^{-1}·K^{-1})=3.40×10^{-2}+6×10^{-4}T(K).

Molecular Weight 219.4994

Wiswesser Line Notation OV1 2 .ZN &QH 2

Evaluation C

$C_4H_6O_5$ (c) 90CEO/SZW

Hydroxybutanedioic acid; Malic acid(DL)

Phase Changes

c,I/liq 402 K, ΔH=33522 J·mol^{-1}

Stable form I.

c,II/liq 396 K, ΔH=30170 J·mol^{-1}

Stable form II.

Molecular Weight 134.0884

Wiswesser Line Notation QVYQ1VQ

Evaluation B

$C_4H_6O_6$ (c) 39SAT/SOG

Tartaric acid

Heat Capacity 323 K, C_p=184.5 J·mol^{-1}·K^{-1}

Temperature range 0 to 100 °C. Mean value.

Molecular Weight 150.0878

Wiswesser Line Notation QVYQYQVQ

Evaluation C

C_4H_7ClO (liq) 1881REI

Butanoyl chloride; Butyryl chloride

Heat Capacity 298 K, C_p=170.7 J·mol^{-1}·K^{-1}

Temperature range 290 to 390 K.

Molecular Weight 106.5517

Wiswesser Line Notation GV3

Evaluation D

C_4H_7ClO (liq) 1881REI

2-Methylpropanoyl chloride; Isobutyryl chloride

Heat Capacity 298 K, C_p=131.8 J·mol^{-1}·K^{-1}

Temperature range 293 to 368 K.

Molecular Weight 106.5517

Wiswesser Line Notation GVY1&1

Evaluation D

$C_4H_7CsO_2$ (c) 75FER/SAN

Cesium butyrate

Phase Changes

c,II/c,I 344 K, ΔH=1460 J·mol^{-1}

ΔS=4.2 J·mol^{-1}·K^{-1}

c,III/c,II 263 K, ΔH=1260 J·mol^{-1}

ΔS=4.8 J·mol^{-1}·K^{-1}

c,I/liq 628 K, ΔH=13810 J·mol^{-1}

ΔS=22.0 J·mol^{-1}·K^{-1}

Molecular Weight 220.0035

Wiswesser Line Notation OV3 .CS

Evaluation C

$C_4H_7KO_2$ (c) 75FER/FRA
Potassium butyrate
Phase Changes
c,V/c,IV 461.4 K
c,IV/c,III 467.2 K, ΔH=1172 J·mol^{-1}
ΔS=2.51 J·mol^{-1}·K^{-1}
Combined values.
c,III/c,II 540.8 K
c,II/c,I 562.2 K, ΔH=4435 J·mol^{-1}
ΔS=8.03 J·mol^{-1}·K^{-1}
Combined values.
c,I/liq 626.1 K, ΔH=10837 J·mol^{-1}
ΔS=17.32 J·mol^{-1}·K^{-1}
Molecular Weight 126.1964
Wiswesser Line Notation OV3 .KA
Evaluation B
Clearing transition at 677.3 K, ΔH=4979 J/mole, ΔS=7.36 J/K·mol.

$C_4H_7KO_2$ (c) 75FER/SAN
Potassium butyrate
Phase Changes
c,VII/c,V 133 K, ΔH=670 J·mol^{-1}
ΔS=5.0 J·mol^{-1}·K^{-1}
Taken as sum of data for transitions at 123 K and 143 K at average temperature.
Molecular Weight 126.1964
Wiswesser Line Notation OV3 .KA
Evaluation C

$C_4H_7KO_2$ (c) 87FRA/NGE
Potassium butyrate
Heat Capacity 298.15 K, C_p=157.97 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S=211.52 J·mol^{-1}·K^{-1}
Phase Changes
c,VII/c,VI 123.85 K, ΔH=409 J·mol^{-1}
ΔS=3.33 J·mol^{-1}·K^{-1}
c,VI/c,VB 142.3 K, ΔH=269 J·mol^{-1}
ΔS=1.88 J·mol^{-1}·K^{-1}
Bifurcated transitions.
c,VB/c,VA
Diffuse anomaly in heat capacity curve.
c,V/c,IV 461.4 K
c,IV/c,III 467.2 K
c,III/c,II 541 K
c,II/c,I 562.2 K
Molecular Weight 126.1964
Wiswesser Line Notation OV3 .KA
Evaluation A
Liquid crystal-isotropic liquid transition at 677.3 K.

$C_4H_7KO_2$ (c) 84FRA/WES2
Potassium 2-methylpropanoate
Heat Capacity 298.15 K, C_p=166.95 J·mol^{-1}·K^{-1}
Temperature range 8 to 350 K.
Entropy 298.15 K, S=192.40 J·mol^{-1}·K^{-1}
Molecular Weight 126.1964
Wiswesser Line Notation OVY1&1 .KA
Evaluation A

$C_4H_7LiO_2$ (c) 85FRA/WES
Lithium butyrate
Heat Capacity 298.15 K, C_p=154.23 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=174.27 J·mol^{-1}·K^{-1}
Molecular Weight 94.0391
Wiswesser Line Notation OV3 .LI
Evaluation A
A gradual thermodynamic transformation occurs from 160 K.

$C_4H_7LiO_2$ (c) 86NGE/WES
Lithium butyrate
Heat Capacity 298.15 K, C_p=153.40 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=173.36 J·mol^{-1}·K^{-1}
Molecular Weight 94.0391
Wiswesser Line Notation OV3 .LI
Evaluation A

$C_4H_7LiO_2$ (c) 93NGE/ABE
Lithium 2-methylpropanoate
Heat Capacity 298.15 K, C_p=146.92 J·mol^{-1}·K^{-1}
Temperature range 7 to 535 K.
Entropy 298.15 K, S=159.06 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 445 K, ΔH=903 J·mol^{-1}
ΔS=2.03 J·mol^{-1}·K^{-1}
c,I/liq 510 K, ΔH=1045 J·mol^{-1}
ΔS=2.05 J·mol^{-1}·K^{-1}
Crystal to isotropic liquid.
Molecular Weight 94.0391
Wiswesser Line Notation OVY1&1 .LI
Evaluation A
Small diffuse hump in the C_p curve was observed from 125 to 250 K

C_4H_7N (liq) 02LOU
Butanenitrile; n-Propyl cyanide
Heat Capacity 340 K, C_p=159 J·mol^{-1}·K^{-1}
Mean value 21 to 113 °C.
Molecular Weight 69.1060
Wiswesser Line Notation NC3
Evaluation D

C_4H_7N (liq) 85GUS/MIR
Butanenitrile; n-Propyl cyanide
Heat Capacity 303.15 K, C_p=134.9 J·mol^{-1}·K^{-1}
Temperature range 303 to 383 K. p=0.1 MPa. Unsmoothed experimental datum given as 1.9520 kJ/kg·K.
Molecular Weight 69.1060
Wiswesser Line Notation NC3
Evaluation B

C_4H_7N (liq) 87MIR/SHA
Butanenitrile; n-Propyl cyanide
Heat Capacity 298.15 K, C_p=134.2 J·mol^{-1}·K^{-1}
Temperature range 173 to 373 K. Unsmoothed experimental datum given as 1.930 kJ/kg·K at 293 K. C_p (liq)=1.8787+0.0018882T/K +7.0408×10^{-6}T^2/K^2 kJ/kg·K (173 to 373 K). Note, second coefficient should be negative.
Molecular Weight 69.1060
Wiswesser Line Notation NC3
Evaluation D

C_4H_7N (liq) 91SVO/ZAB2
3-Methoxypropionitrile
Heat Capacity 300.60 K, C_p=180.6 J·mol^{-1}·K^{-1}
Temperature range 300 to 328 K. C_p(liq)=391.56−1.4014T +2.3268×10^{-3}T^2 J/K·mol (300 to 328 K).
Molecular Weight 69.1060
Wiswesser Line Notation NC2O1
Evaluation B

C_4H_7N (liq) 71HAL/BAL
2-Methylpropionitrile; 2-Cyanopropane; Isopropyl cyanide
Heat Capacity 297 K, C_p=156.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 69.1060
Wiswesser Line Notation NCY1&1
Evaluation C

C_4H_7NO (c) 59KOL/PAU
α-Pyrrolidone
Heat Capacity 290 K, C_p=135.6 J·mol^{-1}·K^{-1}
Temperature range 60 to 335 K.
Entropy 298.15 K, S=136.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 299.082 K, ΔH=13920 J·mol^{-1}
ΔS=46.5 J·mol^{-1}·K^{-1}
Molecular Weight 85.1033
Wiswesser Line Notation T5MVTJ
Evaluation B

C_4H_7NO (liq) 62KOL/PAU
α-Pyrrolidone; 2-Pyrrolidone
Heat Capacity 300.00 K, C_p=169.4 J·mol^{-1}·K^{-1}
Temperature range 60 to 350 K.
Entropy 310.00 K, S=189.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 299.082 K, ΔH=13920 J·mol^{-1}
ΔS=46.5 J·mol^{-1}·K^{-1}
Molecular Weight 85.1033
Wiswesser Line Notation T5MVTJ
Evaluation B

C_4H_7NO (liq) 89STE/CHI3
α-Pyrrolidone; 2-Pyrrolidone
Heat Capacity 300 K, C_p=169.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 85.1033
Wiswesser Line Notation T5MVTJ
Evaluation B

C_4H_7NO (c) 92STE/CHI
Methacrylamide
Heat Capacity 298.15 K, C_p=143.8 J·mol^{-1}·K^{-1}
Temperature range 290 to 385 K. C/R(c)=6.82+0.0352T (290 to 385 K). R=8.31451 J/K·mol.
Phase Changes
c/liq 385.1 K, ΔH=15000 J·mol^{-1}
Molecular Weight 85.1033
Wiswesser Line Notation ZVY1&1
Evaluation A

$C_4H_7NO_4$ (c) 32HUF/BOR
Aminosuccinic acid(L); Aspartic acid(L)
Heat Capacity 293.9 K, C_p=152.7 J·mol^{-1}·K^{-1}
Temperature range 88 to 293 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=173.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 51.09 J·mol^{-1}·K^{-1}.
Molecular Weight 133.1036
Wiswesser Line Notation QVYZ1VQ -L
Evaluation B(C_p),C(S)

$C_4H_7NO_4$ (c) 63HUT/COL2
Aminosuccinic acid(L); Aspartic acid(L)
Heat Capacity 298.15 K, C_p=155.18 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S=170.12 J·mol^{-1}·K^{-1}
Molecular Weight 133.1036
Wiswesser Line Notation QVYZ1VQ -L
Evaluation A

$C_4H_7N_3O$ (c) 32HUF/BOR
Creatinine
Heat Capacity 296.5 K, C_p=138.1 J·mol^{-1}·K^{-1}
Temperature range 87 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=167.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 55.98 J·mol^{-1}·K^{-1}.
Molecular Weight 113.1188
Wiswesser Line Notation T5NYMVTJ A1 BUM
Evaluation B(C_p),C(S)

$C_4H_7NaO_2$ (c) 75FER/FRA
Sodium butyrate
Phase Changes
c,V/c,IV 450.4 K, ΔH=1715 J·mol^{-1}
ΔS=3.81 J·mol^{-1}·K^{-1}
c,IV/c,III 489.8 K, ΔH=544 J·mol^{-1}
ΔS=1.13 J·mol^{-1}·K^{-1}
c,III/c,II 498.3 K, ΔH=753 J·mol^{-1}
ΔS=1.5 J·mol^{-1}·K^{-1}
c,II/c,I 508.4 K, ΔH=1841 J·mol^{-1}
ΔS=3.64 J·mol^{-1}·K^{-1}
c,I/liq 524.5 K, ΔH=10418 J·mol^{-1}
ΔS=19.87 J·mol^{-1}·K^{-1}
Molecular Weight 110.0879
Wiswesser Line Notation OV3 .NA
Evaluation B
Clearing transition at 600.4 K, ΔH=2218 J/mole, ΔS=3.68 J/K·mol.

$C_4H_7O_2Rb$ (c) 75FER/SAN
Rubidium butyrate
Phase Changes
c,IV/c,III 191 K, ΔH=2385 J·mol^{-1}
ΔS=12.5 J·mol^{-1}·K^{-1}
c,III/c,II 346 K, ΔH=1005 J·mol^{-1}
ΔS=2.9 J·mol^{-1}·K^{-1}
c,II/c,I 466 K, ΔH=2340 J·mol^{-1}
ΔS=5.0 J·mol^{-1}·K^{-1}
c,I/liq 652 K, ΔH=15730 J·mol^{-1}
ΔS=24.1 J·mol^{-1}·K^{-1}
Molecular Weight 172.5659
Wiswesser Line Notation OV3 .RB
Evaluation C

$C_4H_7O_2Tl$ (c) 76MEI/SEY
Thallium butyrate
Phase Changes
c/liq 459 K, $\Delta H = 6694\ J \cdot mol^{-1}$
$\Delta S = 14.2\ J \cdot mol^{-1} \cdot K^{-1}$
Solid-mesophase.
Molecular Weight 291.4681
Wiswesser Line Notation OV3 .TL
Evaluation B

$C_4H_7O_2Tl$ (c) 84FER/LOP
Thallium butyrate
Heat Capacity 320 K, $C_p = 175\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 320 to 480 K.
Phase Changes
c/liq 456.7 K, $\Delta H = 7691\ J \cdot mol^{-1}$
$\Delta S = 16.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 291.4681
Wiswesser Line Notation OV3 .TL
Evaluation A

C_4H_8 (liq) 36TOD/PAR
2-Methylpropene; Isobutene
Heat Capacity 253.1 K, $C_p = 121.42\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 93.3 to 253 K. Value is unsmoothed experimental datum.
Entropy 266.0 K, $S = 194\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, $45.23\ J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 132.4 K, $\Delta H = 5920\ J \cdot mol^{-1}$
$\Delta S = 44.71\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 56.1072
Wiswesser Line Notation 1Y1&U1
Evaluation $B(C_p)$,C(S)

C_4H_8 (liq) 71RAB/LEB
2-Methylpropene; Isobutene
Heat Capacity 266.26 K, $C_p = 121.3\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 266 K.
Phase Changes
c/liq 132.38 K
liq/g 266.26 K
Molecular Weight 56.1072
Wiswesser Line Notation 1Y1&U1
Evaluation B

C_4H_8 (liq) 36TOD/PAR
cis-2-Butene
Heat Capacity 266.6 K, $C_p = 118.87\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 93 to 267 K. Value is unsmoothed experimental datum.
Entropy 276.8 K, $S = 212.88\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, $48.95\ J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 133.8 K, $\Delta H = 7318\ J \cdot mol^{-1}$
$\Delta S = 54.69\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 56.1072
Wiswesser Line Notation 2U2 -C
Evaluation $B(C_p)$,C(S)

C_4H_8 (liq) 44SCO/FER
cis-2-Butene
Heat Capacity 298.15 K, $C_p = 126.15\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 15 to 300 K.
Entropy 298.15 K, $S = 219.91\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 134.26 K, $\Delta H = 7309.2\ J \cdot mol^{-1}$
$\Delta S = 54.44\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 56.1072
Wiswesser Line Notation 2U2 -C
Evaluation A

C_4H_8 (liq) 52SCH/SAC
cis-2-Butene
Heat Capacity 299.8 K, $C_p = 130.00\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 80 to 200 °F.
Molecular Weight 56.1072
Wiswesser Line Notation 2U2 -C
Evaluation B

C_4H_8 (liq) 83CHA/HAL
cis-2-Butene
Heat Capacity 298.15 K, $C_p = 127\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 367 K.
Entropy 298.15 K, $S = 220\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 134.26 K, $\Delta H = 7309\ J \cdot mol^{-1}$
$\Delta S = 54.4\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 56.1072
Wiswesser Line Notation 2U2 -C
Evaluation A
A reevaluation of the original measured data from: 36TOD/PAR 44SCO/FER, 52SCH/SAG.

C_4H_8 (liq) 36TOD/PAR
trans-2-Butene
Heat Capacity 259.6 K, $C_p = 122.05\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 93 to 260 K. Value is unsmoothed experimenta datum.
Entropy 274.1 K, $S = 204.97\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, $42.80\ J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 167.3 K, $\Delta H = 9861\ J \cdot mol^{-1}$
$\Delta S = 58.94\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 56.1072
Wiswesser Line Notation 2U2 -T
Evaluation $B(C_p)$,C(S)

C_4H_8 (liq) 45GUT/PI
trans-2-Butene
Heat Capacity 270280 K, $C_p = 122.34\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 15 to 274 K.
Entropy 274.04 K, $S = 205.31\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 167.61 K, $\Delta H = 9757\ J \cdot mol^{-1}$
$\Delta S = 58.21\ J \cdot mol^{-1} \cdot K^{-1}$
liq/g 274.04 K, $\Delta H = 22757\ J \cdot mol^{-1}$
$\Delta S = 83.04\ J \cdot mol^{-1} \cdot K^{-1}$
P = 101.325 kPa
Molecular Weight 56.1072
Wiswesser Line Notation 2U2 -T
Evaluation A

C_4H_8 (liq) 83CHA/HAL
trans-2-Butene
Heat Capacity 280 K, C_p=124.4 J·mol^{-1}·K^{-1}
Temperature range 14 to 271 K.
Entropy 280 K, S=163.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 167.62 K, ΔH=9757 J·mol^{-1}
ΔS=58.2 J·mol^{-1}·K^{-1}
Molecular Weight 56.1072
Wiswesser Line Notation 2U2 -T
Evaluation A
A reevaluation of the original measured data from: 36TOD/PAR, 45GUT/PIT.

$(C_4H_8)_n$ (gls) 64WIL/GRE
Poly(1-butene)
Heat Capacity
Temperature range 213 to 423 K. C_p data given graphically.
Phase Changes
c/liq 407.8 K, ΔH=7008 J·mol^{-1}
Rhombohedral form, 76.0% crystallinity.
c/liq 360 K, ΔH=6502 J·mol^{-1}
Rhombohedral atactic form, 13.0% crystallinity.
c/liq 394.6 K, ΔH=4075 J·mol^{-1}
Tetragonal form, 76.0% crystallinity.
c,II/c,I 394.6 K, ΔH=2933 J·mol^{-1}
Rhombohedral to tetragonal.
Molecular Weight 56.1072
Wiswesser Line Notation /*Y2&1*/
Evaluation C

C_4H_8 (liq) 36TOD/PAR
1-Butene
Heat Capacity 253.4 K, C_p=119.16 J·mol^{-1}·K^{-1}
Temperature range 81 to 253 K. Value is unsmoothed experimental datum.
Molecular Weight 56.1072
Wiswesser Line Notation 3U1
Evaluation B

C_4H_8 (liq) 46AST/FIN
1-Butene
Heat Capacity 260 K, C_p=119.45 J·mol^{-1}·K^{-1}
Temperature range 11.5 to 260 K.
Entropy 266.91 K, S=213.84 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 87.82 K, ΔH=3849 J·mol^{-1}
ΔS=43.83 J·mol^{-1}·K^{-1}
liq/g 266.91 K, ΔH=21866 J·mol^{-1}
ΔS=81.92 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 56.1072
Wiswesser Line Notation 3U1
Evaluation A

C_4H_8 (liq) 49SCH/SAG
1-Butene
Heat Capacity 294 K, C_p=128.6 J·mol^{-1}·K^{-1}
Temperature range 294 to 378 K. C_p given as 0.548 Btu(lb)$^{-1}$(°R)$^{-1}$ at 70 °F at bubble point.
Molecular Weight 56.1072
Wiswesser Line Notation 3U1
Evaluation B

C_4H_8 (liq) 83CHA/HAL
1-Butene
Heat Capacity 298.15 K, C_p=118 J·mol^{-1}·K^{-1}
Temperature range 12 to 360 K.
Entropy 298.15 K, S=227.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 87.82 K, ΔH=3848 J·mol^{-1}
ΔS=43.8 J·mol^{-1}·K^{-1}
Molecular Weight 56.1072
Wiswesser Line Notation 3U1
Evaluation A
A reevaluation of the original measured data from: 36TOD/PAR, 46AST/FIN, 49SCH/SAG.

C_4H_8 (liq) 91TAK/YAM
1-Butene
Heat Capacity 298.15 K, C_p=128.96 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=229.06 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 87.81 K, ΔH=3958.6 J·mol^{-1}
ΔS=45.09 J·mol^{-1}·K^{-1}
Molecular Weight 56.1072
Wiswesser Line Notation 3U1
Evaluation A
T(glass)=60 K.

C_4H_8 (liq) 53RAT/GWI
Cyclobutane
Heat Capacity 285 K, C_p=106.32 J·mol^{-1}·K^{-1}
Temperature range 15 to 285 K.
Entropy 285.66 K, S=175.15 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 145.7 K, ΔH=5707 J·mol^{-1}
ΔS=39.17 J·mol^{-1}·K^{-1}
Transition over about 120 to 145.7 K. Values represent excess over extrapolated C_p curves.
c,I/liq 182.42 K, ΔH=1088 J·mol^{-1}
ΔS=5.96 J·mol^{-1}·K^{-1}
liq/g 285.66 K, ΔH=24188 J·mol^{-1}
ΔS=84.67 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 56.1072
Wiswesser Line Notation L4TJ
Evaluation A

$(C_4H_8)_n$ (liq) 36FER/PAR
Polyisobutylene
Heat Capacity 294.9 K, C_p=109.4 J·mol^{-1}·K^{-1}
Temperature range 121 to 295 K. Annealed sample.
Molecular Weight 56.1072
Wiswesser Line Notation /*1X*1&1/
Evaluation D
T(glass)=197 K.

$(C_4H_8)_n$ (liq) 55FUR/REI
Polyisobutylene
Heat Capacity 300 K, C_p=109.7 J·mol^{-1}·K^{-1}
Temperature range 14 to 380 K. C_p(c)=0.844+3.03×10^{-3}T+2.24×10^{-6}T^2 J/deg·g (210 to 380 K).
Entropy 300 K, S=96.50 J·mol^{-1}·K^{-1}
Molecular Weight 56.1072
Wiswesser Line Notation /*1X*1&1/
Evaluation A
T(glass)=199 K.

$(C_4H_8)_n$ (liq) 56FUR/REI
Polyisobutylene
Heat Capacity 298.15 K, C_p=109.30 J·mol^{-1}·K^{-1}
Temperature range 14 to 380 K. C_p(liq)=0.844+3.03×10^{-3}T +2.24×10^{-6}T^2 J·g^{-1}deg^{-1} (210 to 380 K).
Entropy 298.15 K, S=95.83 J·mol^{-1}·K^{-1}
Molecular Weight 56.1072
Wiswesser Line Notation /*1X*1&1/
Evaluation A
T(glass)=199 K.

$(C_4H_8)_n$ (liq) 71RAB/LEB
Polyisobutylene
Heat Capacity 300 K, C_p=109.7 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Molecular Weight 56.1072
Wiswesser Line Notation /*1X*1&1/
Evaluation A

$(C_4H_8)_n$ (gls) 62DAI/EVA4
Poly(1-butene), isotactic
Heat Capacity 298.15 K, C_p=112.2 J·mol^{-1}·K^{-1}
Temperature range 20 to 310 K.
Entropy 298.15 K, S=103.0 J·mol^{-1}·K^{-1}
When extrapolated to 100% crystallinity, the entropy is 86.6 J·mol^{-1}·K^{-1}.
Phase Changes
c/gls 249 K
Molecular Weight 56.1072
Wiswesser Line Notation /*Y2&1*/
Evaluation A

$C_4H_8Br_2$ (liq) 93SHE
1,4-Dibromobutane
Heat Capacity 298.15 K, C_p=191.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 215.9152
Wiswesser Line Notation E4E
Evaluation B

$C_4H_8Cl_2$ (liq) 92HE/AN
1,2-Dichlorobutane
Heat Capacity 298.15 K, C_p=195.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 127.0132
Wiswesser Line Notation G1YG2
Evaluation B

$C_4H_8Cl_2$ (liq) 85LAI/WIL
1,4-Dichlorobutane
Heat Capacity 298.15 K, C_p=183.59 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 127.0132
Wiswesser Line Notation G4G
Evaluation A

$C_4H_8Cl_2$ (liq) 93HAL
1,4-Dichlorobutane
Heat Capacity 298.15 K, C_p=184.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 127.0132
Wiswesser Line Notation G4G
Evaluation B

$C_4H_8Cl_2O$ (liq) 48TSC
1,5-Dichloro-3-oxapentane; β,β′-Dichlorodiethylether
Heat Capacity 295 K, C_p=253 J·mol^{-1}·K^{-1}
One temperature. C_p is an average of 7 measurements.
Phase Changes
c/liq 226.5 K, ΔH=8385 J·mol^{-1}
Molecular Weight 143.0126
Wiswesser Line Notation G2O2G
Evaluation C

$C_4H_8Cl_2O$ (liq) 87KAL/KOH
1,5-Dichloro-3-oxapentane; β,β′-Dichlorodiethylether
Heat Capacity 293.15 K, C_p=207.81 J·mol^{-1}·K^{-1}
Temperature range 293.15, 313.15 K.
Molecular Weight 143.0126
Wiswesser Line Notation G2O2G
Evaluation B

$C_4H_8Cl_3O_4P$ (c) 89UTS/GAE
Dimethyl 2.2.2-trichloro-1-hydroxyethylphosphonate
Heat Capacity 298 K, C_p=261 J·mol^{-1}·K^{-1}
Temperature range 280 to 330 K. C_p=249+0.502T J·mol^{-1}·K^{-1} (T in °C).
Phase Changes
c,I/liq 350 K, ΔH=20300 J·mol^{-1}
Modification I.
c,II/liq 357 K, ΔH=22400 J·mol^{-1}
Modification II.
c,III/liq 369 K
Modification III.
c,IV/liq 384 K, ΔH=25000 J·mol^{-1}
Modification IV.
Molecular Weight 257.4376
Wiswesser Line Notation
Evaluation B

$C_4H_8N_2$ (liq) 93STE/CHI
1,4,5,6-Tetrahydropyrimidine
Heat Capacity 298.15 K, C_p=157.97 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1206
Wiswesser Line Notation T6NU CMTJ
Evaluation A

$C_4H_8N_2O_2$ (c) 41SAT/SOG
1,4-Butanediamide; Succinamide
Heat Capacity 323 K, C_p=174.0 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 116.1194
Wiswesser Line Notation ZV2VZ
Evaluation C
Same data in 40SAT/SOG5.

$C_4H_8N_2O_2$ (c) 88FER/DEI
N-Acetylglycine amide
Phase Changes
c/liq 408.2 K, ΔH=25600 J·mol^{-1}
ΔS=62.7 J·mol^{-1}·K^{-1}
Molecular Weight 116.1194
Wiswesser Line Notation ZV1MV1
Evaluation A

$C_4H_8N_2O_3$ (c) 41HUF
Glycylglycine
Heat Capacity 293.9 K, C_p=161.80 J·mol^{-1}·K^{-1}
Temperature range 87 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=190.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 56.90 J·mol^{-1}·K^{-1}.
Molecular Weight 132.1188
Wiswesser Line Notation Z1VM1VQ
Evaluation A(C_p),C(S)

$C_4H_8N_2O_3$ (c) 69HUT/COL2
Glycylglycine
Heat Capacity 298.15 K, C_p=163.97 J·mol^{-1}·K^{-1}
Temperature range 11 to 305 K.
Entropy 298.15 K, S=180.3 J·mol^{-1}·K^{-1}
Molecular Weight 132.1188
Wiswesser Line Notation Z1VM1VQ
Evaluation A

$C_4H_8N_2O_3$ (c) 89KUL/KOZ
Glycylglycine
Heat Capacity 298 K, C_p=149.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 132.1188
Wiswesser Line Notation Z1VM1VQ
Evaluation C

$C_4H_8N_2O_3$ (c) 90BAD/KUL
Glycylglycine
Heat Capacity 298 K, C_p=149 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 132.1188
Wiswesser Line Notation Z1VM1VQ
Evaluation D

$C_4H_8N_2O_3$ (c) 32HUF/BOR
Asparagine(L)
Heat Capacity 296.5 K, C_p=159.8 J·mol^{-1}·K^{-1}
Temperature range 85 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=174.5 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 49.79 J·mol^{-1}·K^{-1}.
Molecular Weight 132.1188
Wiswesser Line Notation ZV1YZVQ -L
Evaluation B(C_p),C(S)

$C_4H_8N_2O_3·H_2O$ (c) 32HUF/BOR
Asparagine hydrate(L)
Heat Capacity 296.7 K, C_p=205.9 J·mol^{-1}·K^{-1}
Temperature range 90 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=213.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 56.78 J·mol^{-1}·K^{-1}.
Molecular Weight 150.1340
Wiswesser Line Notation ZV1YZVQ &QH -L
Evaluation B(C_p),C(S)

$C_4H_8N_2O_3·H_2O$ (c) 63HUT/COL2
Asparagine hydrate(L)
Heat Capacity 298.15 K, C_p=207.90 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S=209.62 J·mol^{-1}·K^{-1}
Molecular Weight 150.1340
Wiswesser Line Notation ZV1YZVQ &QH -L
Evaluation A

$C_4H_8N_4O_4$ (c) 71HAL
1,3-Dinitro-1,3-diazacyclohexane
Phase Changes
c,II/c,I 346 K, ΔH=15481 J·mol^{-1}
c,I/liq 353 K, ΔH=2929 J·mol^{-1}
Molecular Weight 200.1536
Wiswesser Line Notation T6N CNTJ ANW CNW
Evaluation C

$C_4H_8N_8O_8$ (c,α) 70LIC
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(α); Octogen(α); HMX
Heat Capacity 298 K, C_p=307 J·mol^{-1}·K^{-1}
Temperature range 203 to 523 K. α-Phase. C_p=0.0991+5×10^{-4}T cal·K^{-1}·g^{-1} (−70 to 250 °C).
Phase Changes
c,II/c,I 193–201 K, ΔH=7398 J·mol^{-1}
α-δ Transition. Data also given for the following transitions: β-δ: T=167 to 183 °C; ΔH=9801 J·mol^{-1}. γ-δ; T=175 to 182 °C; ΔH=2788 J·mol^{-1}.
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation B
Data also given for the following polymorphic forms: β-HMX; C_p(298 K)=301 J·mol^{-1}·K^{-1}; C_p=0.0935+5×10^{-4}T cal·K^{-1}·g^{-1} (−70 to 250 °C); γ-HMX; C_p(298 K)=328 J·mol^{-1}·K^{-1}; C_p=0.1159+5×10^{-4}T cal·K^{-1}·g^{-1} (−70 to 250 °C); δ-HMX; C_p(298 K)=387 J·mol^{-1}·K^{-1}; C_p=0.1642+5×10^{-4}T cal·K^{-1}·g^{-1} (−70 to 250 °C).

$C_4H_8N_8O_8$ (c) 71HAL
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine; Octogen; HMX
Phase Changes
c,II/c,I 471 K, ΔH=7950 J·mol^{-1}
α to δ transition, approximation.
c,III/c,I 460 K, ΔH=9832 J·mol^{-1}
β to δ transition.
c,I/liq 551 K
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation C

$C_4H_8N_8O_8$ (c,α) 73KRI/LIC
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(α); Octogen(α); HMX
Heat Capacity 298 K, C_p=314.2 J·mol^{-1}·K^{-1}
Temperature range 200 to 465 K. Equation only.
Phase Changes
c,α/c,β 466–474 K, ΔH=7406 J·mol^{-1}
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation C

$C_4H_8N_8O_8$ (c,β) 73KRI/LIC
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(β); Octogen(β); HMX
Heat Capacity 298 K, C_p=307.9 J·mol^{-1}·K^{-1}
Temperature range 200 to 452 K. Equation only.
Phase Changes
c,β/c,δ 440–456 K, ΔH=9791 J·mol^{-1}
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation C

$C_4H_8N_8O_8$ (c,γ) 73KRI/LIC
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(γ); Octogen(γ); HMX
Heat Capacity 298 K, C_p=315.9 J·mol^{-1}·K^{-1}
Temperature range 200 to 440 K. Equation only.
Phase Changes
c,γ/c,δ 440–455 K, ΔH=2803 J·mol^{-1}
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation C

$C_4H_8N_8O_8$ (c,δ) 73KRI/LIC
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(δ);Octogen(δ); HMX
Heat Capacity 298 K, C_p=374.5 J·mol^{-1}·K^{-1}
Temperature range 200 to 530 K. Equation only.
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation C

$C_4H_8N_8O_8$ (c,β) 83KOS/SHO
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(β); Octogen(β); HMX
Heat Capacity 315 K, C_p=321.0 J·mol^{-1}·K^{-1}
Temperature range 294 to 486 K. β-phase, powdered blend. C_p given as 1.084 J·g^{-1}·K^{-1}.
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation B

$C_4H_8N_8O_8$ (c) 83KOS/SHO
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine; Octogen; HMX
Heat Capacity 298 K, C_p=293 J·mol^{-1}·K^{-1}
Temperature range 294 to 486 K. Graphical extrapolation of data to 298 K; powdered blend.
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation C

$C_4H_8N_8O_8$ (c,β) 83KOS/SHO
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(β); Octogen(β); HMX
Heat Capacity 298 K, C_p=297 J·mol^{-1}·K^{-1}
Temperature range 294 to 486 K. Graphical extrapolation of data to 298 K; single crystals, beta phase.
Phase Changes
c,II/c,I 453 K
(c,β/c,δ)
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation C

$C_4H_8N_8O_8$ (c) 91YIN/LIU
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine; Octogen; HMX
Heat Capacity 298 K, C_p=290.2 J mol^{-1} K^{-1}
Temperature range 290 to 345 K. C_p value reported at 298 K is 0.980 J/g· K.
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation B

$C_4H_8N_8O_8$ (c) 92MAK
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine; Octogen; HMX
Phase Changes
c/liq 553.15 K, ΔH=69873 J·mol^{-1}
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation B

C_4H_8O (liq) 88BAG/GUR
2-Methoxy-1-propene
Heat Capacity 301.50 K, C_p=162.2 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 72.1066
Wiswesser Line Notation 1YO1U1
Evaluation B

C_4H_8O (liq) 33KOL/UDC
Butanone; Methyl ethyl ketone
Heat Capacity 297.0 K, C_p=160.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation C

C_4H_8O (liq) 34KOL/UDO
Butanone; Methyl ethyl ketone
Heat Capacity 297.0 K, C_p=160.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation C

C_4H_8O (liq) 56PAR/KEN
Butanone; Methyl ethyl ketone
Heat Capacity 298.15 K, C_p=158.41 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.1 K, S=241.4 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 53.47 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 186.1 K, ΔH=8485 J·mol^{-1}
ΔS=45.59 J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation B(C_p),C(S)

C_4H_8O (liq) 64SIN/OE
Butanone; Methyl ethyl ketone
Heat Capacity 298.15 K, C_p=158.91 J·mol^{-1}·K^{-1}
Temperature range 13 to 308 K.
Entropy 298.15 K, S=238.82 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 186.48 K, ΔH=8438.7 J·mol^{-1}
ΔS=45.25 J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation A

C_4H_8O (liq) 67RAS/GA
Butanone; Methyl ethyl ketone
Heat Capacity 293 K, C_p=158.0 J·mol^{-1}·K^{-1}
Temperature range 293 to 353 K.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation C

C_4H_8O (liq) 68AND/COU
Butanone; Methyl ethyl ketone
Heat Capacity 298.15 K, C_p=158.7 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=239.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 186.47 K, ΔH=8385 J·mol^{-1}
ΔS=44.98 J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation A

C_4H_8O (liq) 75GRO/BEN
Butanone; Methyl ethyl ketone
Heat Capacity 298.15 K, C_p=159.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation B

C_4H_8O (liq) 78ROU/PER2
Butanone; Methyl ethyl ketone
Heat Capacity 298.1 K, C_p=158.4 J·mol^{-1}·K^{-1}
Temperature range 277 to 313 K.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation B

C_4H_8O (liq) 84GRO/BEN
Butanone; Methyl ethyl ketone
Heat Capacity 298.15 K, C_p=157.91 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation B

C_4H_8O (liq) 85COS/PAT
Butanone; Methyl ethyl ketone
Heat Capacity 298.15 K, C_p=158.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation B

C_4H_8O (liq) 85COS/PAT2
Butanone; Methyl ethyl ketone
Heat Capacity 298.15 K, C_p=158.4 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation B

C_4H_8O (liq) 86RED
Butanone; Methyl ethyl ketone
Heat Capacity 303.15 K, C_p=162.2 J·mol^{-1}·K^{-1}
Temperature range 303.15, 313.15 K.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation B

C_4H_8O (liq) 92MAL/WOO
Butanone; Methyl ethyl ketone
Heat Capacity 298.15 K, C_p=159 J·mol^{-1}·K^{-1}
Temperature range 278 to 338 K. p=0.1 MPa.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation B

C_4H_8O (liq) 76BON/CER
Tetrahydrofuran; Oxolane
Heat Capacity 298.15 K, C_p=120 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation T5OTJ
Evaluation B

C_4H_8O (liq) 76CON/GIN
Tetrahydrofuran; Oxolane
Heat Capacity 298 K, C_p=120.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation T5OTJ
Evaluation C

C_4H_8O (liq) 77LEB/LIT2
Tetrahydrofuran; Oxolane
Heat Capacity 298.15 K, C_p=123.9 J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K.
Entropy 298.15 K, S=203.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 164.76 K, ΔH=8540 J·mol^{-1}
ΔS=51.83 J·mol^{-1}·K^{-1}
liq/g 338.9 K
Molecular Weight 72.1066
Wiswesser Line Notation T5OTJ
Evaluation A

C_4H_8O (liq) 78LEB/RAB
Tetrahydrofuran; Oxolane
Heat Capacity 298.15 K, C_p=123.9 J·mol^{-1}·K^{-1}
Temperature range 8 to 322 K.
Entropy 298.15 K, S=203.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 164.76 K, ΔH=8540 J·mol^{-1}
ΔS=51.8 J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation T5OTJ
Evaluation A

C_4H_8O (liq) 79KIY/DAR
Tetrahydrofuran; Oxolane
Heat Capacity 298.15 K, C_p=123.56 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation T5OTJ
Evaluation B

C_4H_8O (liq) 79LEB/LIT
Tetrahydrofuran; Oxolane
Heat Capacity 298.15 K
C_p not given. Temperature range 8 to 322 K. Data deposited in VINITI, No. 1077-78. 30 March 1978.
Entropy 298.15 K, S=203.8 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 164.76 K, ΔH=8540 J·mol^{-1}
ΔS=51.83 J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation T5OTJ
Evaluation A

C_4H_8O (liq) 81ING/CAS
Tetrahydrofuran; Oxolane
Heat Capacity 298.15 K, C_p=122.92 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation T5OTJ
Evaluation B

C_4H_8O (liq) 85COS/PAT
Tetrahydrofuran; Oxolane
Heat Capacity 298.15 K, C_p=124.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation T5OTJ
Evaluation B

C_4H_8O (liq) 85COS/PAT2
Tetrahydrofuran; Oxolane
Heat Capacity 298.15 K, C_p=124.1 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 72.1066
Wiswesser Line Notation T5OTJ
Evaluation B

$C_4H_8O·17H_2O$ (c) 82LEA/MUR
Tetrahydrofuran clathrate hydrate
Heat Capacity
Temperature range 120 to 260 K. Data given graphically.
Phase Changes
c/liq 277.4 K, ΔH=98000 J·mol^{-1}
ΔS=353.2 J·mol^{-1}·K^{-1}
Molecular Weight 378.3650
Wiswesser Line Notation T5OTJ &QH 17
Evaluation A
Actual formula: $C_4H_8O·16.9H_2O$

$C_4H_8O·17H_2O$ (c) 84HAN/HAW
Tetrahydrofuran clathrate hydrate
Heat Capacity
Temperature range 85 to 270 K. C_p (85 to 270 K)=0.2562 +0.009446(T/K)−3.3092×10^{-5}(T/K)^2+8.3958×10^{-8}(T/K)^3 J/K·g.
Phase Changes
c/liq 277.3 K, ΔH=98999 J·mol^{-1}
Molecular Weight 378.3650
Wiswesser Line Notation T5OTJ &QH 17
Evaluation A
Actual formula: C4H8O·16.9H2O

$C_4H_8O·17H_2O$ (liq) 85HAN
Tetrahydrofuran clathrate hydrate
Heat Capacity
Temperature range 95 to 260 K.
Phase Changes
c/liq 277.3 K, ΔH=99100 J·mol^{-1}
ΔS=357.4 J·mol^{-1}·K^{-1}
Molecular Weight 378.3650
Wiswesser Line Notation T5OTJ &QH 17
Evaluation A
Actual formula: $C_4H_8O·17H_2O$.

$C_4H_8O·17H_2O$ (liq) 88YAM/OGU
Tetrahydrofuran clathrate hydrate
Heat Capacity 298.15 K, C_p=1523.2 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=1298.7 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 85 K
Glass transition.
c/liq 277.4 K, ΔH=96980 J·mol^{-1}
ΔS=349.6 J·mol^{-1}·K^{-1}
Molecular Weight 378.3650
Wiswesser Line Notation T5OTJ &QH 17
Evaluation A
Actual formula: $C_4H_8O·16.64H_2O$.

C_4H_8O (liq) 56PAR/KEN
Butanal; n-Butyraldehyde
Heat Capacity 298.15 K, C_p=163.51 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.1 K, S=246.9 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 43.93 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 176.8 K, ΔH=11104 J·mol^{-1}
ΔS=62.81 J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation VH3
Evaluation $B(C_p)$,C(S)

C_4H_8O (liq) 89VAS/LEI
Butanal; n-Butyraldehyde
Heat Capacity 298.15 K, C_p=164.7 J·mol^{-1}·K^{-1}
Temperature range 11 to 330 K.
Entropy 298.15 K, S=242.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 176.28 K, ΔH=10773 J·mol^{-1}
ΔS=61.11 J·mol^{-1}·K^{-1}
liq/liq 192.2 K, ΔH=76.9 J·mol^{-1}
ΔS=0.388 J·mol^{-1}·K^{-1}
Temperature range 180 to 210 K.
liq/liq 284.8 K, ΔH=63.4 J·mol^{-1}
ΔS=0.223 J·mol^{-1}·K^{-1}
Temperature range 260 to 280 K.
Molecular Weight 72.1066
Wiswesser Line Notation VH3
Evaluation A

$(C_4H_8O)_n$ (c) 77LEB/LIT
Polytetrahydrofuran
Phase Changes
c,II/c,I 186 K
Glass point.
c/liq 316 K, ΔH=11000 J·mol^{-1}
ΔS=34.8 J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation /*O4*/
Evaluation A

$(C_4H_8O)_n$ (c) 77LEB/LIT
Polytetrahydrofuran
Heat Capacity 200 K, C_p=81.30 J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K. Transition region at 298.15 K.
Entropy 200 K, S=83.06 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 316 K, ΔH=11000 J·mol^{-1}
ΔS=34.8 J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation /*O4*/
Evaluation A
T(glass)=186 K.

$C_4H_8O_2$ (liq) 33PAR/HU
Ethyl acetate; Ethyl ethanoate
Heat Capacity 293.6 K, C_p=169.20 J·mol^{-1}·K^{-1}
Temperature range 92 to 294 K. Value is unsmoothed experiment datum.
Entropy 298.1 K, S=259.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 62.80 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 189.3 K, ΔH=10481 J·mol^{-1}
ΔS=55.27 J·mol^{-1}·K^{-1}
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation B(C_p),C(S)

$C_4H_8O_2$ (liq) 36KUR/VOS
Ethyl acetate; Ethyl ethanoate
Heat Capacity 290 K, C_p=157.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation D

$C_4H_8O_2$ (liq) 45ZHD
Ethyl acetate; Ethyl ethanoate
Heat Capacity 303.61 K, C_p=168.82 J·mol^{-1}·K^{-1}
Temperature range 5 to 46 °C. Value is unsmoothed experimental datum.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation C

$C_4H_8O_2$ (liq) 78ROU/PER2
Ethyl acetate; Ethyl ethanoate
Heat Capacity 298.1 K, C_p=169.5 J·mol^{-1}·K^{-1}
Temperature range 283 to 313 K.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation B

$C_4H_8O_2$ (liq) 79FUC
Ethyl acetate; Ethyl ethanoate
Heat Capacity 298.15 K, C_p=167.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation B

$C_4H_8O_2$ (liq) 85BAL/BRA
Ethyl acetate; Ethyl ethanoate
Heat Capacity 298.15 K, C_p=169.06 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation B

$C_4H_8O_2$ (liq) 85COS/PAT
Ethyl acetate; Ethyl ethanoate
Heat Capacity 298.15 K, C_p=169.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation B

$C_4H_8O_2$ (liq) 85COS/PAT2
Ethyl acetate; Ethyl ethanoate
Heat Capacity 298.15 K, C_p=169.6 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation B

$C_4H_8O_2$ (liq) 86JIM/ROM
Ethyl acetate; Ethyl ethanoate
Heat Capacity 298.15 K, C_p=169.30 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation B

$C_4H_8O_2$ (liq) 87ZAB/HYN
Ethyl acetate; Ethyl ethanoate
Heat Capacity 298.32 K, C_p=170.59 J·mol^{-1}·K^{-1}
Temperature range 294 to 340 K. Unsmoothed experimental datum.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation B

$C_4H_8O_2$ (liq) 88PIN/BRA
Ethyl acetate; Ethyl ethanoate
Heat Capacity 298.15 K, C_p=168.94 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation B

$C_4H_8O_2$ (liq) 79FUC
Methyl propionate; Methyl propanoate
Heat Capacity 298.15 K, C_p=174.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2VO1
Evaluation B

$C_4H_8O_2$ (liq) 84GUS/SHU
Methyl propionate; Methyl propanoate
Heat Capacity 298.38 K, C_p=175.9 J·mol^{-1}·K^{-1}
Temperature range 205 to 348 K. Unsmoothed experimental datum.
Molecular Weight 88.1060
Wiswesser Line Notation 2VO1
Evaluation C

$C_4H_8O_2$ (liq) 85BAL/BRA
Methyl propionate; Methyl propanoate
Heat Capacity 298.15 K, C_p=171.20 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2VO1
Evaluation B

$C_4H_8O_2$ (liq) 86JIM/ROM
Methyl propionate; Methyl propanoate
Heat Capacity 298.15 K, C_p=172.74 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2VO1
Evaluation B

$C_4H_8O_2$ (liq) 87ZAB/HYN
Methyl propionate; Methyl propanoate
Heat Capacity 301.45 K, C_p=174.60 J·mol^{-1}·K^{-1}
Temperature range 296 to 342 K. Unsmoothed experimental datum.
Molecular Weight 88.1060
Wiswesser Line Notation 2VO1
Evaluation B

$C_4H_8O_2$ (liq) 88PIN/BRA
Methyl propionate; Methyl propanoate
Heat Capacity 298.15 K, C_p=171.21 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2VO1
Evaluation B

$C_4H_8O_2$ (liq) 85BAL/BRA
Propyl methanoate; Propyl formate
Heat Capacity 298.15 K, C_p=172.07 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 30VH
Evaluation B

$C_4H_8O_2$ (liq) 86JIM/ROM
Propyl methanoate; Propyl formate
Heat Capacity 298.15 K, C_p=171.42 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 3OVH
Evaluation B

$C_4H_8O_2$ (liq) 88PIN/BRA
Propyl methanoate; Propyl formate
Heat Capacity 298.15 K, C_p=172.10 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 3OVH
Evaluation B

$C_4H_8O_2$ (liq) 1881REI
Butanoic acid; n-Butyric acid
Heat Capacity 298 K, C_p=176.1 J·mol^{-1}·K^{-1}
Temperature range 292 to 448 K.
Molecular Weight 88.1060
Wiswesser Line Notation QV3
Evaluation D

$C_4H_8O_2$ (liq) 26PAR/AND
Butanoic acid; n-Butyric acid
Heat Capacity 290.7 K, C_p=176.1 J·mol^{-1}·K^{-1}
Temperature range 89 to 291292 to 448 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=255.2 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 82.42 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 267.4 K, ΔH=11071 J·mol^{-1}
ΔS=41.40 J·mol^{-1}·K^{-1}
Molecular Weight 88.1060
Wiswesser Line Notation QV3
Evaluation B(C_p),C(S)

$C_4H_8O_2$ (liq) 29PAR/KEL
Butanoic acid; n-Butyric acid
Entropy 298.1 K, S=226.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 53.6 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 88.1060
Wiswesser Line Notation QV3
Evaluation C

$C_4H_8O_2$ (liq) 71KON/WAD
Butanoic acid; n-Butyric acid
Heat Capacity 298.15 K, C_p=178 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation QV3
Evaluation B

$C_4H_8O_2$ (liq) 82MAR/ANL
Butanoic acid; n-Butyric acid
Heat Capacity 298.15 K, C_p=177.7 J·mol^{-1}·K^{-1}
Temperature range 13 to 450 K. Data also given by equation.
Entropy 298.15 K, S=225.3 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 155–230 K, ΔH=1040 J·mol^{-1}
ΔS=5.06 J·mol^{-1}·K^{-1}
c,I/liq 268.03 K, ΔH=11590 J·mol^{-1}
ΔS=43.24 J·mol^{-1}·K^{-1}
Molecular Weight 88.1060
Wiswesser Line Notation QV3
Evaluation A

$C_4H_8O_2$ (liq) 1881RE
Isobutyric acid; 2-Methylpropanoic acid
Heat Capacity 298 K, C_p=171.1 J·mol^{-1}·K^{-1}
Temperature range 291 to 448 K.
Molecular Weight 88.1060
Wiswesser Line Notation QVY1&1
Evaluation D

$C_4H_8O_2$ (liq) 71KON/WAI
Isobutyric acid; 2-Methylpropanoic acid
Heat Capacity 298.15 K, C_p=173 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation QVY1&1
Evaluation B

$C_4H_8O_2$ (liq) *82BIR/SII*
Isobutyric acid; 2-Methylpropanoic acid
Heat Capacity 298.15 K, C_p=181.7 J·mol^{-1}·K^{-1}
Temperature range 270 to 370 K. Equation only. C_p=130.1−0.0815 T+0.0008541 T^2 J·mol^{-1}·K^{-1}.
Molecular Weight 88.1060
Wiswesser Line Notation QVY1&1
Evaluation C

$C_4H_8O_2$ (liq) 76CON/GI
1,3-Dioxane
Heat Capacity 298 K, C_p=143.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O COTJ
Evaluation B

$C_4H_8O_2$·17H_2O (liq) 85HA
1,3-Dioxane clathrate hydrate
Heat Capacity 250 K, C_p=745 J·mol^{-1}·K^{-1}
Temperature range 95 to 250 K.
Phase Changes
c,I/liq 269.6 K, ΔH=89900 J·mol^{-1}
ΔS=333.5 J·mol^{-1}·K^{-1}
Molecular Weight 394.3644
Wiswesser Line Notation T6O COTJ &QH 17
Evaluation A
Actual formula: $C_4H_8O_2$·17H_2O.

$C_4H_8O_2$ (liq) 29HER/LC
1,4-Dioxane
Heat Capacity 296 K, C_p=154.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation C

$C_4H_8O_2$ (liq) 33ROT/MEY
1,4-Dioxane
Heat Capacity 291 K, C_p=146.0 J·mol^{-1}·K^{-1}
Temperature range 8 to 28 °C.
Phase Changes
c/liq 283.2 K, ΔH=11880 J·mol^{-1}
ΔS=41.9 J·mol^{-1}·K^{-1}
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation C

$C_4H_8O_2$ (liq) 34JAC/PAR
1,4-Dioxane
Heat Capacity 298.2 K, C_p=152.97 J·mol^{-1}·K^{-1}
Temperature range 92 to 299 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=196.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 11.12 cal·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 272.9 K, ΔH=2351 J·mol^{-1}
ΔS=8.6 J·mol^{-1}·K^{-1}
c,I/liq 284.1 K, ΔH=12845 J·mol^{-1}
ΔS=45.2 J·mol^{-1}·K^{-1}
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B(C_p),C(S)

$C_4H_8O_2$ (liq) 69SUB/KHA
1,4-Dioxane
Heat Capacity 298 K, C_p=147.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation C

$C_4H_8O_2$ (liq) 71DES/BHA
1,4-Dioxane
Heat Capacity 298 K, C_p=155.6 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 71HYD/SUB
1,4-Dioxane
Heat Capacity 298.15 K, C_p=147.9 J·mol^{-1}·K^{-1}
Temperature range 298, 313 K.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 76BON/CER
1,4-Dioxane
Heat Capacity 298.15 K, C_p=149 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 76CON/GIN
1,4-Dioxane
Heat Capacity 298 K, C_p=140.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 79MUR/SUB
1,4-Dioxane
Heat Capacity 298 K, C_p=149.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 81ING/CAS
1,4-Dioxane
Heat Capacity 298.15 K, C_p=149.73 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 84GRO/ING
1,4-Dioxane
Heat Capacity 298.15 K, C_p=150.65 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 84ING/GRO
1,4-Dioxane
Heat Capacity 298.15 K, C_p=150.77 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 89BAR/KOO2
1,4-Dioxane
Heat Capacity 298.15 K, C_p=149.489 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 91TRE/COS
1,4-Dioxane
Heat Capacity 298.15 K, C_p=150.57 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 93GRO/ROU
1,4-Dioxane
Heat Capacity 298.15 K, C_p=149.65 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$(C_4H_8O_2S)_n$ (c) 62DAI/EVA6
1-Butene polysulphone
Heat Capacity 298.15 K, C_p=155.64 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Molecular Weight 120.1660
Wiswesser Line Notation
Evaluation A

$C_4H_8O_3$ (liq) *83SAN/CIO*
Ethylene glycol monoacetate
Heat Capacity 298.15 K, C_p=203 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K. $C_p°$(kJ·kg^{-1}·K^{-1}) =0.042568T−10.686
Molecular Weight 101.0817
Wiswesser Line Notation Q2OV1
Evaluation D

$C_4H_8O_4$ (c) 69CLE/MEL
Tetroxan
Heat Capacity 298.15 K, C_p=142.22 J·mol^{-1}·K^{-1}
Temperature range 80 TO 420 K.
Entropy 298.15 K, S=167.5 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 50.3 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 385 K, ΔH=22600 J·mol^{-1}
ΔS=58.7 J·mol^{-1}·K^{-1}
Molecular Weight 120.1048
Wiswesser Line Notation T8O CO EO GOTJ
Evaluation B(C_p),C(S)

C_4H_8S (liq) 52HUB/FIN
Thiacyclopentane
Heat Capacity 298.15 K, C_p=140.16 J·mol^{-1}·K^{-1}
Temperature range 13 to 333 K.
Entropy 298.15 K, S=207.82 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 176.98 K, ΔH=7352.1 J·mol^{-1}
ΔS=41.54 J·mol^{-1}·K^{-1}
Molecular Weight *88.1672*
Wiswesser Line Notation T5STJ
Evaluation A

$C_4H_8S_2$ (c) 83DEW/OFF
1,3-Dithiane
Heat Capacity 300 K, C_p=113.9 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c,II/c,I 316.4 K, ΔH=800 J·mol^{-1}
ΔS=2.5 J·mol^{-1}·K^{-1}
c,I/liq 327.2 K, ΔH=14400 J·mol^{-1}
ΔS=44.0 J·mol^{-1}·K^{-1}
Molecular Weight 120.2272
Wiswesser Line Notation T6S CSTJ
Evaluation B

$C_4H_8S_2$ (c) 83DEW/OFF
1,4-Dithiane
Heat Capacity 300 K. C_p=129.8 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c/liq 384.6 K, ΔH=21600 J·mol^{-1}
ΔS=56.2 J·mol^{-1}·K^{-1}
Molecular Weight 120.2272
Wiswesser Line Notation T6S DSTJ
Evaluation B

C_4H_9Br (liq) 48KUR
1-Bromo-2-methylpropane; Isobutyl bromide
Heat Capacity 298 K. C_p=154.4 J·mol^{-1}·K^{-1}
Temperature range 11 to 80°C, mean C_p, two temperatures.
Molecular Weight 137.0191
Wiswesser Line Notation E1Y1&1
Evaluation D

C_4H_9Br (liq) *93SHE*
1-Bromo-2-methylpropane; Isobutyl bromide
Heat Capacity 298.15 K, C_p=163.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 137.0191
Wiswesser Line Notation E1Y1&1
Evaluation B

C_4H_9Br (liq) 31DEI
1-Bromobutane; n-Butyl bromide
Heat Capacity 292.3 K, C_p=152.21 J·mol^{-1}·K^{-1}
Temperature range 94 to 293 K. Value is unsmoothed experimenta datum.
Entropy 298.15 K, S=327.02 J·mol^{-1}·K^{-1}
Extrapolation below 100 K, 42.84 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 160.4 K, ΔH=9234 J·mol^{-1}
ΔS=57.57 J·mol^{-1}·K^{-1}
Molecular Weight 137.0191
Wiswesser Line Notation E4
Evaluation B(C_p),C(S)

C_4H_9Br (liq) 48KUI
1-Bromobutane; n-Butyl bromide
Heat Capacity 298 K, C_p=151.0 J·mol^{-1}·K^{-1}
Temperature range 13 to 100°C, mean C_p, two temperatures.
Molecular Weight 137.0191
Wiswesser Line Notation E4
Evaluation D

C_4H_9Br (liq) 93SHI
1-Bromobutane; n-Butyl bromide
Heat Capacity 298.15 K, C_p=162.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 137.0191
Wiswesser Line Notation E4
Evaluation B

C_4H_9Br (liq) 50KUS/CR(
2-Bromo-2-methylpropane; tert-Butyl bromide
Heat Capacity 265.1 K, C_p=151.0 J·mol^{-1}·K^{-1}
Temperature range 117 to 265 K. Value is unsmoothed experimenta datum.
Phase Changes
c,III/c,II 208.6 K, ΔH=5650 J·mol^{-1}
ΔS=27.1 J·mol^{-1}·K^{-1}
c,II/c,I 231.5 K, ΔH=1045 J·mol^{-1}
ΔS=4.5 J·mol^{-1}·K^{-1}
c,I/liq 256.1 K, ΔH=1965 J·mol^{-1}
ΔS=7.7 J·mol^{-1}·K^{-1}
Molecular Weight 137.0191
Wiswesser Line Notation EX1&1&1
Evaluation B

C_4H_9Br (liq) 93SH
2-Bromo-2-methylpropane; tert-Butyl bromide
Heat Capacity 298.15 K, C_p=165.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 137.0191
Wiswesser Line Notation EX1&1&1
Evaluation B

C_4H_9Cl (liq) 48KUR
1-Chloro-2-methylpropane; Isobutyl chloride
Heat Capacity 298 K, C_p=158.6 J·mol^{-1}·K^{-1}
Temperature range 14 to 59°C, mean C_p, two temperatures.
Molecular Weight 92.5861
Wiswesser Line Notation G1Y1&1
Evaluation D

C_4H_9Cl (liq) 85LAI/WIL
1-Chlorobutane; n-Butyl chloride
Heat Capacity 298.15 K, C_p=159.64 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.5681
Wiswesser Line Notation G4
Evaluation A

C_4H_9Cl (liq) 93GRO/ROU
1-Chlorobutane; n-Butyl chloride
Heat Capacity 298.15 K, C_p=159.53 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.5681
Wiswesser Line Notation G4
Evaluation B

C_4H_9Cl (liq) 93SHE
1-Chlorobutane; n-Butyl chloride
Heat Capacity 298.15 K, C_p=158.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.5681
Wiswesser Line Notation G4
Evaluation B

C_4H_9Cl (liq) 92HE/AN
2-Chlorobutane; sec-Butyl chloride
Heat Capacity 298.15 K, C_p=174.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.5681
Wiswesser Line Notation GY2&1
Evaluation B

C_4H_9Cl (liq) 50KUS/CRO
2-Chloro-2-methylpropane; tert-Butyl chloride
Heat Capacity 259.6 K, C_p=152.7 J·mol^{-1}·K^{-1}
Temperature range 122 to 260 K. Value is unsmoothed experimental datum.
Phase Changes

c,III/c,II	183.1 K,	ΔH=1715 J·mol^{-1}
		ΔS=9.4 J·mol^{-1}·K^{-1}
c,II/c,I	219.6 K,	ΔH=5815 J·mol^{-1}
		ΔS=26.5 J·mol^{-1}·K^{-1}
c,I/liq	248.1 K,	ΔH=2010 J·mol^{-1}
		ΔS=8.1 J·mol^{-1}·K^{-1}

Molecular Weight 92.5681
Wiswesser Line Notation GX1&1&1
Evaluation B

C_4H_9Cl (liq) 66DWO/GUI
2-Chloro-2-methylpropane; tert-Butyl chloride
Heat Capacity 272.73 K, C_p=172.80 J·mol^{-1}·K^{-1}
Temperature range 82 to 273 K. Value is unsmoothed experimental datum.
Phase Changes

c,III/c,II	182.91 K,	ΔH=1874 J·mol^{-1}
		ΔS=10.25 J·mol^{-1}·K^{-1}
c,II/c,I	219.25 K,	ΔH=5883 J·mol^{-1}
		ΔS=26.83 J·mol^{-1}·K^{-1}
c,I/liq	247.53 K,	ΔH=2071 J·mol^{-1}
		ΔS=8.37 J·mol^{-1}·K^{-1}

Molecular Weight 92.5681
Wiswesser Line Notation GX1&1&1
Evaluation A

C_4H_9Cl (liq) 93SHE
2-Chloro-2-methylpropane; tert-Butyl chloride
Heat Capacity 298.15 K, C_p=162.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.5681
Wiswesser Line Notation GX1&1&1
Evaluation B

C_4H_9Cl (liq) 93SHE
2-Chlorobutane; sec-Butyl chloride
Heat Capacity 298.15 K, C_p=160.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.5681
Wiswesser Line Notation GY2&1
Evaluation B

C_4H_9I (liq) 1881REI
1-Iodo-2-methylpropane; Isobutyl iodide
Heat Capacity 298 K, C_p=162.3 J·mol^{-1}·K^{-1}
Temperature range 290 to 417 K
Molecular Weight 184.0196
Wiswesser Line Notation I1Y1&1
Evaluation D

C_4H_9I (liq) 93SHE
1-Iodo-2-methylpropane; Isobutyl iodide
Heat Capacity 298.15 K, C_p=165.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 184.0196
Wiswesser Line Notation I1Y1&1
Evaluation B

C_4H_9I (liq) 93SHE
1-Iodobutane; n-Butyl iodide
Heat Capacity 298.15 K, C_p=164.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 184.0196
Wiswesser Line Notation I4
Evaluation B

C_4H_9I (liq) 93SHE
2-Iodobutane; sec-Butyl iodide
Heat Capacity 298.15 K, C_p=165.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 184.0196
Wiswesser Line Notation IY2&1
Evaluation B

C_4H_9N (liq) 59HIL/SIN
Pyrrolidine
Heat Capacity 298.15 K, C_p=156.57 J·mol^{-1}·K^{-1}
Temperature range 14 to 312 K.
Entropy 298.15 K, S=204.10 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 207.14 K, ΔH=531 J·mol^{-1}
ΔS=2.56 J·mol^{-1}·K^{-1}
c,I/liq 215.31 K, ΔH=8590 J·mol^{-1}
ΔS=39.90 J·mol^{-1}·K^{-1}
Molecular Weight 71.1218
Wiswesser Line Notation T5MTJ
Evaluation A

C_4H_9N (liq) 59MCC/DOU
Pyrrolidine
Heat Capacity 298.15 K, C_p=156.57 J·mol^{-1}·K^{-1}
Temperature range 13 to 350 K.
Entropy 298.15 K, S=204.01 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 207.14 K, ΔH=540.1 J·mol^{-1}
ΔS=2.61 J·mol^{-1}·K^{-1}
c,I/liq 215.31 K, ΔH=8577 J·mol^{-1}
ΔS=39.84 J·mol^{-1}·K^{-1}
Molecular Weight 71.1218
Wiswesser Line Notation T5MTJ
Evaluation A

C_4H_9N (liq) 76CON/GIN
Pyrrolidine
Heat Capacity 298 K, C_p=160.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 71.1218
Wiswesser Line Notation T5MTJ
Evaluation B

C_4H_9NO (liq) 78DEV/HEU
N,N-Dimethylacetamide
Heat Capacity 298.15 K, C_p=178.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 87.1212
Wiswesser Line Notation 1VN1&1
Evaluation B

C_4H_9NO (liq) 71KON/WAD
N-Ethylethanamide; N-Ethylacetamide
Heat Capacity 298.15 K, C_p=180 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 87.1212
Wiswesser Line Notation 2MV1
Evaluation B

C_4H_9NO (liq) 86ZEG/BOE
N-Ethylethanamide; N-Ethylacetamide
Heat Capacity 298.15 K, C_p=180.28 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 87.1212
Wiswesser Line Notation 2MV1
Evaluation B

C_4H_9NO (liq) 71KON/WAD
N-Methylpropanamide
Heat Capacity 298.15 K, C_p=179 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 87.1212
Wiswesser Line Notation 2VM1
Evaluation B

C_4H_9NO (liq) 02LOU
Methyl ethyl ketoxime
Heat Capacity 350 K, C_p=238 J·mol^{-1}·K^{-1}
Mean value 21 to 151 °C.
Molecular Weight 87.1212
Wiswesser Line Notation QNUY1&1
Evaluation D

C_4H_9NO (liq) 42TRI/ENG
Morpholine; Tetrahydro-1,4-isoxazine; Diethyleneimide oxide
Heat Capacity 298 K, C_p=173.89 J·mol^{-1}·K^{-1}
Temperature range 273 to 403 K.
Molecular Weight 87.1212
Wiswesser Line Notation T6M DOTJ
Evaluation C

C_4H_9NO (c) 80LYA
Morpholine; Tetrahydro-1,4-isoxazine; Diethyleneimide oxide
Heat Capacity 298.15 K, C_p=164.8 J·mol^{-1}·K^{-1}
Temperature range 293 to 353 K. Data given graphically. C_p value calculated from equation: C_p(J·g^{-1}·K^{-1})=1.785+0.00427 T(°C).
Molecular Weight 87.1212
Wiswesser Line Notation T6M DOTJ
Evaluation C

C_4H_9NO (c) 89ABB/JIN
2-Methylpropanamide
Heat Capacity 298.15 K, C_p=148.1 J·mol^{-1}·K^{-1}
One temperature; C_p given as 1.70 J·g^{-1}·K^{-1}.
Phase Changes
c/g 298.15 K, ΔH=86000 J·mol^{-1}
ΔS=288.4 J·mol^{-1}·K^{-1}
Molecular Weight 87.1212
Wiswesser Line Notation ZVY1&1
Evaluation A

$C_4H_9NO_2$ (c) 83SKO/SAI
γ-Aminobutyric acid; 4-Aminobutanoic acid
Heat Capacity 298 K, C_p=133.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 103.1206
Wiswesser Line Notation Z3VQ
Evaluation B

$C_4H_9NO_2$ (c) 41SAT/SOG
α-Aminobutyric acid; 2-Aminobutanoic acid
Heat Capacity 323 K, C_p=160.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 103.1206
Wiswesser Line Notation ZY2&QV
Evaluation C
Same data as 40SAT/SOG4.

$C_4H_9NO_2$ (c) 75SPI/WAD
α-Aminobutyric acid(DL); 2-Aminobutanoic acid(DL)
Heat Capacity 298.15 K, C_p=146.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 103.1206
Wiswesser Line Notation ZY2&QV -DI
Evaluation B

$C_4H_9NO_2$ (c) 84GRU/BOU
α-Aminobutyric acid (L); 2-Aminobutanoic acid (L)
Phase Changes
c,II/c,I 356 K, ΔH=530 J·mol^{-1}
ΔS=1.49 J·mol^{-1}·K^{-1}
Molecular Weight 103.1206
Wiswesser Line Notation ZY2&QV -L
Evaluation B

$C_4H_9NO_3$ (c) 70MUR/BRE
2-Methyl-2-nitro-1-propanol
Phase Changes
c,II/c,I 310 K, ΔH=17195 J·mol^{-1}
ΔS=55.6 J·mol^{-1}·K^{-1}
c,I/liq 361 K, ΔH=3738 J·mol^{-1}
ΔS=10.5 J·mol^{-1}·K^{-1}
Molecular Weight 119.1200
Wiswesser Line Notation WNX1&1&1Q
Evaluation A

$C_4H_9NO_4$ (c) 39SAT/SOG
Ammonium acid succinate
Heat Capacity 323 K, C_p=203.8 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 135.1194
Wiswesser Line Notation QV2VQ &ZH
Evaluation C

$C_4H_9NO_4$ (c) 70MUR/BRE
2-Methyl-2-nitro-1,3-propanediol
Phase Changes
c,II/c,I 352 K, ΔH=25723 J·mol^{-1}
ΔS=73.22 J·mol^{-1}·K^{-1}
c,I/liq 424 K, ΔH=3844 J·mol^{-1}
ΔS=9.2 J·mol^{-1}·K^{-1}
Molecular Weight 135.1194
Wiswesser Line Notation WNX1&1Q1Q
Evaluation A

$C_4H_9NO_5$ (c) 70MUR/BRE
2-Hydroxymethyl-2-nitro-1,3-propanediol
Phase Changes
c,II/c,I 354 K, ΔH=22446 J·mol^{-1}
ΔS=63.6 J·mol^{-1}·K^{-1}
457 K
Decomposition.
Molecular Weight 151.1188
Wiswesser Line Notation WNX1Q1Q1Q
Evaluation A

$C_4H_9NO_6$ (c) 39SAT/SOG
Ammonium acid tartrate
Heat Capacity 323 K, C_p=226.8 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 167.1182
Wiswesser Line Notation QVYQYQVQ &ZH
Evaluation C

$C_4H_9N_3O_2$ (c) 32HUF/BOR
Creatine
Heat Capacity 296.3 K, C_p=171.1 J·mol^{-1}·K^{-1}
Temperature range 87 to 295 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=189.5 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 55.69 J·mol^{-1}·K^{-1}.
Molecular Weight 131.1340
Wiswesser Line Notation QV1N1&YZUM
Evaluation B(C_p),C(S)

$C_4H_9N_3O_2$ (c) 41SAT/SOG3
Creatine
Heat Capacity 323 K, C_p=184.5 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 131.1340
Wiswesser Line Notation QV1N1&YZUM
Evaluation C
Same data as 40SAT/SOG4.

$C_4H_9N_3O_2 \cdot H_2O$ (c) 40HUF/FOX
Creatine hydrate
Heat Capacity 298.4 K, C_p=213.59 J·mol^{-1}·K^{-1}
Temperature range 90 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=234.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 68.58 J·mol^{-1}·K^{-1}.
Molecular Weight 149.1492
Wiswesser Line Notation QV1N1&YZUM &QH
Evaluation B(C_p),C(S)

C_4H_{10} (liq) 37PAR/SHO
2-Methylpropane; Isobutane
Heat Capacity 258.3 K, C_p=128.4 J·mol^{-1}·K^{-1}
Temperature range 79 to 261 K. Value is unsmoothed experimental datum.
Entropy 260.9 K, S=198.7 J·mol^{-1}·K^{-1}
Extrapolation below 67 K, 44.02 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 113.2 K, ΔH=4498 J·mol^{-1}
ΔS=39.73 J·mol^{-1}·K^{-1}
Molecular Weight 58.1230
Wiswesser Line Notation 1Y1&1
Evaluation B(C_p),C(S)

C_4H_{10} (liq) 40AST/KEN
2-Methylpropane; Isobutane
Heat Capacity 260 K, C_p=129.70 J·mol^{-1}·K^{-1}
Temperature range 20 to 260 K.
Entropy 261.44 K, S=200.79 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 113.74 K, ΔH=4540 J·mol^{-1}
ΔS=39.92 J·mol^{-1}·K^{-1}
liq/g 261.44 K, ΔH=21297 J·mol^{-1}
ΔS=81.46 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 58.1230
Wiswesser Line Notation 1Y1&1
Evaluation A

C_4H_{10} (liq) 31HUF/PAR
n-Butane
Heat Capacity 261.8 K, C_p=129.7 J·mol^{-1}·K^{-1}
Temperature range 69 to 262 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=229.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 48.95 J·mol^{-1}·K^{-1}.
Extrapolated above 262 K.
Phase Changes
c,II/c,I 107.0 K, ΔH=2117 J·mol^{-1}
ΔS=19.8 J·mol^{-1}·K^{-1}
c,I/liq 134.1 K, ΔH=4372 J·mol^{-1}
ΔS=32.6 J·mol^{-1}·K^{-1}
Molecular Weight 58.1230
Wiswesser Line Notation 4H
Evaluation B(C_p), C(S)

C_4H_{10} (liq) 37PAR/SHO
n-Butane
Entropy 272.5 K, S=226.8 J·mol^{-1}·K^{-1}
Calculated from heat capacity data reported by 31HUF/PAR. Extrapolation below 67 K, 41.34 J·mol^{-1}·K^{-1}.
Molecular Weight 58.1230
Wiswesser Line Notation 4H
Evaluation C

C_4H_{10} (liq) 40AST/MES
n-Butane
Heat Capacity 270 K, C_p=132.42 J·mol^{-1}·K^{-1}
Temperature range 11 to 270 K.
Entropy 298.15 K, S=231.0 J·mol^{-1}·K^{-1}
Using extrapolated values of C_p 273 to 298 K for the superheated liquid.
Phase Changes
c,II/c,I 107.55 K, ΔH=2067 J·mol^{-1}
ΔS=19.22 J·mol^{-1}·K^{-1}
c,I/liq 134.86 K, ΔH=4661 J·mol^{-1}
ΔS=34.56 J·mol^{-1}·K^{-1}
liq/g 272.05 K, ΔH=22389 J·mol^{-1}
ΔS=82.30 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 58.1230
Wiswesser Line Notation 4H
Evaluation A

$C_4H_{10}Cl_2Si$ (liq) 69NAG/DZH
Dichlorodiethylsilane
Heat Capacity 298.16 K, C_p=214.7 J·mol^{-1}·K^{-1}
Temperature range 13 to 298.16 K.
Entropy 298.16 K, S=346.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 174.10 K, ΔH=8958 J·mol^{-1}
ΔS=51.46 J·mol^{-1}·K^{-1}
Molecular Weight 157.1145
Wiswesser Line Notation 2-SI-GG2
Evaluation A

$C_4H_{10}Hg$ (liq) 78BUR/KAM
Diethyl mercury
Heat Capacity 298.15 K, C_p=182.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Phase Changes
c/liq 181.45 K, ΔH=10500 J·mol^{-1}
ΔS=57.87 J·mol^{-1}·K^{-1}
Molecular Weight 258.7130
Wiswesser Line Notation 2-HG-2
Evaluation A

$C_4H_{10}N_2$ (liq) 88BOB/KAM
Piperazine
Heat Capacity 413 K, C_p=237 J·mol^{-1}·K^{-1}
Temperature range 413 to 473 K.
Molecular Weight 86.1364
Wiswesser Line Notation T6M DMTJ
Evaluation D

$C_4H_{10}N_2O$ (c) 87DEL/FEI
1,1,3-Trimethylurea
Phase Changes
c/liq 344.4 K, ΔH=14300 J·mol^{-1}
ΔS=41.5 J·mol^{-1}·K^{-1}
Molecular Weight 102.1358
Wiswesser Line Notation 1MVN1&1
Evaluation A

$C_4H_{10}N_2O$ (c) 87DEL/FEI
Isopropylurea; Monoisopropylurea
Phase Changes
c,II/c,I 375.5 K, ΔH=2310 J·mol^{-1}
c/liq 427.4 K, ΔH=17400 J·mol^{-1}
ΔS=40.7 J·mol^{-1}·K^{-1}
Molecular Weight 102.1358
Wiswesser Line Notation ZVMY1&1
Evaluation A

$C_4H_{10}N_2O$ (c) 87DEL/FE
Propylurea; Monopropylurea
Phase Changes
c/liq 381.0 K, ΔH=14630 J·mol^{-1}
ΔS=38.4 J·mol^{-1}·K^{-1}
Molecular Weight 102.1358
Wiswesser Line Notation ZVM3
Evaluation A

$C_4D_{10}N_2O_8 \cdot D_2O$ (c) 90FUK/MA
Ammonium hydrogen oxalate hemihydrate-d_{12}
Heat Capacity
Temperature range 13 to 300 K; data given graphically.
Phase Changes
c,II/c,I 160.1 K, ΔH=1110 J·mol^{-1}
ΔS=8.23 J·mol^{-1}·K^{-1}
Molecular Weight 244.2416
Wiswesser Line Notation QVVQ &ZH &QH &1/H-2 &4/H-2 &6/H-2 &7/H-2 &9/H-2 &10/H-2
Evaluation A
Note that authors have chosen to define a mole of substance as: × [$(ND_4)DC_2O_4 \cdot 0.5D_2O$].

$C_4H_{10}N_2O_8 \cdot H_2O$ (c) 90FUK/MA
Ammonium hydrogen oxalate hemihydrate
Heat Capacity
Temperature range 13 to 300 K; data given graphically.
Phase Changes
c,II/c,I 145.4 K, ΔH=730 J·mol^{-1}
ΔS=6.01 J·mol^{-1}·K^{-1}
Molecular Weight 232.1468
Wiswesser Line Notation QVVQ &ZH &QH
Evaluation A
Note that authors have chosen to define a mole of substance as: × [$(NH_4)HC_2O_4 \cdot 0.5H_2O$].

$C_4H_{10}O$ (liq) 75AND/MAR

2-Oxa-3-methylbutane; Methyl isopropyl ether

Heat Capacity	298.15 K,	C_p=161.9 J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.		
Entropy	298.15 K,	S=253.7 J·mol^{-1}·K^{-1}
Phase Changes		
c,I/liq	127.93 K,	ΔH=5850 J·mol^{-1}
		ΔS=45.73 J·mol^{-1}·K^{-1}
c,II/liq	123.06 K,	ΔH=5100 J·mol^{-1}
		ΔS=41.44 J·mol^{-1}·K^{-1}

Metastable crystals.
Molecular Weight 74.1224
Wiswesser Line Notation 1Y1&O1
Evaluation A

$C_4H_{10}O$ (liq) 24KEY/BEA

3-Oxapentane; Diethyl ether

Heat Capacity	286.6 K,	C_p=179.1 J·mol^{-1}·K^{-1}
Temperature range 274, 286 K.		
Phase Changes		
liq/g	285.0 K,	ΔH=27530 J·mol^{-1}
		ΔS=96.60 J·mol^{-1}·K^{-1}
		P=101.325 kPa

Molecular Weight 74.1224
Wiswesser Line Notation 2O2
Evaluation B

$C_4H_{10}O$ (liq) 26PAR/HUF

3-Oxapentane; Diethyl ether

Heat Capacity	290.0 K,	C_p=170.7 J·mol^{-1}·K^{-1}
Temperature range 76 to 290 K. Value is unsmoothed experimental datum.		
Entropy	298.1 K,	S=283.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 88.70 J·mol^{-1}·K^{-1}.		
Phase Changes		
c/liq	156.8 K,	ΔH=7301 J·mol^{-1}
		ΔS=46.6 J·mol^{-1}·K^{-1}

Molecular Weight 74.1224
Wiswesser Line Notation 2O2
Evaluation B(C_p), C(S)

$C_4H_{10}O$ (liq) 27BEN/WEN

3-Oxapentane; Diethyl ether

Heat Capacity	308 K,	C_p=179.9 J·mol^{-1}·K^{-1}
Temperature range 308 to 488 K. Value is unsmoothed experimental datum. Pressure 40 atmospheres.		

Molecular Weight 74.1224
Wiswesser Line Notation 2O2
Evaluation B

$C_4H_{10}O$ (liq) 29PAR/KEL

3-Oxapentane; Diethyl ether

Entropy	298.1 K,	S=252.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 58.6 J·mol^{-1}·K^{-1}.		
Revision of previous data.		

Molecular Weight 74.1224
Wiswesser Line Notation 2O2
Evaluation C

$C_4H_{10}O$ (liq) 35AOY/KAN

3-Oxapentane; Diethyl ether

Heat Capacity	255.2 K,	C_p=164.8 J·mol^{-1}·K^{-1}
Temperature range 80 to 255 K. Value is unsmoothed experimental datum.		

Molecular Weight 74.1224
Wiswesser Line Notation 2O2
Evaluation B

$C_4H_{10}O$ (liq) 36KUR/VOS

3-Oxapentane; Diethyl ether

Heat Capacity	290 K,	C_p=167.4 J·mol^{-1}·K^{-1}
One temperature.		

Molecular Weight 74.1224
Wiswesser Line Notation 2O2
Evaluation D

$C_4H_{10}O$ (liq) 39MAZ2

3-Oxapentane; Diethyl ether

Heat Capacity	293.15 K,	C_p=171.88 J·mol^{-1}·K^{-1}
Temperature range −112 to 20 °C.		

Molecular Weight 74.1224
Wiswesser Line Notation 2O2
Evaluation B

$C_4H_{10}O$ (liq) 39MAZ3

3-Oxapentane; Diethyl ether

Heat Capacity	293 K,	C_p=172.0 J·mol^{-1}·K^{-1}
Temperature range −110 to 20 °C.		

Molecular Weight 74.1224
Wiswesser Line Notation 2O2
Evaluation B

$C_4H_{10}O$ (liq) 71COU/LEE

3-Oxapentane; Diethyl ether

Heat Capacity	298.15 K,	C_p=172.5 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.		
Entropy	298.15 K,	S=253.5 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/liq	149.86 K,	ΔH=6820 J·mol^{-1}
		ΔS=45.5 J·mol^{-1}·K^{-1}
c,I/liq	156.92 K,	ΔH=7190 J·mol^{-1}
		ΔS=45.82 J·mol^{-1}·K^{-1}

Metastable crystal.
Molecular Weight 74.1224
Wiswesser Line Notation 2O2
Evaluation A

$C_4H_{10}O$ (liq) 75AND/MAR

2-Oxapentane; Methyl n-propyl ether

Heat Capacity	298.15 K,	C_p=165.4 J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.		
Entropy	298.15 K,	S=262.9 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	133.97 K,	ΔH=7670 J·mol^{-1}
		ΔS=57.25 J·mol^{-1}·K^{-1}

Molecular Weight 74.1224
Wiswesser Line Notation 3O1
Evaluation A

$C_4H_{10}O$ (liq) 75FEN/HAR

2-Oxapentane; Methyl n-propyl ether

Heat Capacity	298.15 K,	C_p=165.3 J·mol^{-1}·K^{-1}
One temperature.		

Molecular Weight 74.1224
Wiswesser Line Notation 3O1
Evaluation B

$C_4H_{10}O$ (liq) *24WIL/DAN*
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 303 K, C_p=187.0 J·mol^{-1}·K^{-1}
Temperature range 303 to 343 K. Equation only.
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation C

$C_4H_{10}O$ (liq) 41ZHD.
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 298.1 K, C_p=184.1 J·mol^{-1}·K^{-1}
Temperature range 5 to 46 °C.
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation C

$C_4H_{10}O$ (liq) 58SWU/ZIE2
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 333 K, C_p=215.1 J·mol^{-1}·K^{-1}
Mean value 21 to 99 °C.
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation C

$C_4H_{10}O$ (liq) 60SWU/ZIE
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 323 K, C_p=201.3 J·mol^{-1}·K^{-1}
Mean value 21 to 78 °C.
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation C

$C_4H_{10}O$ (liq) 68COU/LEE
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 298.15 K, C_p=181.0 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S=214.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 171.18 K, ΔH=6302 J·mol^{-1}
ΔS=36.93 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation A

$C_4H_{10}O$ (gls) 68COU/LEE
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 180 K, C_p=129.2 J·mol^{-1}·K^{-1}
Temperature range 10 to 180 K.
Entropy 180 K, S=140.7 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation A

$C_4H_{10}O$ (liq) 70PAZ/PAZ
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 301.2 K, C_p=185.4 J·mol^{-1}·K^{-1}
Temperature range 28, 40 °C.
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation B

$C_4H_{10}O$ (liq) 78RYB/EME
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 303.15 K, C_p=185.6 J·mol^{-1}·K^{-1}
Temperature range 293.15 to 353.15 K. C_p given as 2504 J·kg^{-1}·K^{-1}.
Molecular Weight 74.1224
Wiswesser Line Notation *Q1Y1&1*
Evaluation C

$C_4H_{10}O$ (liq) 88OKA/OGA
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 298.15 K, C_p=181.05 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation B

$C_4H_{10}O$ (liq) 88PIE/SON
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 298.15 K, C_p=182.01 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation B

$C_4H_{10}O$ (liq) 1881RE
1-Butanol; n-Butyl alcohol
Heat Capacity 298 K, C_p=174.5 J·mol^{-1}·K^{-1}
Temperature range 290 to 390 K.
Molecular Weight 74.1224
Wiswesser Line Notation *Q4*
Evaluation *D*

$C_4H_{10}O$ (liq) 24WIL/DAN
1-Butanol; n-Butyl alcohol
Heat Capacity *303 K,* C_p=180.3 J·mol^{-1}·K^{-1}
Temperature range 303 to 343 K. Equation only.
Molecular Weight 74.1224
Wiswesser Line Notation *Q4*
Evaluation *C*

$C_4H_{10}O$ (liq) 25PAF
1-Butanol; n-Butyl alcohol
Heat Capacity 294.0 K, C_p=175.3 J·mol^{-1}·K^{-1}
Temperature range 90 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=251.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 73.81 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 183.9 K, ΔH=9280 J·mol^{-1}
ΔS=50.46 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B(C_p), C(S)

$C_4H_{10}O$ (liq) 29PAR/KEI
1-Butanol; n-Butyl alcohol
Entropy 298.1 K, S=228.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 46.02 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation *C*

$C_4H_{10}O$ (liq) 33TRE/WAT
1-Butanol; n-Butyl alcohol
Heat Capacity 298 K, C_p=183.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 39PHI
1-Butanol; n-Butyl alcohol
Heat Capacity 302.6 K, C_p=215.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation C
Isomer not specified; normal assumed.

$C_4H_{10}O$ (liq) 60SWI/ZIE
1-Butanol; n-Butyl alcohol
Heat Capacity 323 K, C_p=189.1 J·mol^{-1}·K^{-1}
Mean value 21 to 78 °C.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation C

$C_4H_{10}O$ (liq) 65COU/HAL
1-Butanol; n-Butyl alcohol
Heat Capacity 298.15 K, C_p=177.03 J·mol^{-1}·K^{-1}
Temperature range 11 to 323 K.
Entropy 298.15 K, S=225.73 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 184.5 K, ΔH=9372 J·mol^{-1}
ΔS=50.79 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation A

$C_4H_{10}O$ (liq) 70PAZ/PAZ
1-Butanol; n-Butyl alcohol
Heat Capacity 301.2 K, C_p=179.5 J·mol^{-1}·K^{-1}
Temperature range 28, 40 °C.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 79GRI/YAN
1-Butanol; n-Butyl alcohol
Heat Capacity 303.5 K, C_p=181.6 J·mol^{-1}·K^{-1}
Temperature range 303 to 462 K. p=0.98 bar.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 81ARU/BAG
1-Butanol; n-Butyl alcohol
Heat Capacity 293.15 K, C_p=174.3 J·mol^{-1}·K^{-1}
Temperature range 293 to 373 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.351 kJ/kg·K. C_p given from 293.15 to 533.15 for pressure range 10 to 60 MPa.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 84ZEG/SOM
1-Butanol; n-Butyl alcohol
Heat Capacity 298.15 K, C_p=177.08 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 86GAT/WOO
1-Butanol; n-Butyl alcohol
Heat Capacity 298.15 K, C_p=176.67 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 368.15 K.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation C

$C_4H_{10}O$ (liq) 86KOR/KUK
1-Butanol; n-Butyl alcohol
Heat Capacity 298 K, C_p=177.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 86NAZ/BAS
1-Butanol; n-Butyl alcohol
Heat Capacity 321.05 K, C_p=192.2 J·mol^{-1}·K^{-1}
Temperature range 321.05, 349.20, 373.35 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.5934 kJ/kg·K.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 86OGA/MUR
1-Butanol; n-Butyl alcohol
Heat Capacity 298.15 K, C_p=177.18 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 86ROU/GRO
1-Butanol; n-Butyl alcohol
Heat Capacity 298.15 K, C_p=175.97 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 86TAN/TOY
1-Butanol; n-Butyl alcohol
Heat Capacity 298.15 K, C_p=176.69 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation A

$C_4H_{10}O$ (liq) 88AND/PAT
1-Butanol; n-Butyl alcohol
Heat Capacity 298.15 K, C_p=176.86 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 26PAR/AND
tert-Butyl alcohol; 2-Methyl-2-propanol
Heat Capacity 300 K, C_p=224.7 J·mol^{-1}·K^{-1}
Temperature range 87 to 300 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=197.5 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 53.35 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 298.5 K, ΔH=6782 J·mol^{-1}
ΔS=22.72 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation B(C_p), C(S)

$C_4H_{10}O$ (liq) 29PAR/KEL
tert-Butyl alcohol; 2-Methyl-2-propanol
Entropy 298.1 K, S=189.5 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 45.19 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation C

$C_4H_{10}O$ (c,I) 63OET
tert-Butyl alcohol; 2-Methyl-2-propanol
Heat Capacity 298.15 K, C_p=146.11 J·mol^{-1}·K^{-1}
Temperature range 15 to 330 K.
Entropy 298.15 K, S=170.87 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 286.14 K, ΔH=828 J·mol^{-1}
ΔS=2.89 J·mol^{-1}·K^{-1}
c,III/c,I 294.47 K, ΔH=490 J·mol^{-1}
ΔS=1.66 J·mol^{-1}·K^{-1}
Metastable transition, not always reproducible, c,III,metastable form.
c,I/liq 298.97 K, ΔH=6702.8 J·mol^{-1}
ΔS=22.42 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation A

$C_4H_{10}O$ (liq) 76SKO/SUU
tert-Butyl alcohol; 2-Methyl-2-propanol
Heat Capacity 298.15 K, C_p=218.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation A

$C_4H_{10}O$ (liq) 77DEV/PER
tert-Butyl alcohol; 2-Methyl-2-propanol
Heat Capacity 298.15 K, C_p=210 J·mol^{-1}·K^{-1}
Temperature range 298.15, 313.15, 328.15 K.
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation B

$C_4H_{10}O$ (liq) 77MUR/SUB
tert-Butyl alcohol; 2-Methyl-2-propanol
Heat Capacity 298.15 K, C_p=224.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation B

$C_4H_{10}O$ (liq) 77VIS/PER
tert-Butyl alcohol; 2-Methyl-2-propanol
Heat Capacity 298 K, C_p=210 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation B

$C_4H_{10}O$ (liq) 88CAC/COS
tert-Butyl alcohol; 2-Methyl-2-propanol
Heat Capacity 298.15 K, C_p=215.37 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation B

$C_4H_{10}O$ (liq) 88OKA/OGA
tert-Butyl alcohol; 2-Methyl-2-propanol
Heat Capacity 299.15 K, C_p=221.88 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation B

$C_4H_{10}O$ (liq) 36PAR/THO
2-Butanol; sec-Butyl alcohol
Heat Capacity 281.7 K, C_p=184.9 J·mol^{-1}·K^{-1}
Temperature range 103 to 282 K. Glass at lower temperature. Unsmoothed experimental datum.
Molecular Weight 74.1224
Wiswesser Line Notation QY2&1
Evaluation B

$C_4H_{10}O$ (liq) 76CON/GIN
2-Butanol; sec-Butyl alcohol
Heat Capacity 298 K, C_p=199.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QY2&1
Evaluation B

$C_4H_{10}O$ (liq) 71AND/CON
2-Butanol; sec-Butyl alcohol
Heat Capacity 298.15 K, C_p=197.4 J·mol^{-1}·K^{-1}
Temperature range 11 to 350 K.
Entropy 298.15 K, S=213.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 177.38 K, ΔH=6000 J·mol^{-1}
ΔS=33.83 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation QY2&1
Evaluation A
Optically active form.

$C_4H_{10}O$ (liq) 71AND/CON
2-Butanol; sec-Butyl alcohol
Heat Capacity 298.15 K, C_p=196.8 J·mol^{-1}·K^{-1}
Temperature range 11 to 350 K.
Entropy 298.15 K, S=214.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 184.70 K, ΔH=5970 J·mol^{-1}
ΔS=32.32 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation QY2&1
Evaluation A
Optically inactive form.

$C_4H_{10}O$ (liq) 88OKA/OGA
2-Butanol; sec-Butyl alcohol
Heat Capacity 298.15 K, C_p=198.03 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QY2&1
Evaluation B

$C_4H_{10}O$ (liq) 88PIE/SOM
2-Butanol; sec-Butyl alcohol
Heat Capacity 298.15 K, C_p=196.67 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QY2&1
Evaluation B

$C_4H_{10}O$ (liq) 92STE/CHI
2-Butanol; sec-Butyl alcohol
Heat Capacity 298.15 K, C_p=197.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QY2&1
Evaluation A

$(C_4H_{10}OSi)_n$ (liq) 82KUL/LEB
Poly(diethylsiloxane)
Heat Capacity 298.15 K, C_p=165.5 J·mol^{-1}·K^{-1}
Temperature range 14 to 330 K.
Entropy 298.15 K, S=215.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 203 K, ΔH=2070 J·mol^{-1}
ΔS=10.2 J·mol^{-1}·K^{-1}
Degree of crystallinity=72%.
c/liq 295 K, ΔH=2876 J·mol^{-1}
ΔS=9.75 J·mol^{-1}·K^{-1}
Degree of crystallinity=100%.
Molecular Weight 102.2079
Wiswesser Line Notation /*-SI-2&2&O*/
Evaluation A

$(C_4H_{10}OSi)_n$ (liq) 84LEB/KUL
Poly(diethylsiloxane)
Heat Capacity 298.15 K, C_p=165.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=215.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 203 K, ΔH=2070 J·mol^{-1}
ΔS=10.2 J·mol^{-1}·K^{-1}
Degree of crystallinity=72%.
c,I/liq 295 K, ΔH=2876 J·mol^{-1}
ΔS=9.75 J·mol^{-1}·K^{-1}
Degree of crystallinity=100%.
Molecular Weight 102.2079
Wiswesser Line Notation /*-SI-2&2&O*/
Evaluation A
T(glass)=130 K.

$(C_4H_{10}OSi)_n$ (liq) 88WIE/WUN
Poly(diethylsiloxane)
Phase Changes
c,II/c,I 206 K, ΔH=1700 J·mol^{-1}
ΔS=8.5 J·mol^{-1}·K^{-1}
c,I/liq 276 K, ΔH=1700 J·mol^{-1}
ΔS=6.3 J·mol^{-1}·K^{-1}
Molecular Weight 102.2079
Wiswesser Line Notation /*-SI-2&2&O*/
Evaluation A
T(glass)=135 K.

$(C_4H_{10}OSi)_n$ (amorph) 89VAR/WES
Poly(diethylsiloxane)
Heat Capacity 298.15 K, C_p=164.994 J·mol^{-1}·K^{-1}
Temperature range 0.10 to 550 K. C_p(liq)=0.2365T+93.75 J/(K mol) (290 to 360 K).
Entropy 298.15 K, S=213.697 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 206.7 K, ΔH=2720 J·mol^{-1}
100% crystallinity/condis crystal.
c,II/c,I 282.7 K, ΔH=1840 J·mol^{-1}
Condis crystal/viscous crystal.
c,I/liq 308.5 K, ΔH=231 J·mol^{-1}
Molecular Weight 102.2079
Wiswesser Line Notation /*-SI-2&2&O*/
Evaluation A
T(glass)=135 K.

$(C_4H_{10}OSi)_n$ (c) 89VAR/WES
Poly(diethylsiloxane)
Heat Capacity 298.15 K, C_p=164.994 J·mol^{-1}·K^{-1}
Temperature range 0.10 to 308.50 K.
Entropy 298.15 K, S=212.720 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 206.7 K, ΔH=2720 J·mol^{-1}
100% crystallinity/condis crystal.
c,II/c,I 282.7 K, ΔH=1840 J·mol^{-1}
Condis crystal/viscous crystal.
c,I/liq 308.5 K, ΔH=231 J·mol^{-1}
Molecular Weight 102.2079
Wiswesser Line Notation /*-SI-2&2&O*/
Evaluation A
T(glass)=135 K.

$C_4H_{10}O_2$ (liq) 73KUS/SUU
2,5-Dioxahexane; 1,2-Dimethoxyethane
Heat Capacity 298.15 K, C_p=193.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 90.1218
Wiswesser Line Notation 1O2O1
Evaluation B

$C_4H_{10}O_2$ (liq) 91TRE/COS
2,5-Dioxahexane; 1,2-Dimethoxyethane
Heat Capacity 298.15 K, C_p=191.14 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 90.1218
Wiswesser Line Notation 1O2O1
Evaluation B

$C_4H_{10}O_2$ (liq) 73KUS/SUU
3-Oxa-1-pentanol; 2-Ethoxyethanol
Heat Capacity 298.15 K, C_p=210.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 90.1218
Wiswesser Line Notation Q2O2
Evaluation B

$C_4H_{10}O_2$ (liq) 78ROU/PER
3-Oxa-1-pentanol; 2-Ethoxyethanol
Heat Capacity 298.15 K, C_p=210.5 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K. Data at three temperatures.
Molecular Weight 90.1218
Wiswesser Line Notation Q2O2
Evaluation C

$C_4H_{10}O_2$ (liq) 91SVO/ZAB
3-Oxa-1-pentanol; 2-Ethoxyethanol
Heat Capacity 298.15 K, C_p=209.82 J·mol^{-1}·K^{-1}
Temperature range 298 to 330 K. C_p(liq)=84.928+0.4189(T/K) J·mol^{-1}·K^{-1}. C_p value calculated from equation.
Molecular Weight 90.1218
Wiswesser Line Notation Q2O2
Evaluation B

$C_4H_{10}O_2$ (liq) 72KAW/OTA
1,3-Butanediol; 1,3-Dihydroxybutane
Heat Capacity 303 K, C_p=227.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 90.1218
Wiswesser Line Notation QY1&2Q
Evaluation B

$C_4H_{10}O_2$ (liq) 74PET/TER
1,4-Butanediol; 1,4-Dihydroxybutane
Heat Capacity 297.79 K, C_p=178 J·mol^{-1}·K^{-1}
Temperature range 297 to 470 K. Value is unsmoothed experimental datum.
Molecular Weight 90.1218
Wiswesser Line Notation Q4Q
Evaluation B

$C_4H_{10}O_2$ (liq) 79NIS/BAB
1,4-Butanediol; 1,4-Dihydroxybutane
Heat Capacity 298.15 K, C_p=200.1 J·mol^{-1}·K^{-1}
Temperature range 5 to 320 K.
Entropy 298.15 K, S=223.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 293.58 K, ΔH=18700 J·mol^{-1}
ΔS=63.72 J·mol^{-1}·K^{-1}
Molecular Weight 90.1218
Wiswesser Line Notation Q4Q
Evaluation A

$C_4H_{10}O_2$ (liq) 84VAS/PET
1,4-Butanediol; 1,4-Dihydroxybutane
Heat Capacity 298.15 K, C_p=200.1 J·mol^{-1}·K^{-1}
Temperature range 5 to 450 K.
Entropy 298.15 K, S=223.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 293.58 K, ΔH=18700 J·mol^{-1}
ΔS=63.7 J·mol^{-1}·K^{-1}
Molecular Weight 90.1218
Wiswesser Line Notation Q4Q
Evaluation A

$C_4H_{10}O_2$ (liq) 36KHO/KAL
2,3-Butanediol; 2,3-Dihydroxybutane
Heat Capacity 298.2 K, C_p=213.0 J·mol^{-1}·K^{-1}
Temperature range 26 to 140 °C.
Molecular Weight 90.1218
Wiswesser Line Notation QY1&YQ1
Evaluation C
Extracted from Chem. Abst. 30,4080 (1936).

$C_4H_{10}O_2Se$ (liq) 83GEI/GUS
β-Selenodiglycol
Heat Capacity 298.15 K, C_p=349.9 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=358.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 154.0 K, ΔH=110 J·mol^{-1}
ΔS=0.7 J·mol^{-1}·K^{-1}
Glassy (solid) to liquid.
Molecular Weight 169.0818
Wiswesser Line Notation Q2-SE-2Q
Evaluation A

$C_4H_{10}O_3$ (liq) 79STE/TAN
Diethylene glycol; 1,5-Dihydroxy-3-oxapentane
Heat Capacity 298 K, C_p=287.0 J·mol^{-1}·K^{-1}
Temperature range 273 to 513 K.
Molecular Weight 106.1212
Wiswesser Line Notation Q2O2Q
Evaluation B

$C_4H_{10}O_3$ (liq) 82ZAI
Diethylene glycol; 1,5-Dihydroxy-3-oxapentane
Heat Capacity 298 K, C_p=243.9 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 106.1212
Wiswesser Line Notation Q2O2Q
Evaluation B

$C_4H_{10}O_4$ (c) 26PAR/ANI
1,2,3,4-Tetrahydroxybutane; 1,2,3,4-Butanetetrol; Erythritol
Heat Capacity 291.7 K, C_p=161.9 J·mol^{-1}·K^{-1}
Temperature range 87 to 292 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=177.8 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 55.48 J·mol^{-1}·K^{-1}.
Molecular Weight 122.1206
Wiswesser Line Notation Q1YQYQ1Q
Evaluation B(C_p), C(S)

$C_4H_{10}O_4$ (c) 29PAR/KEL
1,2,3,4-Tetrahydroxybutane; 1,2,3,4-Butanetetrol; Erythritol
Entropy 298.1 K, S=166.5 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 44.35 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 122.1206
Wiswesser Line Notation Q1YQYQ1Q
Evaluation C

$C_4H_{10}O_4$ (c) 32SPA/THO
1,2,3,4-Tetrahydroxybutane; 1,2,3,4-Butanetetrol; Erythritol
Heat Capacity 303 K, C_p=170.7 J·mol^{-1}·K^{-1}
Temperature range 30 to 150 °C.
Phase Changes
c/liq 381.6 K, ΔH=42359 J·mol^{-1}
ΔS=111.0 J·mol^{-1}·K^{-1}
Molecular Weight 122.1206
Wiswesser Line Notation Q1YQYQ1Q
Evaluation B

$C_4H_{10}O_4$ (c) 90BAR/DEL
1,2,3,4-Tetrahydroxybutane; 1,2,3,4-Butanetetrol; Erythritol
Phase Changes
c/liq 390.9 K, $\Delta H = 39400$ J·mol^{-1}
$\Delta S = 100.8$ J·mol^{-1}·K^{-1}
Molecular Weight 122.1206
Wiswesser Line Notation Q1YQYQ1Q
Evaluation A

$C_4H_{10}O_6S_3$ (c) 56DAV/STA
Trimethylsulfonylmethane
Heat Capacity 298.15 K, $C_p = 269.62$ J·mol^{-1}·K^{-1}
Temperature range 22 to 293 K.
Entropy 298.15 K, $S = 304.60$ J·mol^{-1}·K^{-1}
Molecular Weight 250.2994
Wiswesser Line Notation 1SWYSW1&SW1
Evaluation A

$C_4H_{10}S$ (liq) 55MCC/FIN
3-Methyl-2-thiabutane; Isopropyl methyl sulfide
Heat Capacity 298.15 K, $C_p = 172.38$ J·mol^{-1}·K^{-1}
Temperature range 12 to 344 K.
Entropy 298.15 K, $S = 263.09$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 171.65 K, $\Delta H = 9355$ J·mol^{-1}
$\Delta S = 54.50$ J·mol^{-1}·K^{-1}
Molecular Weight 90.1830
Wiswesser Line Notation 1Y1&S1
Evaluation A

$C_4H_{10}S$ (liq) 52SCO/FIN2
3-Thiapentane; Diethyl sulfide
Heat Capacity 298.15 K, $C_p = 171.42$ J·mol^{-1}·K^{-1}
Temperature range 16 to 316 K.
Entropy 298.15 K, $S = 269.28$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 169.21 K, $\Delta H = 11903$ J·mol^{-1}
$\Delta S = 70.35$ J·mol^{-1}·K^{-1}
Molecular Weight 90.1830
Wiswesser Line Notation 2S2
Evaluation A

$C_4H_{10}S$ (liq) 57SCO/FIN
2-Thiapentane; Methyl n-propyl sulfide
Heat Capacity 298.15 K, $C_p = 171.63$ J·mol^{-1}·K^{-1}
Temperature range 12 to 326 K.
Entropy 298.15 K, $S = 272.55$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 160.17 K, $\Delta H = 9912$ J·mol^{-1}
$\Delta S = 61.88$ J·mol^{-1}·K^{-1}
Molecular Weight 90.1830
Wiswesser Line Notation 3S1
Evaluation A

$C_4H_{10}S$ (liq) 58SCO/MCC
2-Methyl-1-propanethiol; Isobutyl mercaptan
Heat Capacity 298.15 K, $C_p = 171.88$ J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, $S = 266.35$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 128.31 K, $\Delta H = 4982.3$ J·mol^{-1}
$\Delta S = 388.3$ J·mol^{-1}·K^{-1}
Molecular Weight 90.1830
Wiswesser Line Notation SH1Y1&1
Evaluation A

$C_4H_{10}S$ (liq) 57SCO/FIN
1-Butanethiol; n-Butyl mercaptan
Heat Capacity 298.15 K, $C_p = 172.30$ J·mol^{-1}·K^{-1}
Temperature range 12 to 314 K.
Entropy 298.15 K, $S = 275.98$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 157.47 K, $\Delta H = 10460$ J·mol^{-1}
$\Delta S = 66.43$ J·mol^{-1}·K^{-1}
Molecular Weight 90.1830
Wiswesser Line Notation SH4
Evaluation A

$C_4H_{10}S$ (liq) 82TUT/GAB
1-Butanethiol; n-Butyl mercaptan
Heat Capacity 300 K, $C_p = 171.39$ J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K. $C_p = 155.76 + 2.780 \times 10^{-2}T + 8.100 \times 10^{-5}T^2$.
Molecular Weight 90.1830
Wiswesser Line Notation SH4
Evaluation B

$C_4H_{10}S$ (liq) 53MCC/SCO
2-Methyl-2-propanethiol; tert-Butyl mercaptan
Heat Capacity 298.15 K, $C_p = 175.06$ J·mol^{-1}·K^{-1}
Temperature range 12 to 329 K.
Entropy 298.15 K, $S = 246.44$ J·mol^{-1}·K^{-1}
Phase Changes
c,IV/c,III 151.6 K, $\Delta H = 4066.8$ J·mol^{-1}
$\Delta S = 26.83$ J·mol^{-1}·K^{-1}
c,III/c,II 157.0 K, $\Delta H = 648.1$ J·mol^{-1}
$\Delta S = 4.13$ J·mol^{-1}·K^{-1}
c,II/c,I 199.4 K, $\Delta H = 970.7$ J·mol^{-1}
$\Delta S = 4.87$ J·mol^{-1}·K^{-1}
c,I/liq 274.42 K, $\Delta H = 2481.9$ J·mol^{-1}
$\Delta S = 9.04$ J·mol^{-1}·K^{-1}
Molecular Weight 90.1830
Wiswesser Line Notation SHX1&1&1
Evaluation A

$C_4H_{10}S$ (liq) 58MCC/FIN
2-Butanethiol; sec-Butyl mercaptan.
Heat Capacity 298.15 K, $C_p = 171.2$ J·mol^{-1}·K^{-1}
Temperature range 12 to 309 K.
Entropy 298.15 K, $S = 271.42$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 133.02 K, $\Delta H = 6477$ J·mol^{-1}
$\Delta S = 48.69$ J·mol^{-1}·K^{-1}
Molecular Weight 90.1830
Wiswesser Line Notation SHY2&1
Evaluation A

$C_4H_{10}S_2$ (liq) 52SCO/FIN
Diethyl disulfide; 3,4-Dithiahexane
Heat Capacity 298.15 K, $C_p = 204.01$ J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, $S = 305.01$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 171.64 K, $\Delta H = 9404.4$ J·mol^{-1}
$\Delta S = 54.79$ J·mol^{-1}·K^{-1}
Molecular Weight 122.2430
Wiswesser Line Notation 2SS2
Evaluation A

$C_4H_{10}Zn$ (liq) 87GIB/GRI
Diethyl zinc
Heat Capacity 298.15 K, C_p=188.9 J·mol^{-1}·K^{-1}
Temperature range 18 to 273 K.
Entropy 298.15 K, S=276.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 239.80 K, ΔH=18050 J·mol^{-1}
ΔS=75.30 J·mol^{-1}·K^{-1}
Molecular Weight 123.5030
Wiswesser Line Notation 2-ZN-2
Evaluation A

$C_4H_{10}Zn$ (liq) 88RAB/NIS
Diethyl zinc
Heat Capacity 298.15 K, C_p=194.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=290.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 148.4 K, ΔH=275.4 J·mol^{-1}
ΔS=2.12 J·mol^{-1}·K^{-1}
c,I/liq 236.98 K, ΔH=16634 J·mol^{-1}
ΔS=70.19 J·mol^{-1}·K^{-1}
Molecular Weight 123.5030
Wiswesser Line Notation 2-ZN-2
Evaluation A

$C_4H_{11}N$ (liq) 36KUR/VOS
Diethylamine
Heat Capacity 290 K, C_p=106.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.1376
Wiswesser Line Notation 2M2
Evaluation D

$C_4H_{11}N$ (liq) 85COS/PAT
Diethylamine
Heat Capacity 298.15 K, C_p=178.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.1376
Wiswesser Line Notation 2M2
Evaluation B

$C_4H_{11}N$ (liq) 85COS/PAT2
Diethylamine
Heat Capacity 298.15 K, C_p=178.1 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 73.1376
Wiswesser Line Notation 2M2
Evaluation B

$C_4H_{11}N$ (liq) 71KON/WAD
2-Methyl-1-aminopropane; Isobutylamine
Heat Capacity 298.15 K, C_p=194 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.1376
Wiswesser Line Notation Z1Y1&1
Evaluation B

$C_4H_{11}N$ (liq) 71KON/WAD
1-Aminobutane; n-Butylamine
Heat Capacity 298.15 K, C_p=188 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.1376
Wiswesser Line Notation Z4
Evaluation B

$C_4H_{11}N$ (liq) 67SMI/GOO2
2-Methyl-2-aminopropane; tert-Butylamine
Heat Capacity 298.15 K, C_p=192.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.1376
Wiswesser Line Notation ZX1&1&1
Evaluation B

$C_4H_{11}N$ (liq) 71KON/WAD
2-Methyl-2-aminopropane; tert-Butylamine
Heat Capacity 298.15 K, C_p=190 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 73.1376
Wiswesser Line Notation ZX1&1&1
Evaluation B

$C_4H_{11}N$ (liq) 72FIN/MES
2-Methyl-2-aminopropane; tert-Butylamine
Heat Capacity 298.15 K, C_p=191.71 J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Entropy 298.15 K, S=233.63 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 91.30 K, ΔH=113.51 J·mol^{-1}
ΔS=1.24 J·mol^{-1}·K^{-1}
c,II/c,I 202.27 K, ΔH=6052.6 J·mol^{-1}
ΔS=29.91 J·mol^{-1}·K^{-1}
c,I/liq 206.19 K, ΔH=882.0 J·mol^{-1}
ΔS=4.28 J·mol^{-1}·K^{-1}
Molecular Weight 73.1376
Wiswesser Line Notation ZX1&1&1
Evaluation A

$C_4H_{11}NO$ (liq) 90STE/CHI
N,N-Diethylhydroxylamine
Heat Capacity 298.15 K, C_p=370.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 89.1370
Wiswesser Line Notation QN2&2
Evaluation B

$C_4H_{11}NO$ (liq) 84GEI/KAR
3-Methoxypropylamine
Heat Capacity 298.15 K, C_p=225.52 J·mol^{-1}·K^{-1}
Temperature range 55 to 300 K.
Entropy 298.15 K, S=257.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 135 K
Glass/liquid transition.
Molecular Weight 89.1370
Wiswesser Line Notation Z3O1
Evaluation B

$C_4H_{11}NO$ (liq) 80ROU/ROB
2-Amino-2-methylpropanol
Heat Capacity 298.15 K, C_p=229.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 89.1370
Wiswesser Line Notation ZX1&1&1Q
Evaluation B

$C_4H_{11}NO_2$ (c) 82MIN/SAB
Diethanolamine
Heat Capacity 298.15 K, C_p=137 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.3 J·K^{-1}·g^{-1}, an estimated value.
Molecular Weight 105.1364
Wiswesser Line Notation Q2M2Q
Evaluation C

$C_4H_{11}NO_2$ (c) 70MUR/BRE
2-Amino-2-methyl-1,3-propanediol
Phase Changes
c,II/c,I 352 K, ΔH=25205 J·mol^{-1}
ΔS=72.0 J·mol^{-1}·K^{-1}
c,I/liq 384 K, ΔH=2991 J·mol^{-1}
ΔS=7.9 J·mol^{-1}·K^{-1}
Molecular Weight 105.1364
Wiswesser Line Notation ZX1&1&1Q1Q
Evaluation A

$C_4H_{11}NO_2$ (c) 90ZHA/YAN
2-Amino-2-methyl-1,3-propanediol
Heat Capacity 301.40 K, C_p=161.37 J·mol^{-1}·K^{-1}
Temperature range 280 to 370 K. Unsmoothed experimental datum.
Phase Changes
c,III/c,II 352.89 K, ΔH=5000 J·mol^{-1}
ΔS=14.2 J·mol^{-1}·K^{-1}
c,II/c,I 353.72 K, ΔH=18460 J·mol^{-1}
ΔS=52.2 J·mol^{-1}·K^{-1}
c,I/liq 384.08 K, ΔH=2780 J·mol^{-1}
ΔS=7.23 J·mol^{-1}·K^{-1}
Molecular Weight 105.1364
Wiswesser Line Notation ZX1&1&1Q1Q
Evaluation B

$C_4H_{11}NO_2$ (c) 91BAR/FON
2-Amino-2-methyl-1,3-propanediol
Heat Capacity
Temperature range 273 to 423 K. Data given graphically.
Phase Changes
c,II/c,I 351.25 K, ΔH=24680 J·mol^{-1}
c,I/liq 383.55 K, ΔH=2731 J·mol^{-1}
Molecular Weight 105.1364
Wiswesser Line Notation ZX1&1&1Q1Q
Evaluation B

$C_4H_{11}NO_3$ (c) 72ARV/WES
Tris(hydroxymethyl)aminomethane; TRIS; THAM
Heat Capacity 298.15 K, C_p=167.19 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=175.44 J·mol^{-1}·K^{-1}
Molecular Weight 121.1358
Wiswesser Line Notation Q1XZ1Q1Q
Evaluation A

$C_4H_{11}NO_3$ (c) 70MUR/BRE
2-Amino-2-hydroxymethyl-1,3-propanediol
Phase Changes
c,II/c,I 405 K, ΔH=34262 J·mol^{-1}
ΔS=84.9 J·mol^{-1}·K^{-1}
c,I/liq 439 K, ΔH=3041 J·mol^{-1}
ΔS=7.1 J·mol^{-1}·K^{-1}
Molecular Weight 121.1358
Wiswesser Line Notation ZX1Q1Q1Q
Evaluation A

$C_4H_{11}NO_3$ (c) 90YIN/LIN
2-Amino-2-hydroxymethyl-1,3-propanediol
Heat Capacity 298.15 K, C_p=171.27 J·mol^{-1}·K^{-1}
Temperature range 290 to 450 K.
Phase Changes
c,II/c,I 407.44 K, ΔH=33416 J·mol^{-1}
Bifurcated transition.
c,II/c,I 407.56 K
c,I/liq 443.4 K, ΔH=2407 J·mol^{-1}
Molecular Weight 121.1358
Wiswesser Line Notation ZX1Q1Q1Q
Evaluation A

$C_4H_{11}N_3O_7$ (c) 85TAR/SAV
Diglycine nitrate
Heat Capacity 298.15 K, C_p=297 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K. Data given graphically. C_p=−0.0108+0.231×10^{-2}T−0.631×10^{-5}T^2+0.830×10^{-8}T^3 cal·g^{-1}·K^{-1} (80 to 300 K). C_p value calculated from equation.
Phase Changes
c,II/c,I 206.5 K, ΔH=1072 J·mol^{-1}
ΔS=5.19 J·mol^{-1}·K^{-1}
Molecular Weight 213.1468
Wiswesser Line Notation Z1VQ 2 &WNQ
Evaluation C

$C_4H_{12}BrN$ (c) 62CHA/WES2
Tetramethylammonium bromide
Heat Capacity 298.15 K, C_p=161.67 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=200.79 J·mol^{-1}·K^{-1}
Molecular Weight 154.0495
Wiswesser Line Notation 1K1&1&1 &E
Evaluation A

$C_4H_{12}BrN$ (c) 74BUR/VER
Tetramethylammonium bromide
Heat Capacity 298 K, C_p=159.4 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
Molecular Weight 154.0495
Wiswesser Line Notation 1K1&1&1 &E
Evaluation B

$C_4H_{12}CdCl_3N$ (c) 87BRA/CHA
Tetramethylammonium trichlorocadmate
Phase Changes
c,IV/c,III 111.3 K, ΔH=143.5 J·mol^{-1}
c,III/c,II 122.7 K, ΔH=714.7 J·mol^{-1}
c,II/c,I 400 K
Molecular Weight 292.9145
Wiswesser Line Notation 1K1&1&1 .CD G3
Evaluation A

$C_4H_{12}CdSe$ (liq) 92LEB/KUL
Dimethylcadmium· dimethylselenium
Heat Capacity 298.15 K, C_p=277.70 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=413.56 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 205.64 K, ΔH=12679 J·mol^{-1}
ΔS=61.61 J·mol^{-1}·K^{-1}
Molecular Weight 251.5088
Wiswesser Line Notation 1-SE-1 &1-CD-1
Evaluation A

$C_4H_{12}CdTe$ (liq) 92LEB/KUL

Dimethyl cadmium· dimethyl tellurium

Heat Capacity	298.15 K,	C_p=275.21 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.		
Entropy	298.15 K,	S=413.06 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/c,I	103.2 K,	ΔH=669 J·mol^{-1}
		ΔS=0.84 J·mol^{-1}·K^{-1}
c,I/liq	210.45 K,	ΔH=10775 J·mol^{-1}·K^{-1}
		ΔS=51.40 J·mol^{-1}·K^{-1}

Molecular Weight 300.1488
Wiswesser Line Notation 1-TE-1 &1-CD-1
Evaluation A

$C_4H_{12}ClN$ (c) 62CHA/WES2

Tetramethylammonium chloride

Heat Capacity	298.15 K,	C_p=156.94 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.		
Entropy	298.15 K,	S=190.71 J·mol^{-1}·K^{-1}
Phase Changes		
c/III/c,II	75.76 K,	ΔH=116.3 J·mol^{-1}
		ΔS=1.54 J·mol^{-1}·K^{-1}
c,II/c,I	184.85 K,	ΔH=108.4 J·mol^{-1}
		ΔS=0.59 J·mol^{-1}·K^{-1}

Transition over range 180 to 190 K.
Molecular Weight 109.5985
Wiswesser Line Notation 1K1&1&1 &G
Evaluation A

$C_4H_{12}ClN$ (c) 70MUR/BRE

Tetramethylammonium chloride

Phase Changes		
c,II/c,I	536 K,	ΔH=9905 J·mol^{-1}
		ΔS=18.4 J·mol^{-1}·K^{-1}

Molecular Weight 109.5985
Wiswesser Line Notation 1K1&1&1 &G
Evaluation A

$C_4H_{12}ClNO_4$ (c) 91ISH/IWA

tert-Butylammonium perchlorate

Phase Changes		
c,III/c,II	327 K,	ΔS=6.9 J·mol^{-1}·K^{-1}
c,II/c,I	394 K,	ΔS=12 J·mol^{-1}·K^{-1}
c,I/liq	414 K,	ΔS=17 J·mol^{-1}·K^{-1}

Molecular Weight 173.5961
Wiswesser Line Notation ZX1&1&1 &QGO 3
Evaluation A

$C_4H_{12}Cl_3MnN$ (c) 83DUN/JEW

Tetramethylammonium trichloromanganate(II)

Heat Capacity	299.55 K,	C_p=240.0 J·mol^{-1}·K^{-1}
Temperature range 1.5 to 300 K. Value is unsmoothed experimental datum.		
Phase Changes		
c,II/c,I	126.52 K	
Monoclinic-hexagonal.		

Molecular Weight 235.4425
Wiswesser Line Notation 1K1&1&1 .MN G3
Evaluation A

$C_4H_{12}Cl_3MnN$ (c) 87BRA/CHA

Tetramethylammonium trichloromanganate(II)

Phase Changes		
c,II/c,I	132.1 K	
Monoclinic-hexagonal.		

Molecular Weight 235.4425
Wiswesser Line Notation 1K1&1&1 .MN G3
Evaluation A

$C_4H_{12}Cl_4FeN$ (c) 87RUI/LOP

Tetramethylammonium tetrachloroferrate (III)

Heat Capacity		
Temperature range 60 to 350 K. Data given graphically.		
Phase Changes		
c,VI/c,V	236.1 K,	ΔH=498.9 J·mol^{-1}
		ΔS=1.98 J·mol^{-1}·K^{-1}
c,V/c,IV	291.4 K,	ΔH=2524 J·mol^{-1}
		ΔS=10.7 J·mol^{-1}·K^{-1}
c,IV/c,III	307.4 K,	ΔH=734.3 J·mol^{-1}
		ΔS=2.38 J·mol^{-1}·K^{-1}
c,III/c,II	347.0 K,	ΔH=713.1 J·mol^{-1}
		ΔS=2.05 J·mol^{-1}·K^{-1}
c,II/c,I	381.0 K,	ΔH=5319.6 J·mol^{-1}
		ΔS=14.0 J·mol^{-1}·K^{-1}

Molecular Weight 271.8045
Wiswesser Line Notation 1K1&1&1 .FE G4
Evaluation A

$C_4H_{12}Ge$ (liq) 70VAL/KIL

Tetramethylgermane

Heat Capacity	300 K,	C_p=196.9 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.		
Entropy	300 K,	S=296.80 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	184.368 K,	ΔH=7447.1 J·mol^{-1}
		ΔS=40.39 J·mol^{-1}·K^{-1}
liq/g	285 K,	ΔH=28125 J·mol^{-1}
		ΔS=98.7 J·mol^{-1}·K^{-1}
		P=1 atm

Molecular Weight 132.7288
Wiswesser Line Notation 1-GE-1&1&1
Evaluation A

$C_4H_{12}IN$ (c) 40COU/PIT

Tetramethylammonium iodide

Heat Capacity	298.15 K,	C_p=160.79 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.		
Entropy	298.15 K,	S=207.9 J·mol^{-1}·K^{-1}

Molecular Weight 201.0500
Wiswesser Line Notation 1K1&1&1 &I
Evaluation A

$C_4H_{12}IN$ (c) 88NAG/SAK

Tetramethylammonium iodide

Heat Capacity	298.15 K,	C_p=161 J·mol^{-1}·K^{-1}
One temperature.		

Molecular Weight 201.0500
Wiswesser Line Notation 1K1&1&1 &I
Evaluation B

$C_4H_{12}N_2$ (liq) 75MES/FIN

1,2-Diamino-2-methylpropane

Heat Capacity 298.15 K, C_p=234.56 J·mol^{-1}·K^{-1}

Temperature range 11 to 375 K.

Entropy 298.15 K, S=259.53 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 237.5 K, ΔH=15464 J·mol^{-1}

ΔS=65.11 J·mol^{-1}·K^{-1}

c,I/liq 256.1 K, ΔH=2230 J·mol^{-1}

ΔS=8.71 J·mol^{-1}·K^{-1}

Molecular Weight 88.1423

Wiswesser Line Notation ZX1&1&1Z

Evaluation A

$C_4H_{12}N_2O_4$ (c) 39SAT/SOG

Ammonium succinate

Heat Capacity 323 K, C_p=258.2 J·mol^{-1}·K^{-1}

Temperature range 0 to 100 °C. Mean value.

Molecular Weight 152.1498

Wiswesser Line Notation QV2VQ &ZH 2

Evaluation C

$C_4H_{12}N_2O_6$ (c) 39SAT/SOG

Ammonium tartrate

Heat Capacity 323 K, C_p=284.5 J·mol^{-1}·K^{-1}

Temperature range 0 to 100 °C. Mean value.

Molecular Weight 184.1486

Wiswesser Line Notation QVYQYQVQ &ZH 2

Evaluation C

$C_4H_{12}O_4Si$ (liq) 08KAII/KOE

Tetramethyl silicate; Methyl silicate

Heat Capacity C_p=319 J·mol^{-1}·K^{-1}

Temperature range 296 to 388 K. One value given for the entire temperature range. C_p given as 0.5011 cal·g^{-1}·K^{-1}.

Phase Changes

liq/g 394 K, ΔH=30900 J·mol^{-1}

ΔS=78.4 J·mol^{-1}·K^{-1}

Molecular Weight 152.2219

Wiswesser Line Notation 1O-SI-O1&O1&O1

Evaluation D

$C_4H_{12}O_4Si$ (liq) 85NKI/CHA

Tetramethyl silicate; Methyl silicate

Heat Capacity 298.15 K, C_p=240.5 J·mol^{-1}·K^{-1}

One temperature.

Molecular Weight 152.2219

Wiswesser Line Notation 1O-SI-O1&O1&O1

Evaluation B

$C_4H_{12}Pb$ (liq) 54STA/WAR

Tetramethyl lead

Phase Changes

c/liq 242.92 K, ΔH=10799 J·mol^{-1}

ΔS=44.43 J·mol^{-1}·K^{-1}

Molecular Weight 267.3388

Wiswesser Line Notation 1-PB-1&1&1

Evaluation B

$C_4H_{12}Pb$ (liq) 59GOO/SCO

Tetramethyl lead

Heat Capacity 298.15 K, C_p=202.5 J·mol^{-1}·K^{-1}

One temperature.

Entropy 298.15 K, S=319.99 J·mol^{-1}·K^{-1}

Molecular Weight 267.3388

Wiswesser Line Notation 1-PB-1&1&1

Evaluation B

$C_4H_{12}SZn$ (liq) 93LEB/KUL

Dimethylzinc dimethylsulfide complex

Heat Capacity 298.15 K, C_p=291.75 J·mol^{-1}·K^{-1}

Temperature range 5 to 330 K.

Entropy 298.15 K, S=389.53 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 238.08 K, ΔH=16521 J·mol^{-1}

ΔS=69.43 J·mol^{-1}·K^{-1}

Molecular Weight 157.5788

Wiswesser Line Notation 1-ZN-1 &1S1

Evaluation A

$C_4H_{12}SeZn$ (liq) 90LEB/KUL

Dimethylzinc dimethylselenium complex

Heat Capacity 298.15 K, C_p=287.18 J·mol^{-1}·K^{-1}

Temperature range 5 to 330 K.

Entropy 298.15 K, S=401.09 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 216.60 K, ΔH=14442 J·mol^{-1}

ΔS=66.673 J·mol^{-1}·K^{-1}

Molecular Weight 204.4788

Wiswesser Line Notation 1-ZN-1 &1-SE-1

Evaluation A

$C_4H_{12}Si$ (liq) 41AST/KEN

Tetramethylsilane; Silicon tetramethyl

Heat Capacity 290 K, C_p=197.90 J·mol^{-1}·K^{-1}

Temperature range 11 to 290 K.

Entropy 298.15 K, S=277.27 J·mol^{-1}·K^{-1}

Phase Changes

c,I/liq 171.04 K, ΔH=5969.7 J·mol^{-1}

ΔS=34.90 J·mol^{-1}·K^{-1}

c,II/liq 174.12 K, ΔH=6895 J·mol^{-1}

ΔS=39.60 J·mol^{-1}·K^{-1}

liq/g 299.80 K, ΔH=24204 J·mol^{-1}

ΔS=80.73 J·mol^{-1}·K^{-1}

P=101.325 kPa

Molecular Weight 88.2243

Wiswesser Line Notation 1-SI-1&1&1

Evaluation A

$C_4H_{12}Si$ (liq) 73SHI/ENO

Tetramethylsilane; Silicon tetramethyl

Heat Capacity 177.45 K, C_p=164.56 J·mol^{-1}·K^{-1}

Temperature range 2 to 26 K and 106 to 277.5 K.

Phase Changes

c,II/liq 70.983 K, ΔH=5840.9 J·mol^{-1}

ΔS=34.16 J·mol^{-1}·K^{-1}

Metastable form.

c,I/liq 174.049 K, ΔH=6741.3 J·mol^{-1}

ΔS=38.73 J·mol^{-1}·K^{-1}

Stable form.

Molecular Weight 88.2243

Wiswesser Line Notation 1-SI-1&1&1

Evaluation A

$C_4H_{12}Si$ (liq) 77HAR/ATA
Tetramethylsilane; Silicon tetramethyl
Heat Capacity 290 K, C_p=189.84 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 290 K, S=272.04 J·mol^{-1}·K^{-1}
Phase Changes
c,α/liq 165.920 K, ΔH=703 J·mol^{-1}
ΔS=4.24 J·mol^{-1}·K^{-1}
c,β/liq 171.016 K, ΔH=5878 J·mol^{-1}
ΔS=34.37 J·mol^{-1}·K^{-1}
c,γ/liq 174.074 K, ΔH=6874 J·mol^{-1}
ΔS=39.51 J·mol^{-1}·K^{-1}
Molecular Weight 88.2243
Wiswesser Line Notation 1-SI-1&1&1
Evaluation A

$C_4H_{12}Sn$ (liq) 54STA/WAR
Tetramethyl tin; Tetramethyl stannane
Phase Changes
c/liq 218.18 K, ΔH=9439 J·mol^{-1}
ΔS=43.26 J·mol^{-1}·K^{-1}
Molecular Weight 178.8488
Wiswesser Line Notation 1-SN-1&1&1
Evaluation B

$C_4H_{12}Sn$ (liq) 89SHE/RAB
Tetramethyl tin; Tetramethyl stannane
Heat Capacity 298.15 K, C_p=197.9 J·mol^{-1}·K^{-1}
Temperature range 5 to 313 K.
Entropy 298.15 K, S=310.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 218.05 K, ΔH=9234 J·mol^{-1}
ΔS=42.35 J·mol^{-1}·K^{-1}
Molecular Weight 178.8488
Wiswesser Line Notation 1-SN-1&1&1
Evaluation A

$C_4H_{12}TeZn$ (liq) 90LEB/KUL
Dimethylzinc dimethyltellerium complex
Heat Capacity 298.15 K, C_p=284.02 J·mol^{-1}·K^{-1}
Temperature range 13.87 to 300 K.
Entropy 298.15 K, S=420.71 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 195.34 K, ΔH=10942 J·mol^{-1}
ΔS=56.014 J·mol^{-1}·K^{-1}
Molecular Weight 253.1188
Wiswesser Line Notation 1-ZN-1 &1-TE-1
Evaluation A

$C_4H_{13}Cl_2N$ (c) 62CHA/WES3
Tetramethylammonium hydrogen dichloride
Heat Capacity 298.15 K, C_p=205.31 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K. Corrected for decomposition above 250 K.
Entropy 298.15 K, S=253.68 J·mol^{-1}·K^{-1}
Molecular Weight 146.0594
Wiswesser Line Notation 1K1&1&1 &G &GH
Evaluation A

$C_4H_{13}N_3$ (liq) 88BOB/KAM
Diethylenetriamine
Heat Capacity 313 K, C_p=254 J·mol^{-1}·K^{-1}
Temperature range 313 to 493 K.
Molecular Weight 103.1668
Wiswesser Line Notation Z2M2Z
Evaluation D

$C_4H_{16}Cl_4MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(ethylammonium) manganese II
Phase Changes
c,III/c,II 222 K, ΔH=43.6 J·mol^{-1}
ΔS=0.20 J·mol^{-1}·K^{-1}
c,II/c,I 424 K, ΔH=4.1 J·mol^{-1}
ΔS=0.009 J·mol^{-1}·K^{-1}
Molecular Weight 288.9338
Wiswesser Line Notation 2ZH2 .MN G4
Evaluation B

$C_4H_{20}Br_2N_4Pt$ (c) 89PAL/KUZ
Tetrakis(methylamine)platinum dibromide
Heat Capacity 298.15 K, C_p=299.00 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=399.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 164.5 K, ΔH=245 J·mol^{-1}
ΔS=1.49 J·mol^{-1}·K^{-1}
Molecular Weight 479.1268
Wiswesser Line Notation Z1 4 .PT E2
Evaluation A

$C_4H_{20}Br_4N_4Pt$ (c) 90PAL/KUZ
trans-Tetrakis(methylamine)platinum tetrabromide
Heat Capacity 300 K, C_p=351.20 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Molecular Weight 638.9348
Wiswesser Line Notation Z1 4 .PT E4 -T
Evaluation A

$C_4H_{20}I_2N_4Pt$ (c) 90PAL/KUZ
Tetramethylammonium platinum iodide
Heat Capacity 298.15 K, C_p=310.82 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=416.80 J·mol^{-1}·K^{-1}
Molecular Weight 573.1278
Wiswesser Line Notation Z1 4 .PT I2
Evaluation A

$C_5F_{11}N$ (liq) 63GOO/TOI
Perfluoropiperidine
Heat Capacity 298.15 K, C_p=296.77 J·mol^{-1}·K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=393.38 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 161.0 K, ΔH=6627.5 J·mol^{-1}
ΔS=41.16 J·mol^{-1}·K^{-1}
c,II/c,I 171.9 K, ΔH=1838.9 J·mol^{-1}
ΔS=10.70 J·mol^{-1}·K^{-1}
c,I/liq 274.12 K, ΔH=2816 J·mol^{-1}
ΔS= 10.27 J·mol^{-1}·K^{-1}
Molecular Weight 283.0441
Wiswesser Line Notation T6NTJ AF BF BF CF CF DF DF EF EF FF F
Evaluation A

C_5F_{12} (liq) 83CAM/DL
n-Perfluoropentane
Heat Capacity 293 K, C_p=188.3 J·mol^{-1}·K^{-1}
Interpolated data.
Molecular Weight 288.0358
Wiswesser Line Notation FXFFXFFXFFXFFXFFF
Evaluation C

$C_5F_{13}N$ (liq) 80ZHO/KOS
Perfluoromethyldiethylamine
Heat Capacity 298.15 K, C_p=337.46 J· mol^{-1}· K^{-1}
Temperature range 6 to 300 K.
Entropy 298.15 K, S=475.09 J· mol^{-1}· K^{-1}
Phase Changes
c,III/c,II 102.4 K
Metastable phase is a supercooled liquid in the range 102.4 to 126.0 K and forms a glass at 102.4 K.
c,II/c,I 126.0 K, ΔH=5532.1 J· mol^{-1}
ΔS=43.89 J· mol^{-1}· K^{-1}
c,I/liq 149.64 K, ΔH=7157.6 J· mol^{-1}
ΔS= 47.86 J· mol^{-1}· K^{-1}
Monotropic transition from metastable to stable phase.
Molecular Weight 321.0409
Wiswesser Line Notation FXFFXFF 2NXFFF
Evaluation A

$C_5F_{13}N$ (liq) 84GOL/KOL
Perfluoromethyldiethylamine
Phase Changes
c/liq 150.1 K, ΔH=4600 J· mol^{-1}
ΔS= 30.6 J· mol^{-1}· K^{-1}
Molecular Weight 321.0409
Wiswesser Line Notation FXFFXFF 2NXFFF
Evaluation A

$C_5H_3F_7O_2$ (liq) 84GOL/KOL
Methyl perfluorobutanoate
Phase Changes
c/liq 191.4 K, ΔH=11770 J· mol^{-1}
ΔS= 61.5 J· mol^{-1}· K^{-1}
Molecular Weight 228.0663
Wiswesser Line Notation XFFFXFFXFFVO1
Evaluation A

$C_5H_4N_4$ (c) 84KIR/DOM
Purine
Heat Capacity 298.15 K, C_p=106.9 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 120.1134
Wiswesser Line Notation T56 BN DM GN INJ
Evaluation B

$C_5H_4N_4O$ (c) 35STI/HUF
Hypoxanthine
Heat Capacity 298.5 K, C_p=134.52 J· mol^{-1}· K^{-1}
Temperature range 85 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=145.6 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 45.56 J· mol^{-1}· K^{-1}.
Molecular Weight 136.1128
Wiswesser Line Notation T56 BM DN FVM INJ
Evaluation B (Cp),C(S)

$C_5H_4N_4O_2$ (c) 35STI/HUF
Xanthine
Heat Capacity 298.5 K, C_p=151.34 J·mol^{-1}· K^{-1}
Temperature range 85 to 299 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=161.1 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 48.87 J· mol^{-1}· K^{-1}.
Molecular Weight 152.1122
Wiswesser Line Notation T56 BM DN FMVMVJ
Evaluation B (Cp),C(S)

$C_5H_4N_4O_3$ (c) 35STI/HUF
Uric acid
Heat Capacity 297.1 K, C_p=166.15 J· mol^{-1}· K^{-1}
Temperature range 85 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=173.2 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 50.25 J· mol^{-1}· K^{-1}.
Molecular Weight 168.1116
Wiswesser Line Notation T56 BMVM FMVMVJ
Evaluation B (Cp),C(S)

$C_5H_4O_2$ (liq) 1881REI
Furfural; Furfuraldehyde
Heat Capacity 298 K, C_p=158.2 J· mol^{-1}· K^{-1}
Temperature range 290 to 347 K.
Molecular Weight 96.0854
Wiswesser Line Notation T5OJ BVH
Evaluation D

$C_5H_4O_2$ (liq) 35MIL
Furfural; Furfuraldehyde
Heat Capacity
Temperature range 100 to 298 K. C_p data in thesis only.
Entropy 298.15 K, S=218.0 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 52.38 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 235.1 K, ΔH=14368 J· mol^{-1}
ΔS=61.1 J· mol^{-1}· K^{-1}
Molecular Weight 96.0854
Wiswesser Line Notation T5OJ BVH
Evaluation C

$C_5H_4O_2$ (liq) 62OME
Furfural; Furfuraldehyde
Heat Capacity 298.15 K, C_p=162.8 J· mol^{-1}· K^{-1}
Temperature range 288 to 412 K.
Molecular Weight 96.0854
Wiswesser Line Notation T5OJ BVH
Evaluation B

$C_5H_4O_2$ (liq) 67RAS/GAN
Furfural; Furfuraldehyde
Heat Capacity 293 K, C_p=159.5 J· mol^{-1}· K^{-1}
Temperature range 293 to 373 K.
Molecular Weight 96.0854
Wiswesser Line Notation T5OJ BVH
Evaluation C

$C_5H_5F_3O_2$ (liq) 84GOL/KOL
Trifluoromethyl (2-hydroxy-1-propenyl) ketone
Phase Changes
c/liq 232.4 K, ΔH=8450 J· mol^{-1}
ΔS=36.4 J· mol^{-1}· K^{-1}
Molecular Weight 154.0885
Wiswesser Line Notation QY1&U1VXFFF
Evaluation A

C_5H_5N (liq) 71HAL/BAL
1-Bicyclobutyl cyanide; 1-Cyanobicyclobutane
Heat Capacity 297 K, C_p=132.1 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 79.1012
Wiswesser Line Notation L33TJ ACN
Evaluation C

C_5H_5N (liq) 16BRA
Pyridine
Heat Capacity 283 K, C_p=130.5 J· mol^{-1}· K^{-1}
Mean value, 0 to 20°C.
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation C

C_5H_5N (liq) 17MAT/KRA
Pyridine
Heat Capacity 294 K, C_p=129.33 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation B

C_5H_5N (liq) 31SWI/RYB
Pyridine
Heat Capacity 290 K, C_p=135.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation B

C_5H_5N (liq) 31SWI/RYB2
Pyridine
Heat Capacity 273.4 K, C_p=135.35 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation B

C_5H_5N (liq) 34RAD/JUL
Pyridine
Heat Capacity 289 K, C_p=129.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation C

C_5H_5N (liq) 36PAR/TOD
Pyridine
Heat Capacity 298.1 K, C_p=134.93 J· mol^{-1}· K^{-1}
Temperature range 90 to 300 K.
Entropy 298.1 K, S=179.1 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 50.04 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 231.1 K, ΔH=8272 J· mol^{-1}
ΔS=35.79 J· mol^{-1}· K^{-1}
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation B(Cp),C(S)

C_5H_5N (liq) 36PEA/BAK
Pyridine
Heat Capacity 298.1 K, C_p=133.30 J· mol^{-1}· K^{-1}
Temperature range 90 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=210.41 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 89.33 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 230.38 K, ΔH=3100 J· mol^{-1}
ΔS=13.46 J· mol^{-1}· K^{-1}
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation B (Cp),C(S)

C_5H_5N (liq) 57MCC/DOU
Pyridine
Heat Capacity 298.15 K, C_p=132.72 J· mol^{-1}· K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S=177.90 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 231.49 K, ΔH=8278.5 J· mol^{-1}
ΔS=35.76 J· mol^{-1}· K^{-1}
Includes energy of anomaly at about 210 K.
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation A

C_5H_5N (liq) 58SWI/ZI
Pyridine
Heat Capacity 332 K, C_p=146.9 J· mol^{-1}· K^{-1}
Mean value 22 to 96°C.
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation C

C_5H_5N (liq) 61HUB/FR
Pyridine
Heat Capacity 298.15 K, C_p=133 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation B

C_5H_5N (liq) 67RAS/GA
Pyridine
Heat Capacity 293 K, C_p=193.4 J· mol^{-1}· K^{-1}
Temperature range 293 to 353 K.
Molecular Weight 79.1012
Wiswesser Line Notation T6NJ
Evaluation C

$C_5H_5N_5$ (c) 35STI/HU
Adenine
Heat Capacity 298.1 K, C_p=143.13 J· mol^{-1}· K^{-1}
Temperature range 88 to 298 K. Value is unsmoothed experiment datum.
Entropy 298.15 K, S=151.01 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 46.69 J· mol^{-1}· K^{-1}.
Molecular Weight 135.1280
Wiswesser Line Notation T56 BM DN FN HNJ IZ
Evaluation
B(Cp),C(S)

$C_5H_5N_5$ (c) 78K
Adenine
Heat Capacity 298 K, C_p=147.0 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 135.1280
Wiswesser Line Notation T56 BM DN FN HNJ IZ
Evaluation C

$C_5H_5N_5O$ (c) 35STI/HUF
Guanine
Heat Capacity 296.7 K, C_p=156.94 J· mol^{-1}· K^{-1}
Temperature range 84 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=160.2 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 45.06 J· mol^{-1}· K^{-1}.
Molecular Weight 151.1274
Wiswesser Line Notation T56 BN DM FN HNJ GZ IQ
Evaluation
B(Cp),C(S)

$C_5H_5N_5O$ (c) 81KIL
Guanine
Heat Capacity 298 K, C_p=160.7 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 151.1274
Wiswesser Line Notation T56 BN DM FN HNJ GZ IQ
Evaluation C

C_5H_6 (liq) 77LEB/LIT4
Cyclopentadiene
Heat Capacity 298.15 K, C_p=115.3 J· mol^{-1}· K^{-1}
Temperature range 14 to 330 K.
Entropy 298.15 K, S=182.7 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 176.60 K, ΔH=8010 J· mol^{-1}
ΔS=45.4 J· mol^{-1}· K^{-1}
Molecular Weight 66.1024
Wiswesser Line Notation L5 AHJ
Evaluation A

$C_5H_6F_6NP$ (c) 93HAN/OHT
Pyridium hexafluorophosphate
Heat Capacity 299.27 K, C_p=243.6 J· mol^{-1}· K^{-1}
Temperature range 4 to 320 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 217.83 K, ΔH=5040 J· mol^{-1}
ΔS= 25.0 J· mol^{-1}· K^{-1}
Assumption A.
c,II/c,I 217.83 K, ΔH=9740 J·mol^{-1}
ΔS= 36.0 J· mol^{-1}· K^{-1}
Assumption B.
Molecular Weight 225.0733
Wiswesser Line Notation T6NJ &HPFFFFFF
Evaluation A
Assumption A: crystal is completely in the disordered state at 320 K. Assumption B: disordered stae in the crystal is a function of the β/T^2 term, where β is the fitting parameter and short range order completely disappears at infinite temperature.

C_5H_6IN (c) 93HAN/OHT
Pyridium iodide
Heat Capacity 299.83 K, C_p=139.2 J· mol^{-1}· K^{-1}
Temperature range 4 to 320 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 249.65 K, ΔH=4070 J· mol^{-1}
ΔS=18.6 J· mol^{-1}· K^{-1}
Assumption A.
c,II/c,I 249.65 K, ΔH=7260 J· mol^{-1}
ΔS= 21.8 J·mol^{-1}· K^{-1}
Assumption B.
Molecular Weight 193.0069
Wiswesser Line Notation T6NJ &HI
Evaluation A
Assumption A: crystal is completely in the disordered state at 320 K. Assumption B: disordered state in the crystal is a function of β/T^2 term, where the fitting parameter and short range order completely disappears at infinite temperature.

$(C_5H_6NNaO_3)_n$ (c) 91ROL
Poly-L-glutamic acid, sodium salt
Heat Capacity 300 K, C_p=157.4 J·mol^{-1}· K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 151.0971
Wiswesser Line Notation /*V2YVO &-NA- &M*/ -L
Evaluation B

$(C_5H_6NNaO_3)_n$ (c) 93ROL/XEN
Poly-L-glutamic acid, sodium salt
Heat Capacity 300 K, C_p=157.4 J· mol^{-1}· K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 151.0971
Wiswesser Line Notation /*V2YVO &-NA- &M*/ -L
Evaluation B

$C_5H_6N_2$ (liq) 65CLE/WUL
Glutaronitrile; 1,3-Dicyanopropane
Heat Capacity 298.15 K, C_p=186.26 J· mol^{-1}· K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=239.45 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 244.21 K, ΔH=12585 J·mol^{-1}
ΔS=51.53 J· mol^{-1}· K^{-1}
Molecular Weight 94.1158
Wiswesser Line Notation NC3CN
Evaluation A

$C_5H_6N_2$ (c,II) 67RIB/WES
Dimethylmalonitrile; 2,2-Dicyanopropane
Heat Capacity 298.15 K, C_p=179.49 J·mol^{-1}· K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=187.95 J·mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 302.60 K, ΔH=9866 J· mol^{-1}
ΔS=32.60 J· mol^{-1}·K^{-1}
c,I/liq 307.47 K, ΔH=4054 J· mol^{-1}
ΔS=13.19 J·mol^{-1}· K^{-1}
Molecular Weight 94.1158
Wiswesser Line Notation NCX1&1&CN
Evaluation A

$C_5H_6N_2O_2$ (c) 1889EYK
Thymine
Phase Changes
c/liq 321.3 K, ΔH=17510 J· mol^{-1}
Molecular Weight 126.1146
Wiswesser Line Notation T6MVMVJ E1
Evaluation C

$C_5H_6N_2O_2$ (c) 73ALV/BIL
Thymine
Heat Capacity 298.15 K, C_p=151.4 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 126.1146
Wiswesser Line Notation T6MVMVJ E1
Evaluation C

$C_5H_6N_2O_2$ (c) 78KIL2
Thymine
Heat Capacity 298 K, C_p=150.2 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 126.1146
Wiswesser Line Notation T6MVMVJ E1
Evaluation C

C_5H_6O (liq) 65CAR/WES2
2-Methylfuran
Heat Capacity 298.15 K, C_p=143.72 J· mol^{-1}· K^{-1}
Temperature range 5 to 310 K.
Entropy 298.15 K, S=213.89 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 181.90 K, ΔH=8552 J· mol^{-1}
ΔS=47.01 J· mol^{-1}· K^{-1}
Molecular Weight 82.1018
Wiswesser Line Notation T5OJ B1
Evaluation A

$C_5H_6O_2$ (liq) 35MIL
Furfuryl alcohol
Entropy 298.15 K, S=215.5 J·mol^{-1}· K^{-1}
Extrapolation below 90 K, 42.97 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 253.5 K, ΔH=14811 J· mol^{-1}
ΔS=58.4 J· mol^{-1}· K^{-1}
Molecular Weight 98.1012
Wiswesser Line Notation T5OJ B1Q
Evaluation C

$C_5H_6O_2$ (liq) 50HOU/MAS
Furfuryl alcohol
Heat Capacity 303 K, C_p=193.3 J· mol^{-1}· K^{-1}
Temperature range 303 to 333 K.
Molecular Weight 98.1012
Wiswesser Line Notation T5OJ B1Q
Evaluation B

$C_5H_6O_2$ (liq) 56PAR/KEN
Furfuryl alcohol
Heat Capacity 298.15 K, C_p=204.01 J· mol^{-1}· K^{-1}
Temperature range 90 to 300 K.
Entropy 298.1 K, S=215.9 J· mol^{-1}· K^{-1}
Extrapolation below 80 K, 48.99 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 258.6 K, ΔH=13129 J· mol^{-1}
ΔS=50.77 J· mol^{-1}· K^{-1}
Molecular Weight 98.1012
Wiswesser Line Notation T5OJ B1Q
Evaluation B
(C_p),C(S)

C_5H_6S (gls) 68CAR/WES
2-Methylthiophene
Heat Capacity 199.70 K, C_p=97.91 J·mol^{-1}· K^{-1}
Temperature range 110 to 200 K. Value is unsmoothed experimental datum.
Molecular Weight 98.1624
Wiswesser Line Notation T5SJ B1
Evaluation A Data for glass transition region.

C_5H_6S (liq) 56PEN/FIN
2-Methylthiophene
Heat Capacity 298.15 K, C_p=149.83 J·mol^{-1}·K^{-1}
Temperature range 12 to 340 K.
Entropy 298.15 K, S=218.49 J·mol^{-1}· K^{-1}
Phase Changes
c/liq 207.79 K, ΔH=11142 J· mol^{-1}
ΔS=53.62 J· mol^{-1}· K^{-1}
Molecular Weight 98.1624
Wiswesser Line Notation T5SJ B1
Evaluation A

C_5H_7N (liq) 71HAL/BAL
Cyclobutyl cyanide; Cyanocyclobutane
Heat Capacity 297 K, C_p=146.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 81.1170
Wiswesser Line Notation L4TJ ACN
Evaluation C

C_5H_7N (liq) 86STE/CHE
N-Methylpyrrole
Heat Capacity 298.15 K, C_p=150.06 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=200.48 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 216.912 K
Molecular Weight 81.1170
Wiswesser Line Notation T5NJ A1
Evaluation A

C_5H_7N (liq) 87MES/TOL
N-Methylpyrrole
Heat Capacity 298.15 K, C_p=150.06 J· mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=200.48 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 216.912 K, ΔH=7824.8 J· mol^{-1}
ΔS=36.07 J· mol^{-1}· K^{-1}
Molecular Weight 81.1170
Wiswesser Line Notation T5NJ A1
Evaluation A

C_5H_7N (liq) 88MES/TOL
N-Methylpyrrole
Heat Capacity 298.150 K, C_p=150.058 J·mol^{-1}· K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S=200.519 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 216.912 K, ΔH=7824.77 J·mol^{-1}
Molecular Weight 81.1170
Wiswesser Line Notation T5NJ A1
Evaluation A

$(C_5H_7NO)_n$ (c) 91ROI
Poly-L-proline
Heat Capacity 300 K, C_p=115.7 J· mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 97.1164
Wiswesser Line Notation /T5NTJ A* BV*/ -L
Evaluation B

$(C_5H_7NO)_n$ (c) 93ROL/XEN
Poly-L-proline
Heat Capacity 300 K, C_p=115.7 J· mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 97.1164
Wiswesser Line Notation /T5NTJ A* BV*/ -L
Evaluation B

$C_5H_7NO_2$ (liq) 87KHO/BUG
Ethyl cyanoacetate
Heat Capacity 298.15 K, C_p=220.22 J· mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 298.15 K, S=177.45 J·mol^{-1}· K^{-1}
S value does not agree with 91ISK/ISM.
Phase Changes
c,II/c,I 162.5 K
Glass transition. Transition temperature estimated from graph.
c,I/liq 246.8 K, ΔH=11780 J· mol^{-1}
ΔS=47.73 J·mol^{-1}· K^{-1}
Molecular Weight 113.1158
Wiswesser Line Notation NC1VO2
Evaluation A

$C_5H_7NO_2$ (liq) 91ISK/ISM
Ethyl cyanoacetate
Heat Capacity 300 K, C_p=222.04 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 300 K, S=275.33 J·mol^{-1}· K^{-1}
S value does not agree with 87 KHO/BUG.
Molecular Weight 113.1158
Wiswesser Line Notation NC1VO2
Evaluation A T(glass)=160 K.

C_5H_8 (liq) 36PAR/TOD2
1,4-Pentadiene
Heat Capacity 292.5 K, C_p=146.61 J·mol^{-1}· K^{-1}
Temperature range 82 to 293 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=338.7 J· mol^{-1}· K^{-1}
Extrapolation below 80 K, 47.11 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 124.3 K, ΔH=6142 J· mol^{-1}
ΔS=49.41 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation 1U3U1
Evaluation B (C_p),C(S)

C_5H_8 (liq) 70MES/TOD
1,4-Pentadiene
Heat Capacity 298.15 K, C_p=146.82 J· mol^{-1}·K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=248.86 J·mol^{-1}· K^{-1}
Phase Changes
c/liq 124.9 K, ΔH=6073.1 J· mol^{-1}
ΔS=48.620 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation 1U3U1
Evaluation A

C_5H_8 (liq) 37BEK/WOO
2-Methyl-1,3-butadiene; Isoprene
Heat Capacity 298.2 K, C_p=152.6 J· mol^{-1}· K^{-1}
Temperature range 20 to 300 K.
Entropy 298.2 K, S=229.3 J· mol^{-1}·K^{-1}
Phase Changes
c/liq 126.4 K, ΔH=4830 J· mol^{-1}
ΔS=38.21 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation 1UY1&1U1
Evaluation A

C_5H_8 (liq) 65WAR/PET
2-Methyl-1,3-butadiene; Isoprene
Heat Capacity 298.15 K, C_p=152.5 J· mol^{-1}· K^{-1}
Temperature range 20 to 300 K. A reexamination of 37BEK/WOO.
Entropy 298.15 K, S=229.2 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 126.4 K, ΔH=4830 J· mol^{-1}
ΔS=38.21 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation 1UY1&1U1
Evaluation A

C_5H_8 (liq) 70MES/TOD
2-Methyl-1,3-butadiene; Isoprene
Heat Capacity 298.15 K, C_p=151.08 J· mol^{-1}· K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=228.28 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 127.27 K, ΔH=4924.6 J· mol^{-1}
ΔS=38.694 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation 1UY1&1U1
Evaluation A

C_5H_8 (liq) 69GOO
3-Methyl-1,2-butadiene
Heat Capacity 298.15 K, C_p=151.1 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 68.1182
Wiswesser Line Notation 1Y1&UCU1
Evaluation B

C_5H_8 (liq) 70MES/TOD
3-Methyl-1,2-butadiene
Heat Capacity 298.15 K, C_p=152.42 J· mol^{-1}· K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=231.79 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 159.53 K, ΔH=7956.3 J· mol^{-1}
ΔS=49.873 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation 1Y1&UCU1
Evaluation A

C_5H_8 (liq) 70MES/TOD
1-cis-3-Pentadiene
Heat Capacity 298.15 K, C_p=146.57 J· mol^{-1}· K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=233.25 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 132.35 K, ΔH=5638.8 J· mol^{-1}
ΔS=42.605 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation 2U2U1 -C
Evaluation A

C_5H_8 (liq) 70MES/TOD
1-trans-3-Pentadiene
Heat Capacity 298.15 K, C_p=149.33 J· mol^{-1}· K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=227.11 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 185.71 K, ΔH=7143.8 J· mol^{-1}
ΔS=38.468 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation 2U2U1 -T
Evaluation A

C_5H_8 (liq) 70MES/TOD
2,3-Pentadiene
Heat Capacity 298.15 K, C_p=152.34 J· mol^{-1}· K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=237.32 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 147.52 K, ΔH=6127.9 J· mol^{-1}
ΔS=44.929 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation 2UCU2
Evaluation A

C_5H_8 (liq) 70MES/TOD
1,2-Pentadiene
Heat Capacity 298.15 K, C_p=150.83 J· mol^{-1}·K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=244.97 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 135.89 K, ΔH=7559.2 J· mol^{-1}
ΔS=55.628 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation 3UCU1
Evaluation A

C_5H_8 (liq) 50SCO/FIN2
Spiropentane
Heat Capacity 298.15 K, C_p=134.52 J· mol^{-1}· K^{-1}
Temperature range 12 to 312 K.
Entropy 298.15 K, S=193.68 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 166.14 K, ΔH=6433.3 J·mol^{-1}
ΔS=38.72 J· mol^{-1}· K^{-1}
liq/g 312.13 K, ΔH=26748 J· mol^{-1}
ΔS= 85.70 J· mol^{-1}· K^{-1}
P=101.325 kPa
Molecular Weight 68.1182
Wiswesser Line Notation L3XT J A-& AL3XTJ
Evaluation A

C_5H_8 (liq) 75LEB/LEB
Methylenecyclobutane
Heat Capacity 298.15 K, C_p=133.6 J· mol^{-1}· K^{-1}
Temperature range 6 to 320 K.
Entropy 298.15 K, S=210.6 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 138.621 K. ΔH=5756 J· mol^{-1}
ΔS=41.6 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation L4YTJ AU1
Evaluation A

C_5H_8 (liq) 78LEB/TSV
Methylenecyclobutane
Heat Capacity 298.15 K, C_p=133.6 J· mol^{-1}· K^{-1}
Temperature range 12 to 315 K.
Entropy 298.15 K, S=210.6 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 138.62 K, ΔH=5755 J· mol^{-1}
ΔS=41.6 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation L4YTJ AU1
Evaluation A Q

C_5H_8 (liq) 78LEB/TSV
Methylenecyclobutane
Heat Capacity 298.15 K, C_p=133.6 J· mol^{-1}· K^{-1}
Temperature range 12 to 315 K.
Entropy 298.15 K, S=210.6 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 138.62 K, ΔH=5755 J· mol^{-1}
ΔS=41.6 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation L4YTJ AU1
Evaluation A

C_5H_8 (liq) 81FIN/ME
Methylenecyclobutane
Heat Capacity 298.15 K, C_p=131.1 J· mol^{-1}· K^{-1}
Temperature range 12 to 301 K. Equation also given for temperatur
range 146 to 301 K.
Entropy 298.15 K, S=210.2 J· mol^{-1}· K^{-1}
Phase Changes
c,I/liq 138.535 K, ΔH=5861.4 J· mol^{-1}
ΔS=42.31 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation L4YTJ AU1
Evaluation A

C_5H_8 (liq) 48HUF/EA
Cyclopenten
Heat Capacity 298.15 K. C_p=122.38 J· mol^{-1}· K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=201.25 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 87.07 K, ΔH=479.5 J· mol^{-1}
ΔS=9.51 J· mol^{-1}· K^{-1}
c,I/liq 138.13 K, ΔH=3363.4 J· mol^{-1}
ΔS= 24.35 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation L5UTJ
Evaluation A

$(C_5H_8)_n$ (c) 35BEK/MA
Rubber; Late
Heat Capacity 280 K, C_p=122.9 J· mol^{-1}· K^{-1}
Temperature range 15 to 280 K. Values per C_5H_8 unit.
Phase Changes
c/amorp 284 K, ΔH=4761 J· mol^{-1}
ΔS=16.8 J· mol^{-1}· K^{-1}
Corrected for premelting, 255 to 284 K. Value per C_5H_8 unit. 'Fusio
actually transition to amorphous form.
Molecular Weight 68.1182
Wiswesser Line Notation /*Y1&U3*-C/
Evaluation C
Latex digested with steam at 190°C, and extracted with alcohol and wate

$(C_5H_8)_n$ (amorp) 35BEK/MAT
Rubber; Latex
Heat Capacity 298.15 K, C_p=128.1 J· mol^{-1}· K^{-1}
Temperature range 14 to 320 K. Value per C_5H_8 unit.
Entropy 298.15 K, S=128.1 J· mol^{-1}· K^{-1}
From graphical integration of C_p data of crystal, entropy of fusion, and C_p data of amorphous above 284 K.
Molecular Weight 68.1182
Wiswesser Line Notation /*Y1&U3*-C/
Evaluation C
Latex digested with steam at 190°C, and extracted with alcohol and water.

$(C_5H_8)_n$ (amorp) 65WAR/PET
Rubber; Latex
Heat Capacity 298.15 K, C_p=128.3 J· mol^{-1}· K^{-1}
Temperature range 14 to 320 K. A reexamination of 35BER/MAT.
Entropy 298.15 K, S=128.6 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation /*Y1&U3*-C/
Evaluation A T(glass)=199 K.

$(C_5H_8)_n$ (liq) 76LEB/RAB2
Polypentenamer
Heat Capacity 298.15 K, C_p=132.5 J· mol^{-1}· K^{-1}
Temperature range 14 to 322 K.
Entropy 298.15 K, S=149.7 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 293 K, ΔH=8080 J· mol^{-1}
ΔS= 27.58 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation /*YU4*/
Evaluation A
T(glass)=173.5 K.

$(C_5H_8)_n$ (gls) 77LEB/LIT3
cis-Polypentenamer
Heat Capacity 298.15 K, C_p=128.5 J· mol^{-1}· K^{-1}
Temperature range 7 to 325 K.
Entropy 298.15 K, S=140.4 J mol^{-1} K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation /*YU4* -C/
Evaluation A
T(glass)=158 K, transition from glass to highly elastic phase.

$(C_5H_8)_n$ (gls) 77LEB/RAB3
cis-Polypentenamer
Heat Capacity 300 K, C_p=130 J· mol^{-1}· K^{-1}
Temperature range 7 to 330 K. Glassy state. Data given graphically. Value estimated from graph.
Entropy 300 K, S=152 J· mol^{-1}· K^{-1}
Highly elastic state.
Phase Changes
c/liq 232 K, ΔH=5200 J· mol^{-1}
ΔS=22.4 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation /*YU4* -C/
Evaluation B
T(glass)=156 K.

$(C_5H_8)_n$ (gls) 77LEB/RAB3
trans-Polypentenamer
Heat Capacity 300 K, C_p=136 J· mol^{-1}· K^{-1}
Temperature range 7 to 330 K. Glassy state. Data given graphically. Value estimated from graph.
Entropy 300 K, S=150 J mol^{-1} K^{-1}
Highly elastic state.
Phase Changes
c/liq 310 K, ΔH=8900 J· mol^{-1}
ΔS=28.7 J· mol^{-1}· K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation /*YU4* -T/
Evaluation B
T(glass)=175 K.

$C_5H_8Br_4$ (c) 59WES
2,2-Bis(bromomethyl)-1,3-dibromopropane; Pentaerythrityl tetrabromide
Heat Capacity 298.15 K, C_p=213.80 J· mol^{-1}· K^{-1}
Based on data 10 to 350 K, to be reported elsewhere.
Entropy 298.15 K, S=291.12 J· mol^{-1}· K^{-1}
Molecular Weight 387.7342
Wiswesser Line Notation E1X1E1E1E
Evaluation B

$C_5H_8Br_4$ (c) 62PAY/WES
2,2-Bis(bromomethyl)-1,3-dibromopropane; Pentaerythrityl tetrabromide
Heat Capacity 298.15 K, C_p=213.80 J· mol^{-1}· K^{-1}
Temperature range 6 to 300 K. Anomalous region, 260 to 290 K.
Entropy 298.15 K, S=291.12 J· mol^{-1}· K^{-1}
Molecular Weight 387.7342
Wiswesser Line Notation E1X1E1E1E
Evaluation A

$C_5H_8Br_4$ (c) 65CLE/WON
2,2-Bis(bromomethyl)-1,3-dibromopropane; Pentaerythrityl tetrabromide
Heat Capacity 298.15 K, C_p=218.57 J· mol^{-1}· K^{-1}
Temperature range 250 to 460 K.
Entropy 298.15 K, S=297.12 J· mol^{-1}· K^{-1}
Based on low temperature data of 62PAY/WES.
Phase Changes
c/liq 433.45 K, ΔH=27966 J· mol^{-1}
ΔS= 64.52 J· mol^{-1}· K^{-1}
Molecular Weight 387.7342
Wiswesser Line Notation E1X1E1E1E
Evaluation A

$C_5H_8Cl_2O$ (liq) 62DAI/EVA2
3,3-Bis-(chloromethyl)oxacyclobutane
Heat Capacity 300 K, C_p=218.7 J· mol^{-1}· K^{-1}
Temperature range 20 to 310 K.
Entropy 300 K, S=274.4 J· mol^{-1}· K^{-1}
Phase Changes
c,l/liq 292.16 K, ΔH=16944 J· mol^{-1}
ΔS=58.00 J· mol^{-1}· K^{-1}
Premelting occurs above 250 K.
Molecular Weight 155.0236
Wiswesser Line Notation T4OTJ C1G C1G
Evaluation A

$(C_5H_8Cl_2O)_n$ (c) 62DAI/EVA2
3,3-Bis-(chloromethyl)polyoxacyclobutane; Penton
Heat Capacity 300 K, C_p=179.8 J· mol^{-1}· K^{-1}
Temperature range 20 to 310 K.
Entropy 300 K, S=191.0 J· mol^{-1}· K^{-1}
Molecular Weight 155.0236
Wiswesser Line Notation /*T4OTJ C1G C1G*/
Evaluation A

$C_5H_8Cl_2O_2$ (liq) 1881REI
Ethyl 2,3-dichloropropanoate; Ethyl α,β- dichloropropionate
Heat Capacity 298 K, C_p=248.9 J· mol^{-1}· K^{-1}
Temperature range 290 to 465 K.
Molecular Weight 171.0230
Wiswesser Line Notation G1YGVO2
Evaluation D

$C_5H_8Cl_4$ (c) 59WES
2,2-Bis(chloromethyl)-1,3-dichloropropane; Pentaerythrityl tetrachloride
Heat Capacity 298.15 K, C_p=198.49 J· mol^{-1}· K^{-1}
Based on data 10 to 350 K, to be reported elsewhere.
Entropy 298.15 K, S=257.48 J· mol^{-1}· K^{-1}
Molecular Weight 209.9302
Wiswesser Line Notation G1X1G1G1G
Evaluation B

$C_5H_8Cl_4$ (c) 62PAY/WES
2,2-Bis(chloromethyl)-1,3-dichloropropane; Pentaerythrityl tetrachloride
Heat Capacity 298.15 K, C_p=198.49 J· mol^{-1}· K^{-1}
Temperature range 6 to 300 K. Anomalous region, 220 to 240 K.
Entropy 298.15 K, S=257.48 J· mol^{-1}· K^{-1}
Molecular Weight 209.9302
Wiswesser Line Notation G1X1G1G1G
Evaluation A

$C_5H_8Cl_4$ (c,II) 65CLE/WON
2,2-Bis(chloromethyl)-1,3-dichloropropane; Pentaerythrityl tetrachloride
Heat Capacity 298.15 K, C_p=186.94 J· mol^{-1}· K^{-1}
Temperature range 290 to 420 K.
Entropy 298.15 K, S=240.62 J·mol^{-1}· K^{-1}
Based on low temperature data of 62PAY/WES.
Phase Changes
c,II/c,I 368.23 K, ΔH=22259 J· mol^{-1}
ΔS=60.45 J· mol^{-1}· K^{-1}
Molecular Weight 209.9302
Wiswesser Line Notation G1X1G1G1G
Evaluation A

$C_5H_8F_4$ (c,I) 59WES
2,2-Bis(fluoromethyl)-1,3-difluoropropane; Pentaerythrityl tetrafluoride
Heat Capacity 298.15 K, C_p=212.55 J· mol^{-1}· K^{-1}
Based on data 10 to 350 K, to be reported elsewhere.
Entropy 298.15 K, S=290.16 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 249.40 K, ΔH=13210 J· mol^{-1}
ΔS=53.0 J· mol^{-1}· K^{-1}
Lambda transition, no details.
Molecular Weight 144.1118
Wiswesser Line Notation F1X1F1F1F
Evaluation B

$C_5H_8F_4$ (c) 64TRO/WES
2,2-Bis(fluoromethyl)-1,3-difluoropropane; Pentaerythrityl tetrafluoride
Heat Capacity
Data on solid and liquid 295 to 385 K, supplementing previous work of Westrum and Payne.
Phase Changes
c,I/liq 367.43 K, ΔH=5142 J· mol^{-1}
ΔS=13.99 J· mol^{-1}· K^{-1}
Molecular Weight 144.1118
Wiswesser Line Notation F1X1F1F1F
Evaluation B

$C_5H_8I_4$ (c) 59WE
2,2-Bis(iodomethyl)-1,3-diiodopropane; Pentaerythrityl tetraiodide
Heat Capacity 298.15 K, C_p=207.69 J· mol^{-1}· K^{-1}
Based on data 10 to 350 K, to be reported elsewhere.
Molecular Weight 575.7362
Wiswesser Line Notation I1X1I1I1I
Evaluation B

$C_5H_8I_4$ (c) 62PAY/WE
2,2-Bis(iodomethyl)-1,3-diiodopropane; Pentaerythrityl tetraiodide
Heat Capacity 298.15 K, C_p=207.70 J· mol^{-1}· K^{-1}
Temperature range 6 to 300 K.
Entropy 298.15 K, S=316.73 J· mol^{-1}· K^{-1}
Molecular Weight 575.7362
Wiswesser Line Notation I1X1I1I1I
Evaluation A

$C_5H_8I_4$ (c) 65CLE/WO
2,2-Bis(iodomethyl)-1,3-diiodopropane; Pentaerythrityl tetraiodide
Heat Capacity 298.15 K, C_p=209.62 J· mol^{-1}· K^{-1}
Temperature range 260 to 420 K.
Entropy 298.15 K, S=316.94 J· mol^{-1}· K^{-1}
Based on low temperature data of 62PAY/WES
Molecular Weight 575.7362
Wiswesser Line Notation I1X1I1I1I
Evaluation A

$C_5H_8N_2$ (c) 92JIM/RC
2-Ethylimidazole
Heat Capacity 298.15 K, C_p=147.08 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 96.1316
Wiswesser Line Notation T5N CMJ B2
Evaluation A

$C_5H_8N_4O_{12}$ (c) 91YIN/L
Petaerythritol tetranitrate; PETN
Heat Capacity 298 K, C_p=353.8 J· mol^{-1}· K^{-1}
Temperature range 293 to 333 K. C_p value reported at 298 K is 1.1 J/g· K.
Molecular Weight 316.1378
Wiswesser Line Notation WNO1X1ONW&1ONQ&1ONW
Evaluation B
Desensitized PETN.

$C_5H_8O_2$ (liq) 52ERD/J
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 293 K, C_p=188.49 J· mol^{-1}· K^{-1}
Temperature range 20 to 50°C.
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation C

$C_5H_8O_2$ (c) 58SOC/TI
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 210 K, C_p=150.2 J· mol^{-1}· K^{-1}
Temperature range 60 to 210 K.
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation B

$C_5H_8O_2$ (liq) 62MEL
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 298.15 K, C_p=210.55 J· mol^{-1}· K^{-1}
Temperature range 60 to 300 K.
Phase Changes
c/liq 225 K, ΔS=54.4 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation B

$C_5H_8O_2$ (liq) 71LEB/RAB
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 300 K, C_p=192.4 J· mol^{-1}· K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, S=266.2 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 225.59 K, ΔH=14435 J· mol^{-1}
ΔS=64.0 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation B

$C_5H_8O_2$ (liq) 84VAS/PET
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 300 K, C_p=192.42 J· mol^{-1}· K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, S=266.2 J· mol^{-1}· K^{-1}
Phase Changes
c,l/liq 225.59 K
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation B

$C_5H_8O_2$ (liq) 85KAR/ABD
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 298.15 K, C_p=215.3 J· mol^{-1}· K^{-1}
Temperature range 225 to 350 K. Equation only. C_p (J· kg^{-1}· K^{-1})=114.1+6.8299 T. C_p data calculated from equation.
Phase Changes
c/liq 225.6 K
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation B

$C_5H_8O_2$ (liq) 85KAR/ABD2
Methyl 2-methylpropenoate; Methyl methacrylate
Phase Changes
c/liq 225.5 K, ΔH=13451 J· mol^{-1}
ΔS=59.65 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation A

$C_5H_8O_2$ (liq) 85KAR/SAI
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 298.15 K, C_p=215.3 J· mol^{-1}· K^{-1}
Temperature range 90 to 350 K. C_p(c)=280.01+ 4.96T J/kg· K (103 to 212 K). C_p(liq)=114.12+6.83T J/kg· K (225.6 to 350 K). C_p data calculated from equation.
Phase Changes
c/liq 225.6 K
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation B

$C_5H_8O_2$ (liq) 86ZHA/BEN
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 298.15 K, C_p=191.09 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation A

$C_5H_8O_2$ (liq) 1881REI
2-Propenyl ethanoate; Allyl acetate
Heat Capacity 298 K, C_p=184.1 J· mol^{-1}· K^{-1}
Temperature range 292 to 382 K.
Molecular Weight 100.1170
Wiswesser Line Notation 1VO2U1
Evaluation D

$C_5H_8O_2$ (liq) 69MEL/MER
Acetylacetone, enol form
Heat Capacity 298.15 K, C_p=208.2 J· mol^{-1}· K^{-1}
Temperature range 80 to 300 K. C_{sat}(liq)=0.8978+3.964×10^{-3}T J·K^{-1}·g^{-1} (260 to 300 K); C_{sat}(298.15 K) given as 2.080 J· K^{-1}· g^{-1}.
Entropy 298.15 K, S=261.4 J· mol^{-1}· K^{-1}
Extrapolated below 90 K. S(298.15 K) given as 2.611 J· K^{-1}· g^{-1}.
Phase Changes
c/liq 254.8 K, ΔH=14497 J· mol^{-1}
ΔS=56.90 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation QY1&U1V1
Evaluation A
(C_p), B(S) C_p(solid)=0.4257 + 3.674×10^{-3} T J· K^{-1}· g^{-1} (90 to 200 K).

$C_5H_8O_2$ (liq) 81EVS/LEB
δ-Valerolactone
Heat Capacity 298.15 K, C_p=171.6 J· mol^{-1}· K^{-1}
Temperature range 5 to 340 K.
Entropy 298.15 K, S=219.0 J· mol^{-1}· K^{-1}
Phase Changes
c,IV/c,III 118.1 K, ΔH=457 J· mol^{-1}
ΔS=3.88 J· mol^{-1}· K^{-1}
c,III/c,II 122-155 K, ΔH=310 J· mol^{-1}
ΔS= 2.2 J· mol^{-1}· K^{-1}
c,II/c,I 180-225 K, ΔH=205 J· mol^{-1}
ΔS=0.90 J· mol^{-1}· K^{-1}
c,I/liq 262.82 K, ΔH=10530 J· mol^{-1}
ΔS= 39.46 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation T6OVTJ
Evaluation A

$C_5H_8O_2$ (liq) 82YEV/LEB
δ-Valerolactone
Heat Capacity 298.15 K, C_p=171.6 J· mol^{-1}· K^{-1}
Temperature range 5 to 340 K.
Entropy 298.15 K, S=219.0 J· mol^{-1}· K^{-1}
Phase Changes
c,IV/c,III 118 K, ΔH=457 J· mol^{-1}
ΔS=3.88 J· mol^{-1}· K^{-1}
c,III/c,II 122-155 K, ΔH=310 J· mol^{-1}
ΔS= 2.2 J· mol^{-1}· K^{-1}
c,II/c,I 180-225 K, ΔH=205 J· mol^{-1}
ΔS=0.90 J· mol^{-1}· K^{-1}
c,I/liq 262.82 K, ΔH=10530 J· mol^{-1}
ΔS= 39.46 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation T6OVTJ
Evaluation A

$C_5H_8O_2$ (liq) 83LEB/YEV
δ-Valerolactone
Heat Capacity 298.15 K, C_p=171.6 J· mol^{-1}· K^{-1}
Temperature range 13.8 to 340 K.
Entropy 298.15 K, S=219.0 J· mol^{-1}· K^{-1}
Phase Changes
c,IV/c,III 118.1 K, ΔH=457 J· mol^{-1}
ΔS=3.88 J· mol^{-1}· K^{-1}
c,III/c,II 122-155 K, ΔH=310 J· mol^{-1}
ΔS=2.2 J· mol^{-1}· K^{-1}
c,II/c,I 180-225 K, ΔH=205 J· mol^{-1}
ΔS=0.90 J· mol^{-1}· K^{-1}
c,I/liq 262.82 K, ΔH=10530 J· mol^{-1}
ΔS= 39.46 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation T6OVTJ
Evaluation A

$(C_5H_8O_2)_n$ (c) 58SOC/TRA
Poly(methyl methacrylate); PMMA
Heat Capacity 260 K, C_p=111.7 J· mol^{-1}· K^{-1}
Temperature range 60 to 260 K. Values per monomer unit.
Molecular Weight 100.1170
Wiswesser Line Notation /*1X*1&VO1/
Evaluation B

$(C_5H_8O_2)_n$ (c) 62MEL
Poly(methyl methacrylate); PMMA
Heat Capacity 298.15 K, C_p=130.8 J· mol^{-1}· K^{-1}
Temperature range 16 to 300 K. C_p(c)=0.0437 + 0.00118T - 1.25×10^{-6}T^2 cal· deg^{-1}· g^{-1} (200 to 300 K).
Entropy 298.15 K, S=157.6 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation /*1X*1&VO1/
Evaluation B

$(C_5H_8O_2)_n$ (c) 67PAV/RAB
Poly(methyl methacrylate); PMMA
Heat Capacity 298 K, C_p=125.6 J· mol^{-1}· K^{-1}
Temperature range 298 to 463 K. C_p=0.265 + 1.39×10^{-3}T cal· g· °C (20 to 90°C). Value calculated from equation.
Molecular Weight 100.1170
Wiswesser Line Notation /*1X*1&VO1/
Evaluation B T(glass)=378 K.

$(C_5H_8O_2)_n$ (c) 71LEB/RAB
Poly(methyl methacrylate); PMMA
Heat Capacity 300 K, C_p=131.8 J· mol^{-1}· K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, S=145.1 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation /*1X*1&VO1/
Evaluation B

$(C_5H_8O_2)_n$ (c) 91YIN/LIU
Poly(methylmethacrylate); PMMA
Heat Capacity 298 K, C_p=137.9 J· mol^{-1}· K^{-1}
Temperature range 290 to 375 K. C_p value reported at 298 K is 1.377 J/g· K.
Molecular Weight 100.1170
Wiswesser Line Notation /*X*1&VO1/
Evaluation B

$(C_5H_8O_2)_n$ (c) 81EVS/LEB
Poly-δ-valerolactone
Heat Capacity 298.15 K, C_p=136.3 J· mol^{-1}· K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=153.6 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 331 K, ΔH=18200 J· mol^{-1}
ΔS= 54.9 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation /*OV4*/
Evaluation A

$(C_5H_8O_2)_n$ (c) 82YEV/LEI
Poly-δ-valerolactone
Heat Capacity 298 K, C_p=136.3 J· mol^{-1}· K^{-1}
Temperature range 13.8 to 340 K.
Entropy 298 K, S=153.6 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 331 K, ΔH=18200 J· mol^{-1}
ΔS= 54.9 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation /*OV4*/
Evaluation A T(glass)=207 K.

$(C_5H_8O_2)_n$ (gls) 81EVS/LEI
Poly-δ-valerolactone
Heat Capacity 298.15 K, C_p=183.2 J· mol^{-1}· K^{-1}
Temperature range 5 to 331 K.
Entropy 298.15 K, S=204.0 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation /*OV4*/
Evaluation A T(glass)=207 K.

$(C_5H_8O_2)_n$ (gls) 82YEV/LEI
Poly-δ-valerolactone
Heat Capacity 298.15 K, C_p=183.2 J· mol^{-1}· K^{-1}
Temperature range 5 to 331 K.
Entropy 298.15 K, S=204.0 J· mol^{-1}· K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation /*OV4*/
Evaluation A T(glass)=207 K.

$C_5H_8O_4$ (liq) 92VER/BE
Malonic acid dimethyl ester
Heat Capacity 298.15 K, C_p=210.1 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 132.1158
Wiswesser Line Notation 1OV1VO1
Evaluation B

$C_5H_8O_4$ (c) 74CIN/BE
Glutaric acid
Phase Changes
c,II/c,I 348.5 K, ΔH=2464 J· mol^{-1}
ΔS= 7.07 J· mol^{-1}· K^{-1}
c,I/liq 371.0 K, ΔH=20899 J· mol^{-1}
ΔS= 56.32 J· mol^{-1}· K^{-1}
Molecular Weight 132.1158
Wiswesser Line Notation QV3VQ
Evaluation B

$C_5H_8O_4$ (c) 88PET/TSY
Glutaric acid
Phase Changes
c,II/c,I 338.0 K, ΔH=2400 J· mol^{-1}
ΔS= 7.1 J· mol^{-1}· K^{-1}
Molecular Weight 132.1158
Wiswesser Line Notation QV3VQ
Evaluation A

$C_5H_8O_4$ (c) 39SAT/SOG
Pyrotartaric acid; 2-Methylsuccinic acid
Heat Capacity 323 K, C_p=199.6 J· mol^{-1}· K^{-1}
Temperature range 0 to 100°C. Mean value.
Molecular Weight 132.1158
Wiswesser Line Notation QVY1&1VQ
Evaluation C

C_5H_9Cl (liq) 93DIK/KAB
Chlorocyclopentane
Heat Capacity 298.15 K, C_p=152.40 J· mol^{-1}· K^{-1}
Temperature range 6 to 301 K.
Entropy 298.15 K, S=238.04 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 169.35 K, ΔH=7630.6 J· mol^{-1}
ΔS=45.06 J· mol^{-1}· K^{-1}
c,I/liq 180.0 K, ΔH=637.3 J· mol^{-1}
ΔS= 3.54 J· mol^{-1}· K^{-1}
liq/g 298.15 K, ΔH=38790 J· mol^{-1}
ΔS= 130.1 J· mol^{-1}· K^{-1}
Molecular Weight 104.5791
Wiswesser Line Notation L5TJ AG
Evaluation A

C_5H_9ClO (liq) 1881REI
Pentanoyl chloride; Valeryl chloride
Heat Capacity 298 K, C_p=187.9 J· mol^{-1}· K^{-1}
Temperature range 291 to 400 K.
Molecular Weight 120.5785
Wiswesser Line Notation GV4
Evaluation D

$C_5H_9ClO_2$ (liq) 1881REI
Ethyl 2-chloropropanoate; Ethyl α-chlorpropionate
Heat Capacity 298 K, C_p=220.5 J· mol^{-1}· K^{-1}
Temperature range 291 to 431 K.
Molecular Weight 136.5779
Wiswesser Line Notation GY1&VO2
Evaluation D

$C_5H_9LiO_2$ (c) 86FRA/NGE
Lithium n-pentanoate
Heat Capacity 298.15 K, C_p=224.07 J· mol^{-1}· K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=198.55 J· mol^{-1}· K^{-1}
Phase Changes
c,III/c,II 209.3 K, ΔH=665 J· mol^{-1}
ΔS=3.24 J· mol^{-1}· K^{-1}
c,II/c,I 319.06 K, ΔH=2745 J· mol^{-1}
ΔS=16.13 J· mol^{-1}· K^{-1}
Molecular Weight 108.0659
Wiswesser Line Notation OV4 .LI
Evaluation A

C_5H_9N (liq) 01KAH
Valeronitrile
Heat Capacity
C_p=180.8 J· mol^{-1}· K^{-1}
Temperature range 294.15 to 403.15 K. Heat capacity is an average value over the temperature range.
Molecular Weight 83.1328
Wiswesser Line Notation NC4
Evaluation D

C_5H_9N (liq) 67WES/RIB
2,2-Dimethylpropionitrile; 2-Cyano-2-methylpropane; tert-Butyl cyanide
Heat Capacity 298.15 K, C_p=179.37 J· mol^{-1}· K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=232.00 J· mol^{-1}· K^{-1}
Phase Changes
c,III/c,II 213 K, ΔH=230 J· mol^{-1}
ΔS=1.08 J· mol^{-1}· K^{-1}
c,II/c,I 232.74 K, ΔH=1912 J· mol^{-1}
ΔS= 7.78 J· mol^{-1}· K^{-1}
ΔS not equal to $\Delta H/T$, see article.
c,I/liq 292.13 K, ΔH=9288 J· mol^{-1}
ΔS= 31.79 J· mol^{-1}· K^{-1}
Molecular Weight 83.1328
Wiswesser Line Notation NCX1&1&1
Evaluation A

C_5H_9N (liq) 71HAL/BAL
2,2-Dimethylpropionitrile; 2-Cyano-2-methylpropane; tert-Butyl cyanide
Heat Capacity 297 K, C_p=153.3 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 83.1328
Wiswesser Line Notation NCX1&1&1
Evaluation C

C_5H_9NO (liq) 78MAR/CIO
1-Methyl-2-pyrrolidone
Heat Capacity 298 K, C_p=307.8 J· mol^{-1}· K^{-1}
Temperature range 298 to 461 K.
Molecular Weight 99.1322
Wiswesser Line Notation T5NVJ A1
Evaluation D

C_5H_9NO (liq) 90STE/CHI
1-Methyl-2-pyrrolidone
Heat Capacity 298.15 K, C_p=412.4 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 99.1322
Wiswesser Line Notation T5NVJ A1
Evaluation B

C_5H_9NO (c) 59KOL/PAU
α-Piperidone
Heat Capacity 290 K, C_p=189.8 J· mol^{-1}· K^{-1}
Temperature range 60 to 350 K.
Entropy 298.15 K, S=164.8 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 311.85 K, ΔH=10493 J· mol^{-1}
ΔS=33.6 J· mol^{-1}· K^{-1}
Molecular Weight 99.1299
Wiswesser Line Notation T6MVTJ
Evaluation B

C_5H_9NO (c) 62KOL/PAU
α-Piperidone
Heat Capacity 295.00 K, C_p=208.3 J· mol^{-1}· K^{-1}
Temperature range 60 to 350 K.
Entropy 298.15 K, S=165.0 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 311.85 K, ΔH=10502 J· mol^{-1}
ΔS=33.7 J· mol^{-1}· K^{-1}
Molecular Weight 99.1299
Wiswesser Line Notation T6MVTJ
Evaluation B

$(C_5H_9NO)_n$ (c) 91ROL
Poly-L-valine
Heat Capacity 300 K, C_p=144.2 J· mol^{-1}· K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 99.1241
Wiswesser Line Notation /*VYM*&Y1&1/ -L
Evaluation B

$(C_5H_9NO)_n$ (c) 91ROL/WUN
Poly-L-valine
Heat Capacity 300 K, C_p=144.2 J· mol^{-1}· K^{-1}
Temperature range 230 to 390 K.
Molecular Weight 99.1241
Wiswesser Line Notation /*VYM*&Y1&1/ -L
Evaluation B

$(C_5H_9NOS)_n$ (c) 91ROL
Poly-L-methionine
Heat Capacity 300 K, C_p=176.7 J· mol^{-1}· K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 131.1922
Wiswesser Line Notation /*VY2S1&M*/ -L
Evaluation B

$(C_5H_9NOS)_n$ (c) 93ROL/XEN
Poly-L-methionine
Heat Capacity 300 K, C_p=176.7 J· mol^{-1}· K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 131.1922
Wiswesser Line Notation /*VY2S1&M*/ -L
Evaluation B

$C_5H_9NO_2$ (c) 40HUF/FOX
Proline(L); Pyrrolidine-2-carboxylic acid(L)
Heat Capacity 300.4 K, C_p=149.12 J· mol^{-1}· K^{-1}
Temperature range 90 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=170.7 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 56.07 J· mol^{-1}· K^{-1}.
Molecular Weight 115.1316
Wiswesser Line Notation T5MTJ BVQ -L
Evaluation C

$C_5H_9NO_2$ (c) 63COL/HUT
Proline(L); Pyrrolidine-2-carboxylic acid(L)
Heat Capacity 298.15 K, C_p=151.17 J· mol^{-1}· K^{-1}
Temperature range 11 to 305 K.
Entropy 298.15 K, S=164.06 J· mol^{-1}· K^{-1}
Molecular Weight 115.1316
Wiswesser Line Notation T5MTJ BVQ -L
Evaluation A

$C_5H_9NO_2$ (c) 75SPI/WA
Proline(L); Pyrrolidine-2-carboxylic acid(L)
Heat Capacity 298.15 K, C_p=150.4 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 115.1316
Wiswesser Line Notation T5MTJ BVQ -L
Evaluation B

$C_5H_9NO_4$ (c) 75SAK/SE
Glutamic acid
Heat Capacity 298 K, C_p=175.08 J· mol^{-1}· K^{-1}
One temperature. C_p given as 1.19 J· g^{-1}· K^{-1}.
Molecular Weight 147.1304
Wiswesser Line Notation QVYZ2VQ
Evaluation B C_p same for D and L forms.

$C_5H_9NO_4$ (c) 32HUF/BC
Glutamic acid(D)
Heat Capacity 294.6 K, C_p=172.8 J· mol^{-1}· K^{-1}
Temperature range 91 to 295 K. Value is unsmoothed experimen datum.
Entropy 298.1 K, S=191.2 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 54.39 J· mol^{-1}· K^{-1}.
Molecular Weight 147.1304
Wiswesser Line Notation QVYZ2VQ -D
Evaluation B(C_p),C(S)

$C_5H_9NO_4$ (c) 63HUT/COl
Glutamic acid(L)
Heat Capacity 298.15 K, C_p=175.06 J· mol^{-1}· K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S=188.20 J· mol^{-1}· K^{-1}
Molecular Weight 147.1304
Wiswesser Line Notation QVYZ2VQ -L
Evaluation A

$C_5H_9O_2Tl$ (c) 76MEI/SE
Thallium pentanoate
Phase Changes
c,II/c,I 354.6 K, ΔH=2259 J· mol^{-1}
ΔS= 6.28 J· mol^{-1}· K^{-1}
c,I/liq 455 K, ΔH=5439 J· mol^{-1}
ΔS=12.1 J· mol^{-1}· K^{-1}
Solid-mesophase. liq/liq 487 K, ΔH=3054 J· mol^{-1} ΔS= 6.28 mol^{-1}· K^{-1} Mesophase-isotropic.
Molecular Weight 305.4949
Wiswesser Line Notation OV4 .TL
Evaluation B

$C_5H_9O_2Tl$ (c) 84FER/L
Thallium pentanoate
Heat Capacity 320 K, C_p=216 J· mol^{-1}· K^{-1}
Temperature range 320 to 480 K.
Phase Changes
c,II/c,I 353.0 K, ΔH=2104 J· mol^{-1}
ΔS= 5.99 J· mol^{-1}· K^{-1}
c,I/liq 455.0 K, ΔH=5704 J· mol^{-1}
ΔS= 12.5 J· mol^{-1}· K^{-1}
Solid to mesophase.
liq/liq 488.0 K, ΔH=3051 J· mol^{-1}
ΔS= 6.24 J· mol^{-1}· K^{-1}
Mesophase to isotropic.
Molecular Weight 305.4949
Wiswesser Line Notation OV4 .TL
Evaluation A

C_5H_{10} (liq) 47TOD/OLI
3-Methyl-1-butene
Heat Capacity 298.15 K, C_p=156.06 J· mol^{-1}· K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=253.30 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 104.712 K, ΔH=5359.3 J· mol^{-1}
ΔS=51.18 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 1Y1&1U1
Evaluation A

C_5H_{10} (liq) 83CHA/HAL
3-Methyl-1-butene
Heat Capacity 298.15 K, C_p=156.1 J· mol^{-1}· K^{-1}
Temperature range 13 to 298 K.
Entropy 298.15 K, S=253.5 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 104.71 K, ΔH=5359 J· mol^{-1}
ΔS=51.18 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 1Y1&1U1
Evaluation A
A reevaluation of the original measured data from: 47TOD/OLI.

C_5H_{10} (liq) 30PAR/HUF2
2-Methyl-2-butene
Heat Capacity 293.9 K, C_p=146.4 J· mol^{-1}· K^{-1}
Temperature range 93 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=248.9 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 13.12 cal· mol^{-1}· K^{-1}.
Phase Changes
c/liq 138.9 K, ΔH=7435 J· mol^{-1}
ΔS=5.35 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 2UY1&1
Evaluation B (C_p),C(S)

C_5H_{10} (liq) 47TOD/OLI
2-Methyl-2-butene
Heat Capacity 298.15 K, C_p=152.80 J· mol^{-1}· K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=251.04 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 139.42 K, ΔH=7597.3 J· mol^{-1}
ΔS=54.49 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 2UY1&1
Evaluation A

C_5H_{10} (liq) 83CHA/HAL
2-Methyl-2-butene
Heat Capacity 298.15 K, C_p=152.8 J· mol^{-1}· K^{-1}
Temperature range 13 to 301 K.
Entropy 298.15 K, S=251.2 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 139.40 K, ΔH=7579 J· mol^{-1}
ΔS=54.37 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 2UY1&1
Evaluation A
A reevaluation of the original measured data from: 47TOD/OLI, 30PAR/HUF.

C_5H_{10} (liq) 47TOD/OLI
2-Methyl-1-butene
Heat Capacity 298.15 K, C_p=157.19 J· mol^{-1}· K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=253.97 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 135.62 K, ΔH=7910.3 J· mol^{-1}
ΔS=58.33 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 2Y1&U1
Evaluation A

C_5H_{10} (liq) 83CHA/HAL
2-Methyl-1-butene
Heat Capacity 298.15 K, C_p=157.3 J· mol^{-1}· K^{-1}
Temperature range 12 to 293 K.
Entropy 298.15 K, S=254.0 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 135.60 K, ΔH=7911 J· mol^{-1}
ΔS=58.34 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 2Y1&U1
Evaluation A
A reevaluation of the original measured data from: 47TOD/OLI.

C_5H_{10} (liq) 1881REI
2-Pentene
Heat Capacity 298 K, C_p=195.8 J· mol^{-1}· K^{-1}
Temperature range 290 to 322 K.
Molecular Weight 70.1340
Wiswesser Line Notation 3U2
Evaluation D

C_5H_{10} (liq) 30PAR/HUF2
2-Pentene
Heat Capacity 289.1 K, C_p=151.13 J· mol^{-1}· K^{-1}
Temperature range 136 to 289 K. Value is unsmoothed experimental datum.
Molecular Weight 70.1340
Wiswesser Line Notation 3U2
Evaluation B

C_5H_{10} (liq) 47TOD/OLI
cis-2-Pentene
Heat Capacity 298.15 K, C_p=151.71 J· mol^{-1}· K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=258.61 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 121.80 K, ΔH=7111.5 J· mol^{-1}
ΔS=58.39 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 3U2 -C
Evaluation A

C_5H_{10} (liq) 83CHA/HAL
cis-2-Pentene
Heat Capacity 298.15 K, C_p=151.8 J· mol^{-1}· K^{-1}
Temperature range 13 to 295 K.
Entropy 298.15 K, S=258.8 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 121.78 K, ΔH=7112 J· mol^{-1}
ΔS=58.40 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 3U2 -C
Evaluation A
A reevaluation of the original measured data from: 47TOD/OLI.

C_5H_{10} (liq) 47TOD/OLI
trans-2-Pentene
Heat Capacity 298.15 K, C_p=156.98 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=256.52 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 132.95 K, ΔH=8351 J· mol^{-1}
ΔS=62.81 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 3U2 -T
Evaluation A

C_5H_{10} (liq) 83CHA/HAL
trans-2-Pentene
Heat Capacity 298.15 K, C_p=157.0 J· mol^{-1}· K^{-1}
Temperature range 12 to 302 K.
Entropy 298.15 K, S=256.6 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 132.93 K, ΔH=8352 J· mol^{-1}
ΔS=62.83 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 3U2 -T
Evaluation A
A reevaluation of the original measured data from: 47TOD/OLI.

C_5H_{10} (liq) 47TOD/OLI
1-Pentene
Heat Capacity 298.15 K, C_p=155.31 J· mol^{-1}· K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=262.55 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 107.9 K, ΔH=5807 J· mol^{-1}
ΔS=53.82 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 4U1
Evaluation A

C_5H_{10} (liq) 49SCH/SAG
1-Pentene
Heat Capacity 294 K, C_p=154.3 J· mol^{-1}· K^{-1}
Temperature range 294 to 378 K. C_p given as 0.526 Btu(lb)$^{-1}$(°R)$^{-1}$ at 70°F
Molecular Weight 70.1340
Wiswesser Line Notation 4U1
Evaluation B

C_5H_{10} (liq) 83CHA/HAL
1-Pentene
Heat Capacity 298.15 K, C_p=154 J· mol^{-1}· K^{-1}
Temperature range 12 to 353 K.
Entropy 298.15 K, S=262.6 J·mol^{-1}· K^{-1}
Phase Changes
c/liq 107.90 K, ΔH=5807 J· mol^{-1}
ΔS=53.82 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 4U1
Evaluation A
A reevaluation of the original measured data from: 47TOD/OLI, 49SCH/SAG.

C_5H_{10} (liq) 90MES/TO
1-Pentene
Heat Capacity 298.15 K, C_p=154.87 J· mol^{-1}· K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=262.60 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 108.016 K, ΔH=5937.39 J· mol^{-1}
ΔS=54.97 J· mol^{-1}· K^{-1}
c/liq 107.797 K, ΔH=5881.68 J· mol^{-1}
ΔS=54.56 J· mol^{-1}· K^{-1}
c(metastable)/liq
Molecular Weight 70.1340
Wiswesser Line Notation 4U1
Evaluation A

C_5H_{10} (gls) 90TAK/OC
1-Pentene
Phase Changes
c/gls 71.7 K
Molecular Weight 70.1340
Wiswesser Line Notation 4U1
Evaluation A

C_5H_{10} (liq) 34JAC/PA
Cyclopentane
Heat Capacity 293.7 K, C_p=125.90 J· mol^{-1}· K^{-1}
Temperature range 93 to 294 K. Value is unsmoothed experimen datum.
Entropy 298 K, S=206.7 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 53.09 J· mol^{-1}· K^{-1}.
Phase Changes
c,III/c,II 121.6 K, ΔH=4745 J· mol^{-1}
ΔS=39.02 J· mol^{-1}· K^{-1}
c,II/c,I 137.1 K, ΔH=358.2 J· mol^{-1}
ΔS= 2.61 J· mol^{-1}· K^{-1}
c,I/liq 179.0 K, ΔH=604.6 J· mol^{-1}
ΔS= 3.38 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation L5TJ
Evaluation B (C_p),C(S)

C_5H_{10} (liq) 43AST/F
Cyclopentane
Heat Capacity 298.15 K, C_p=128.83 J· mol^{-1}· K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=204.47 J· mol^{-1}· K^{-1}
Phase Changes
c,III/c,II 122.39 K, ΔH=4874 J· mol^{-1}
ΔS=39.82 J· mol^{-1}· K^{-1}
c,II/c,I 138.07 K, ΔH=346.4 J· mol^{-1}
ΔS= 2.51 J· mol^{-1}· K^{-1}
c,I/liq 179.69 K, ΔH=602 J· mol^{-1}
ΔS= 3.35 J· mol^{-1}· K^{-1}
liq/g 298.15 K, ΔH=29213 J· mol^{-1}
ΔS= 97.98 J· mol^{-1}· K
P=41.10 kPa
Molecular Weight 70.1340
Wiswesser Line Notation L5TJ
Evaluation A

C_5H_{10} (liq) 46DOU/HUF2
Cyclopentane
Heat Capacity 298.15 K, C_p=126.78 J· mol^{-1}· K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=204.14 J· mol^{-1}· K^{-1}
Phase Changes
c,III/c,II 122.39 K, ΔH=4884.0 J· mol^{-1}
ΔS=39.91 J· mol^{-1}· K^{-1}
c,II/c,I 138.09 K, ΔH=344.43 J· mol^{-1}
ΔS= 2.49 J· mol^{-1}· K^{-1}
c,I/liq 179.71 K, ΔH=608.94 J· mol^{-1}
ΔS= 3.38 J· mol^{-1}· K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation L5TJ
Evaluation A

C_5H_{10} (liq) 47SZA/MOR
Cyclopentane
Heat Capacity 300 K, C_p=127.44 J·mol^{-1}· K^{-1}
Temperature range 14 to 300 K.
Phase Changes
c,III/c,II 122.36 K, ΔH=4884.4 J· mol^{-1}
ΔS=39.92 J· mol^{-1}· K^{-1}
c,II/c,I 138.07 K, ΔH=342.7 J· mol^{-1}
ΔS= 2.48 J· mol^{-1}· K^{-1}
Temperature from 43AST/FIN.
c,I/liq 179.69 K, ΔH=603.8 J· mol^{-1}
ΔS=3.36 J· mol^{-1}· K^{-1}
Temperature from 43AST/FIN.
Molecular Weight 70.1340
Wiswesser Line Notation L5TJ
Evaluation A

C_5H_{10} (liq) 75JOL/BOI
Cyclopentane
Heat Capacity 298.15 K, C_p=127.28 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 70.1340
Wiswesser Line Notation L5TJ
Evaluation B

C_5H_{10} (liq) 79FOR/DAR
Cyclopentane
Heat Capacity 298.15 K, C_p=126.873 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 70.1340
Wiswesser Line Notation L5TJ
Evaluation B

C_5H_{10} (liq) 83SID/SVE
Cyclopentane
Heat Capacity 293.15 K, C_p=126.17 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 70.1340
Wiswesser Line Notation L5TJ
Evaluation B

C_5H_{10} (liq) 85TAN
Cyclopentane
Heat Capacity 298.15 K, C_p=126.74 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 70.1340
Wiswesser Line Notation L5TJ
Evaluation A

C_5H_{10} (liq) 92RAH/GME
Cyclopentane
Heat Capacity
Temperature range 15 to 300 K. Data given graphically.
Phase Changes
c,III/c,II 121.95 K, ΔH=5195 J· mol^{-1}
c,II/c,I 138.22 K, ΔH=361 J· mol^{-1}
c,I/liq 179.21 K, ΔH=615 J· mol^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation L5TJ
Evaluation A

$C_5H_{10}ClNO_4$ (c) 40HUF/ELL
Glutamic acid hydrochloride
Heat Capacity 296.8 K, C_p=208.49 J· mol^{-1}· K^{-1}
Temperature range 85 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=248.24 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 76.94 J· mol^{-1}· K^{-1}.
Molecular Weight 183.5913
Wiswesser Line Notation QVYZ2VQ &GH
Evaluation A (C_p),C(S)

$C_5H_{10}Cl_2$ (liq) 93HAL
1,5-Dichloropentane
Heat Capacity 298.15 K, C_p= 213.4 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 141.0400
Wiswesser Line Notation G5G
Evaluation B

$C_5H_{10}N_2$ (liq) 82DZH/KAR
β-Dimethylaminopropionitrile
Heat Capacity 298.15 K, C_p=212.5 J· mol^{-1}· K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=266.4 J· mol^{-1}· K^{-1}
Molecular Weight 98.1474
Wiswesser Line Notation NC2N1&1
Evaluation A

$C_5H_{10}N_2O_2$ (c) 91ABA/DEL
2-(Acetylamino)-N-methylethanamide;
N-Acetylglycine-N'-methylamide
Heat Capacity 298 K, C_p= 177.75 J· mol^{-1}· K^{-1}
Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 130.1462
Wiswesser Line Notation 1VM1VM1
Evaluation C

$C_5H_{10}N_2O_2$ (c) 88FER/DEL
N-Acetyl-L-alanine amide
Phase Changes
c/liq 431.0 K, ΔH=21700 J· mol^{-1}
ΔS= 50.3 J· mol^{-1}· K^{-1}
Molecular Weight 130.1462
Wiswesser Line Notation ZVY1&MV1
Evaluation A

$C_5H_{10}N_2O_3$ (c) 63HUT/COL2
Glutamine(L)
Heat Capacity 298.15 K, C_p = 184.18 J· mol^{-1}· K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S=195.06 J· mol^{-1}· K^{-1}
Molecular Weight 146.1456
Wiswesser Line Notation ZV2YZVQ -L
Evaluation A

$C_5H_{10}N_2O_3$ (c) 89KUL/KOZ
Alanylglycine
Heat Capacity 298 K, C_p=168.0 J· mol^{-1}· K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 146.1456
Wiswesser Line Notation ZY1&VM1VQ
Evaluation C

$C_5H_{10}N_2O_3$ (c) 90BAD/KUL
β-Alanylglycine
Heat Capacity 298 K, C_p=168 J· mol^{-1}· K^{-1}
Temperature range 298, 313, 333, 348 K.
Phase Changes
c/liq 507.95 K, ΔH=56600 J· mol^{-1} Melting with decomposition.
Molecular Weight 146.1456
Wiswesser Line Notation Z2VM1VQ
Evaluation D

$C_5H_{10}N_2O_3$ (c) 41HUF
Alanylglycine(DL)
Heat Capacity 296.4 K, C_p=181.79 J·mol^{-1}· K^{-1}
Temperature range 85 to 296 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=213.4 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 66.27 J· mol^{-1}· K^{-1}.
Molecular Weight 146.1456
Wiswesser Line Notation ZY1&VM1VQ -DL
Evaluation A (C_p),C(S)

$C_5H_{10}N_4O_4$ (c) 71HAL
1,3-Dinitro-1,3-diazacycloheptane
Phase Changes
c,II/c,I 373 K, ΔH=23430 J· mol^{-1}
An approximation.
c,I/liq 376 K, ΔH=3975 J· mol^{-1}
An approximation.
Molecular Weight 190.1584
Wiswesser Line Notation T7N CNTJ ANW CNW
Evaluation C

$C_5H_{10}O$ (liq) 84BAG/BAE
2-Methyl-3-buten-2-ol
Heat Capacity 298.05 K, C_p=240.7 J· mol^{-1}· K^{-1}
Temperature range 273 to 343 K. C_p(liq)=−0.96211+0.017280T−1.6×10^{-5}T^2 kJ/kg· K (273 to 343 K).
Molecular Weight 86.1334
Wiswesser Line Notation 1XQ1U1
Evaluation B

$C_5H_{10}O$ (liq) 88BAG/GUR
2-Methyl-3-buten-2-ol
Heat Capacity 298.05 K, C_p=241.2 J· mol^{-1}· K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 86.1334
Wiswesser Line Notation 1XQ1U1
Evaluation B

$C_5H_{10}O$ (liq) 68AND/COU
3-Methyl-2-butanone; Isopropyl methyl ketone
Heat Capacity 298.15 K, C_p=179.9 J· mol^{-1}· K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=268.5 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 180.01 K, ΔH=9343 J· mol^{-1}
ΔS=51.90 J· mol^{-1}· K^{-1}
Molecular Weight 86.1334
Wiswesser Line Notation 1Y1&V1
Evaluation A

$C_5H_{10}O$ (liq) 70HAR/HE
3-Methyl-2-butanone; Isopropyl methyl ketone
Heat Capacity 298.15 K, C_p=180.0 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 1Y1&V1
Evaluation B

$C_5H_{10}O$ (liq) 68AND/COU
3-Pentanone; Diethyl ketone
Heat Capacity 298.15 K, C_p=190.9 J· mol^{-1}· K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=266.0 J· mol^{-1}· K^{-1}
Phase Changes
c,III/c,II 118.5 K, ΔH=110.9 J· mol^{-1}
ΔS=0.96 J· mol^{-1}· K^{-1}
c,II/c,I 180 K, ΔH=9.6 J· mol^{-1}
ΔS=0.04 J· mol^{-1}· K^{-1}
c,I/liq 234.16 K, ΔH=11594 J· mol^{-1}
ΔS=49.51 J· mol^{-1}· K^{-1}
Molecular Weight 86.1334
Wiswesser Line Notation 2V2
Evaluation A

$C_5H_{10}O$ (liq) 70HAR/HE
3-Pentanone; Diethyl ketone
Heat Capacity 298.15 K, C_p=200.7 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 2V2
Evaluation B

$C_5H_{10}O$ (liq) 79SAL/PE
3-Pentanone; Diethyl ketone
Heat Capacity 298.15 K, C_p=190.0 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 2V2
Evaluation B

$C_5H_{10}O$ (liq) 84BAG/BA
3-Pentanone; Diethyl ketone
Heat Capacity 298.15 K, C_p=195.7 J· mol^{-1}· K^{-1}
Temperature range 273 to 334 K. C_p(liq)=−1.8555+0.025782T−4.0×10^{-5}T^2 kJ/kg·K (273 to 335 K).
Molecular Weight 86.1334
Wiswesser Line Notation 2V2
Evaluation B

$C_5H_{10}O$ (liq) 84GRO/BEN
3-Pentanone; Diethyl ketone
Heat Capacity 298.15 K, C_p=190.30 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 2V2
Evaluation B

$C_5H_{10}O$ (liq) 88BAG/GUR
3-Pentanone; Diethyl ketone
Heat Capacity 298.15 K, C_p=196.4 J· mol^{-1}· K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 86.1334
Wiswesser Line Notation 2V2
Evaluation B

$C_5H_{10}O$ (liq) 65OET
2-Pentanone; n-Propyl methyl ketone
Heat Capacity 298.15 K, C_p=184.35 J· mol^{-1}· K^{-1}
Temperature range 12 to 330 K.
Entropy 298.15 K, S=272.42 J·mol^{-1}· K^{-1}
Phase Changes
c/liq 196.35 K, ΔH=10623 J· mol^{-1}
ΔS=54.10 J· mol^{-1}· K^{-1}
Molecular Weight 86.1334
Wiswesser Line Notation 3V1
Evaluation A

$C_5H_{10}O$ (liq) 68AND/COU
2-Pentanone; n-Propyl methyl ketone
Heat Capacity 298.15 K, C_p=184.2 J· mol^{-1}· K^{-1}
Temperature range 10 to 360 K.
Entropy 298.15 K, S=274.1 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 110 K, ΔH=237.7 J· mol^{-1}
ΔS=2.18 J· mol^{-1}· K^{-1}
Apparently a typographic error in ΔH in paper; given as 137.7 J· mol^{-1}.
c,I/liq 196.31 K, ΔH=10632 J· mol^{-1}
ΔS= 54.16 J· mol^{-1}· K^{-1}
Molecular Weight 86.1334
Wiswesser Line Notation 3V1
Evaluation A

$C_5H_{10}O$ (liq) 70HAR/HEA
2-Pentanone; n-Propyl methyl ketone
Heat Capacity 298.15 K, C_p=184.3 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 3V1
Evaluation B

$C_5H_{10}O$ (liq) 75GRO/BEN
2-Pentanone; n-Propyl methyl ketone
Heat Capacity 298.15 K, C_p=185.1 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 3V1
Evaluation B

$C_5H_{10}O$ (liq) 79SAL/PEA
2-Pentanone; n-Propyl methyl ketone
Heat Capacity 298.15 K, C_p=185.4 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 3V1
Evaluation B

$C_5H_{10}O$ (liq) 56PAR/KEN
Cyclopentanol
Heat Capacity 298.15 K, C_p=184.14 J·mol^{-1}· K^{-1}
Temperature range 80 to 300 K.
Entropy 298.1 K, S=206.3 J·mol^{-1}· K^{-1}
Extrapolation below 80 K, 48.79 J· mol^{-1}· K^{-1}.
Phase Changes
c,II/c,I 202.8 K, ΔH=3707 J· mol^{-1}
ΔS=18.28 J· mol^{-1}· K^{-1}
c,I/liq 257.4 K, ΔH=1536 J· mol^{-1}
ΔS= 5.97 J· mol^{-1}· K^{-1}
Molecular Weight 86.1334
Wiswesser Line Notation L5TJ AQ
Evaluation B (C_p),C(S)

$C_5H_{10}O$ (liq) 76CON/GIN
Cyclopentanol
Heat Capacity 298 K, C_p= 185.4 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation L5TJ AQ
Evaluation B

$C_5H_{10}O$ (liq) 86BEN/DAR
Cyclopentanol
Heat Capacity 298.15 K, C_p=181.57 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation L5TJ AQ
Evaluation B

$C_5H_{10}O$ (liq) 86BEN/DAR2
Cyclopentanol
Heat Capacity 298.15 K, C_p=181.57J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation L5TJ AQ
Evaluation B

$C_5H_{10}O$ (liq) 64MOE/THO
Tetrahydropyran; Oxane
Heat Capacity 297.62 K, C_p=151.13 J·mol^{-1}· K^{-1}
Temperature range 297 to 327 K.
Molecular Weight 86.1334
Wiswesser Line Notation T6OTJ
Evaluation B

$C_5H_{10}O$ (liq) 76CON/GIN
Tetrahydropyran; Oxane
Heat Capacity 298 K, C_p=140.6 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation T6OTJ
Evaluation B

$C_5H_{10}O$ (liq) 81ING/CAS
Tetrahydropyran; Oxane
Heat Capacity 298.15 K, C_p=149.21 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation T6OTJ
Evaluation B

$C_5H_{10}O$ (liq) 84ING/GRO
Tetrahydropyran; Oxane
Heat Capacity 298.15 K, C_p=149.60 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation T6OTJ
Evaluation B

$C_5H_{10}O$ (liq) 1881REI
Valeraldehyde; n-Pentanal; Valeral
Heat Capacity 298 K, C_p=171.5 J· mol^{-1}· K^{-1}
Temperature range 290 to 385 K.
Molecular Weight 86.1334
Wiswesser Line Notation VH4
Evaluation D

$C_5H_{10}O$ (liq) 82DYA/VAS
Valeraldehyde; n-Pentanal; Valeral
Entropy 298.15 K, S=273.6 J·mol^{-1}· K^{-1}
Molecular Weight 86.1334
Wiswesser Line Notation VH4
Evaluation B

$C_5H_{10}O$ (liq) 83KOR/DYA
Valeraldehyde; n-Pentanal; Valeral
Heat Capacity 298.15 K, C_p=174.39 J· mol^{-1}· K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S=273.59 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 191.59 K
Molecular Weight 86.1334
Wiswesser Line Notation VH4
Evaluation B

$C_5H_{10}O$ (liq) 84VAS/PET
Valeraldehyde; n-Pentanal; Valeral
Heat Capacity 298.15 K, C_p=174.39 J· mol^{-1}· K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S=273.59 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 191.59 K
Molecular Weight 86.1334
Wiswesser Line Notation VH4
Evaluation A

$C_5H_{10}O$ (liq) 83KOR/DYA
2,2-Dimethylpropanal; Pivalaldehyde; tert-Butylaldehyde
Heat Capacity 298.15 K, C_p=185.58 J· mol^{-1}· K^{-1}
Temperature range 50 to 350 K.
Entropy 298.15 K, S=262.05 J· mol^{-1}· K^{-1}
Phase Changes
c,I/liq 274.15 K Second order transitions observed at 62.5, 69.0, 110.8, 162.5, and 183.3 K.
Molecular Weight 86.1334
Wiswesser Line Notation VHX1&1&1
Evaluation C

$C_5H_{10}O$ (liq) 88WHI/PER
2,2-Dimethylpropanal; Pivalaldehyde; tert-Butylaldehyde
Heat Capacity 298.43 K, C_p=192.8 J· mol^{-1}· K^{-1}
Temperature range 29 to 298 K. Value is unsmoothed experimental datum.
Phase Changes
c,III/c,II 158.5 K, ΔH=499 J· mol^{-1}; ΔS=3.34 J· mol^{-1}· K^{-1}
c,II/c,I 183.9 K, ΔH=4809 J· mol^{-1}; ΔS= 26.22 J· mol^{-1}· K^{-1}
c,I/liq 272.1 K, ΔH=2520 J· mol^{-1}; ΔS= 9.3 J· mol^{-1}· K^{-1}
Molecular Weight 86.1334
Wiswesser Line Notation VHX1&1&1
Evaluation C_p(B), transitions (A).

$C_5H_{10}O_2$ (liq) 79FUC
1-Methylethyl ethanoate; Isopropyl acetate
Heat Capacity 298.15 K, C_p=196.6 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation 1Y1&OV1
Evaluation B

$C_5H_{10}O_2$ (liq) 86JIM/ROM
Ethyl propionate; Ethyl propanoate
Heat Capacity 298.15 K, C_p=200.90 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation 2VO2
Evaluation B

$C_5H_{10}O_2$ (liq) 87ZAB/HYN
Ethyl propionate; Ethyl propanoate
Heat Capacity 298.33 K, C_p=199.58 J· mol^{-1}· K^{-1}
Temperature range 294 to 349 K. Unsmoothed experimental datum.
Molecular Weight 102.1328
Wiswesser Line Notation 2VO2
Evaluation B

$C_5H_{10}O_2$ (liq) 1881RE
Propyl ethanoate; n-Propyl acetate
Heat Capacity 298 K, C_p=194.1 J· mol^{-1}· K^{-1}
Temperature range 292 to 382 K.
Molecular Weight 102.1328
Wiswesser Line Notation 3OV1
Evaluation D

$C_5H_{10}O_2$ (liq) 86JIM/ROM
Propyl ethanoate; n-Propyl acetate
Heat Capacity 298.15 K, C_p=196.07 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation 3OV1
Evaluation B

$C_5H_{10}O_2$ (liq) 79FUC
Methyl butanoate; Methyl butyrate
Heat Capacity 298.15 K, C_p=200.8 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation 3VO1
Evaluation B

$C_5H_{10}O_2$ (liq) 88PIN/BRA
Methyl butanoate; Methyl butyrate
Heat Capacity 298.15 K, C_p=198.16 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation 3VO1
Evaluation B

$C_5H_{10}O_2$ (liq) 86JIM/ROM
n-Butyl methanoate
Heat Capacity 298.15 K, C_p=200.25 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation 4OVH
Evaluation B

$C_5H_{10}O_2$ (liq) 1881REI
3-Methylbutanoic acid; Isovaleric acid
Heat Capacity 298 K, C_p=197.1 J· mol^{-1}· K^{-1}
Temperature range 290 to 470 K.
Molecular Weight 102.1328
Wiswesser Line Notation QV1Y1&1
Evaluation D

$C_5H_{10}O_2$ (liq) 65MCD/KIL
Pentanoic acid; n-Valeric acid
Heat Capacity 298.15 K, C_p=210.33 J· mol^{-1}· K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=259.83 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 239.49 K, ΔH=14161.6 J· mol^{-1}
ΔS=59.13 J· mol^{-1}· K^{-1}
Molecular Weight 102.1328
Wiswesser Line Notation QV4
Evaluation A

$C_5H_{10}O_2$ (liq) 71KON/WAD
Pentanoic acid; n-Valeric acid
Heat Capacity 298.15 K, C_p=197 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation QV4
Evaluation B

$C_5H_{10}O_2$ (c) 70BRE/BRE
2,2-Dimethylpropanoic acid; Pivalic acid
Phase Changes
c,II/c,I ΔH=8759.92 J· mol^{-1}
c,I/liq ΔH=2101.8 J· mol^{-1}
Molecular Weight 102.1328
Wiswesser Line Notation QVX1&1&1
Evaluation C

$C_5H_{10}O_2$ (c) 70MUR/BRE
2,2-Dimethylpropanoic acid; Pivalic acid
Phase Changes
c,II/c,I 281 K, ΔH=8760 J· mol^{-1}
ΔS=31.4 J· mol^{-1}· K^{-1}
c,I/liq 307 K, ΔH=2479 J· mol^{-1}
ΔS=7.9 J· mol^{-1}· K^{-1}
Molecular Weight 102.1328
Wiswesser Line Notation QVX1&1&1
Evaluation A

$C_5H_{10}O_2$ (c) 71KON/WAD
2,2-Dimethylpropanoic acid; Pivalic acid
Heat Capacity 298.15 K, C_p=178 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation QVX1&1&1
Evaluation B

$C_5H_{10}O_2$ (c) 90SIN/GLI
2,2-Dimethylpropanoic acid; Pivalic acid
Heat Capacity 298.15 K, C_p=192.2 J· mol^{-1}· K^{-1}
Temperature range 295 to 319 K. C_p(c)=13.38 + 0.1092T cal· mol^{-1} · K^{-1} (295 to 300 K). C_p value calculated from equation. C_p(liq)=16.19 + 0.1042T cal· mol^{-1}· K^{-1}.
Phase Changes
c,II/c,I 278.3 K, ΔH=8184 J· mol^{-1}
c,I/liq 309.085 K, ΔH=2268 J· mol^{-1}
Molecular Weight 102.1328
Wiswesser Line Notation QVX1&1&1
Evaluation B
Suspected error by authors for C_p(c) equation; they report C_p(c)=13.38 + 0.1902T cal/mol· K.

$C_5H_{10}O_2$ (liq) 35MIL
Tetrahydrofurfuryl alcohol
Heat Capacity Temperature range 100 to 298 K. Data in thesis only.
Entropy 298.15 K, S=219.2 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 45.23 J· mol^{-1}· K^{-1}.
Molecular Weight 102.1328
Wiswesser Line Notation T5OTJ B1Q
Evaluation C

$C_5H_{10}O_2$ (liq) 76BON/CER
Tetrahydrofurfuryl alcohol
Heat Capacity 298.15 K, C_p=190 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation T5OTJ B1Q
Evaluation B

$C_5H_{10}O_2$ (liq) 76CON/GIN
1,3-Dioxepane
Heat Capacity 298 K, C_p=167 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation T7O COTJ
Evaluation C

$C_5H_{10}O_2$ (liq) 36KUR/VOS
2-Methylpropyl methanoate; Isobutyl formate
Heat Capacity 290 K, C_p=214.2 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation VHO1Y1&1
Evaluation D

$C_5H_{10}O_3$ (liq) 83SAN/CIO
2-Methoxyethanol acetate
Heat Capacity 298.15 K, C_p=310 J· mol^{-1}· K^{-1}
Temperature range 273.15 to 323.15 K. C_p(kJ· kg^{-1}· K^{-1})=0.024460T −4.667
Molecular Weight 118.1322
Wiswesser Line Notation 1VO2O1
Evaluation D

$C_5H_{10}O_3$ (liq) 1881REI
Diethyl carbonate
Heat Capacity 298 K, C_p= 182.0 J· mol^{-1}· K^{-1}
Temperature range 297 to 416 K.
Molecular Weight 118.1322
Wiswesser Line Notation 2OVO2
Evaluation D

$C_5H_{10}O_3$ (liq) 33KOL/UDO
Diethyl carbonate
Heat Capacity 294.7 K, C_p = 210.9 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 118.1322
Wiswesser Line Notation 2OVO2
Evaluation C

$C_5H_{10}O_3$ (liq) 34KOL/UDO2
Diethyl carbonate
Heat Capacity 294.2 K, C_p = 210.9 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 118.1322
Wiswesser Line Notation 2OVO2
Evaluation C

$C_5H_{10}O_4$ (c) 70MUR/BRE
2,2-Bis(hydroxymethyl)propionic acid
Phase Changes
c,II/c,I 426 K, ΔH=38499 J· mol^{-1}
ΔS=90.8 J· mol^{-1}· K^{-1}
c,I/liq 468 K, ΔH=3592 J· mol^{-1}
ΔS=7.5 J· mol^{-1}· K^{-1}
Molecular Weight 134.1316
Wiswesser Line Notation QVX1&1Q1Q
Evaluation A

$C_5H_{10}O_5$ (c) 69CLE/MEL3
Pentoxane; Pentacycloformaldehyde
Heat Capacity 298.15 K, C_p=171.4 J· mol^{-1}· K^{-1}
Temperature range 180 to 400 K.
Entropy 298.15 K, S=187.7 J· mol^{-1}· K^{-1}
Extrapolation below 180 K, 119.0 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 334 K, ΔH=21900 J· mol^{-1}
ΔS=65.6 J· mol^{-1}· K^{-1}
Molecular Weight 150.1310
Wiswesser Line Notation T-10-O CO EO GO IOTJ
Evaluation B (C_p),C(S)

$C_5H_{10}O_5$ (c) 35MIL
α-Xylose(D)
Heat Capacity C_p data in thesis only.
Temperature range 100 to 298 K.
Entropy 298.15 K, S=143.5 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 31.38 J· mol^{-1}· K^{-1}.
Molecular Weight 150.1310
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ -A&BCE -B&D
Evaluation C

$C_5H_{10}O_5$ (c) 81KAW/KUS
Xylose(D)
Heat Capacity 303 K, C_p=184 J· mol^{-1}· K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 150.1310
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ -A&BCE -B&D
Evaluation B

$C_5H_{10}O_5$ (c) 81KAW/KUS
Arabinose(L)
Heat Capacity 303 K, C_p=184 J· mol^{-1}· K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 150.1310
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ -A&C -B&BDE
Evaluation B

$C_5H_{10}O_5$ (c) 81KAW/KUS
Arabinose(D)
Heat Capacity 303 K, C_p=184 J· mol^{-1}· K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 150.1310
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ -A&DE -B&BC
Evaluation B

$C_5H_{10}O_5$ (c) 81KAW/KUS
Ribose(D)
Heat Capacity 303 K, C_p=187 J· mol^{-1}· K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 150.1310
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ -A&CDE -B&B
Evaluation B

$C_5H_{10}S$ (liq) 61BER/SCC
Cyclopentanethiol; Cyclopentyl mercaptan
Heat Capacity 298.15 K, C_p=265.23 J· mol^{-1}· K^{-1}
Temperature range 12 to 367 K. For metastable crystals 12 to 137 K.
Entropy 298.15 K, S=256.86 J· mol^{-1}· K^{-1}
Phase Changes
c,I/liq 155.39 K, ΔH=7830.8 J· mol^{-1}
ΔS=50.39 J· mol^{-1}· K^{-1}
Molecular Weight 102.1940
Wiswesser Line Notation L5TJ ASH
Evaluation A
From enthalpy data at 102 to 162 K calculate enthalpy of fusion c metastable crystals at 155.39 K as 7381 J· mol^{-1}· K^{-1}. Adiabati transition from metastable to stable crystals, ΔH(155.39 K)=452 J mol^{-1}. Sum gives ΔH_{fusion}=7833 J· mol^{-1}.

$C_5H_{10}S$ (liq) 74MES/FI
2-Methylthiolane; 2-Methylcyclothiapentane
Heat Capacity 298.15 K, C_p=171.80 J· mol^{-1}· K^{-1}
Temperature range 10 to 380 K.
Entropy 298.15 K, S=245.31 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 172.39 K, ΔH=8875.9 J· mol^{-1}
ΔS=51.49 J· mol^{-1}· K^{-1}
Molecular Weight 102.1940
Wiswesser Line Notation T5STJ B1
Evaluation A

$C_5H_{10}S$ (liq) 74MES/FI
3-Methylthiolane; 3-Methylcyclothiapentane
Heat Capacity 298.15 K, C_p=171.80 J· mol^{-1}· K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S=241.00 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 192.00 K, ΔH=10370.5 J· mol^{-1}
ΔS=54.01 J· mol^{-1}· K^{-1}
Molecular Weight 102.1940
Wiswesser Line Notation T5STJ C1
Evaluation A

$C_5H_{10}S$ (liq) 54MCC/FIN
Thiacyclohexane
Heat Capacity 298.15 K, C_p=163.30 J·mol^{-1}· K^{-1}
Temperature range 13 to 340 K.
Entropy 298.15 K, S=218.24 J· mol^{-1}· K^{-1}
Phase Changes
c,III/c,II 201.4 K, ΔH=1097.9 J· mol^{-1}
ΔS=5.45 J· mol^{-1}· K^{-1}
c,II/c,I 240.02 K, ΔH=7775.1 J· mol^{-1}
ΔS= 32.39 J· mol^{-1}· K^{-1}
c,I/liq 292.25 K, ΔH=2448.5 J· mol^{-1}
ΔS= 8.38 J· mol^{-1}· K^{-1}
Molecular Weight 102.1940
Wiswesser Line Notation T6STJ
Evaluation A

$C_5H_{11}Br$ (liq) 48KUR
1-Bromo-3-methylbutane; Isoamyl bromide
Heat Capacity 298 K, C_p=187.0 J· mol^{-1}· K^{-1}
Temperature range 12 to 100· C, mean C_p, two temperatures.
Molecular Weight 151.0459
Wiswesser Line Notation E2Y1&1
Evaluation D

$C_5H_{11}Br$ (liq) 31DEE
1-Bromopentane; n-Amyl bromide; n-Pentyl bromide
Heat Capacity 290.7 K, C_p=171.59 J· mol^{-1}· K^{-1}
Temperature range 96 to 291 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=406.77 J· mol^{-1}· K^{-1}
Extrapolation below 100 K, 56.82 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 185.1 K, ΔH=14364 J· mol^{-1}
ΔS=77.60 J· mol^{-1}· K^{-1}
Molecular Weight 151.0459
Wiswesser Line Notation E5
Evaluation B (C_p),C(S)

$C_5H_{11}Br$ (liq) 50KUS/CRO
1-Bromopentane; n-Amyl bromide; n-Pentyl bromide
Heat Capacity 206.6 K, C_p=174.9 J· mol^{-1}· K^{-1}
Temperature range 122 to 207 K. Value is unsmoothed experimental datum.
Phase Changes
c/liq 185.1 K, ΔH=11465 J· mol^{-1}
ΔS=62.0 J· mol^{-1}· K^{-1}
Molecular Weight 151.0459
Wiswesser Line Notation E5
Evaluation B

$C_5H_{11}Br$ (liq) 93SHE
1-Bromopentane; n-Amyl bromide; n-Pentyl bromide
Heat Capacity 298.15 K, C_p=219.7 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 151.0459
Wiswesser Line Notation E5
Evaluation B

$C_5H_{11}CaCl_2NO_2$· $2H_2O$ (c) 90BRI/GME
Betaine calcium chloride dihydrate
Heat Capacity 300 K, C_p=300 J· mol^{-1}· K^{-1}
Temperature range 2 to 300 K. C_p value estimated graphically.
Phase Changes
c,VI/c,V 47 K, ΔH=5.08 J· mol^{-1}
ΔS= 0.11 J· mol^{-1}· K^{-1}
c,V/c,IV 76 K, ΔH=11.90 J· mol^{-1}
ΔS=0.16 J· mol^{-1}· K^{-1}
c,IV/c,III 116 K, ΔH=5.60 J· mol^{-1}
ΔS=0.05 J· mol^{-1}· K^{-1}
c,III/c,II 127 K, ΔH=1.58 J· mol^{-1}
ΔS=0.01 J·mol^{-1}· K^{-1}
c,II/c,I 164 K, ΔH=187.4 J· mol^{-1}
ΔS=1.28 J· mol^{-1}· K^{-1}
Molecular Weight 264.1638
Wiswesser Line Notation OV1K1&1&1 .CA G 2 &QH 2
Evaluation A

$C_5H_{11}Cl$ (liq) 48KUR
1-Chloro-1-methylbutane; Isoamyl chloride
Heat Capacity 298 K, C_p=179.5 J· mol^{-1}· K^{-1}
Temperature range 14 to 98°C, mean C_p, two temperatures.
Molecular Weight 106.5949
Wiswesser Line Notation G2Y1&1
Evaluation D

$C_5H_{11}Cl$ (liq) 93SHE
1-Chloropentane; n-Amyl cloride; n-Pentyl cloride
Heat Capacity 298.15 K, C_p=187.7 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 106.5949
Wiswesser Line Notation G5
Evaluation B

$C_5H_{11}I$ (liq) 48KUR
1-Iodo-3-methylbutane; Isoamyl iodide
Heat Capacity 298 K, C_p=178.7 J· mol^{-1}· K^{-1}
Temperature range 13 to 137°C, mean C_p.
Molecular Weight 198.0464
Wiswesser Line Notation I2Y1&1
Evaluation D

$C_5H_{11}I$ (liq) 93SHE
1-Iodopentane; n-Amyl iodide; n-Pentyl iodide
Heat Capacity 298.15 K, C_p=193.6 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 198.0464
Wiswesser Line Notation I5
Evaluation B

$C_5H_{11}N$ (liq) 86STE/CHI
3-Methylpyrrolidine
Heat Capacity 298.15 K, C_p=188.28 J·mol^{-1}· K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=236.43 J·mol^{-1}· K^{-1}
Phase Changes
c/liq 170.402 K
Molecular Weight 85.1486
Wiswesser Line Notation T5MTJ C1
Evaluation A

$C_5H_{11}N$ (liq) 76CON/GIN
1-Methylpyrrolidine
Heat Capacity 298 K, C_p=161.1 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 85.1486
Wiswesser Line Notation T5NTJ A1
Evaluation B

$C_5H_{11}N$ (liq) 34RAD/JUL
Piperidine
Heat Capacity 290 K, C_p=170.7 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 85.1486
Wiswesser Line Notation T6MTJ
Evaluation C

$C_5H_{11}N$ (liq) 36KUR/VOS
Piperidine
Heat Capacity 290 K, C_p=186.2 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 85.1486
Wiswesser Line Notation T6MTJ
Evaluation D

$C_5H_{11}N$ (liq) 64MOE/THO
Piperidine
Heat Capacity 297.39 K, C_p=182.76 J·mol^{-1}· K^{-1}
Temperature range 297 to 327 K.
Molecular Weight 85.1486
Wiswesser Line Notation T6MTJ
Evaluation B

$C_5H_{11}N$ (liq) 76CON/GIN
Piperidine
Heat Capacity 298 K, C_p=181.6 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 85.1486
Wiswesser Line Notation T6MTJ
Evaluation B

$C_5H_{11}N$ (liq) 86STE/CHI
Piperidine
Heat Capacity 298.15 K, C_p=179.86 J·mol^{-1}· K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=209.94 J·mol^{-1}· K^{-1}
Phase Changes
c/liq 262.124 K
Molecular Weight 85.1486
Wiswesser Line Notation T6MTJ
Evaluation A

$C_5H_{11}N$ (liq) 87MES/TOD
Piperidine
Heat Capacity 298.15 K, C_p=179.85 J·mol^{-1}· K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=209.94 J·mol^{-1}· K^{-1}
Phase Changes
c/liq 262.124 K, ΔH=14847.9 J· mol^{-1}
ΔS=56.64 J·mol^{-1}· K^{-1}
Molecular Weight 85.1486
Wiswesser Line Notation T6MTJ
Evaluation A

$C_5H_{11}N$ (liq) 88MES/TOD
Piperidine
Heat Capacity 298.150 K, C_p=179.857 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S=209.972 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 262.124 K, ΔH=14853.69 J· mol^{-1}
ΔS=56.67 J·mol^{-1}· K^{-1}
Molecular Weight 85.1486
Wiswesser Line Notation T6MTJ
Evaluation A

$C_5H_{11}N$ (liq) 81FIN/MES
Cyclopentylamine
Heat Capacity 298 K, C_p=181.21 J·mol^{-1}·K^{-1}
Temperature range 12 to 349 K. Equation also given for temperature range 197 to 349 K.
Entropy 298.15 K, S=241.04 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 184.5 K, ΔH=475.3 J· mol^{-1}
ΔS=2.58 J· mol^{-1}· K^{-1}
Lambda type transition.
c,I/liq 190.45 K, ΔH=8312.8 J· mol^{-1}
ΔS=43.65 J·mol^{-1}· K^{-1}
Molecular Weight 85.1486
Wiswesser Line Notation L5TJ AZ
Evaluation A

$C_5H_{11}NO$ (liq) 71KON/WAI
N-(1-Methylethyl)ethanamide; N-Isopropylacetamide
Heat Capacity 298.15 K, C_p=211 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 101.1480
Wiswesser Line Notation 1Y1&MV1
Evaluation B

$C_5H_{11}NO$ (liq) 71KON/WAI
N,N-Dimethylpropanamide
Heat Capacity 298.15 K, C_p=209 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 101.1480
Wiswesser Line Notation 1Y1&VM1
Evaluation B

$C_5H_{11}NO$ (liq) 71KON/WAI
N-(n-Propyl)ethanamide; N-(n-Propyl)acetamide
Heat Capacity 298.15 K, C_p=207 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 101.1480
Wiswesser Line Notation 3MV1
Evaluation B

$C_5H_{11}NO$ (liq) 86ZEG/BOI
N-(n-Propyl)ethanamide; N-(n-Propyl)acetamide
Heat Capacity 298.15 K, C_p=207.94 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 101.1480
Wiswesser Line Notation 3MV1
Evaluation B

$C_5H_{11}NO$ (liq) 71KON/WAD
N-Methylbutanamide
Heat Capacity 298.15 K, C_p=207 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 101.1480
Wiswesser Line Notation 3VM1
Evaluation B

$C_5H_{11}NO$ (liq) 89ABB/JIM
2,2-Dimethylpropanamide
Heat Capacity 298.150 K, C_p=159.8 J·mol^{-1}· K^{-1}
One temperature; C_p given as 1.58 J· g^{-1}· K^{-1}.
Phase Changes
c/g 298.15 K, ΔH=86600 J· mol^{-1}
ΔS=290.5 J·mol^{-1}· K^{-1}
Molecular Weight 101.1480
Wiswesser Line Notation ZVX1&1&1
Evaluation A

$C_5H_{11}NO_2$ (liq) 92VER/BEC
N,N-Dimethylaminoethanoic acid methyl ester
Heat Capacity 298.15 K, C_p=284.3 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 117.1474
Wiswesser Line Notation 1OV1N1&1
Evaluation B

$C_5H_{11}NO_2$ (c) 84GRU/BOU
Norvaline (L); α-Aminovaleric acid (L)
Phase Changes
c,II/c,I 273 K, ΔH=40 J· mol^{-1}
ΔS=0.16 J· mol^{-1}· K^{-1}
Molecular Weight 117.1474
Wiswesser Line Notation QVYZ3 -L
Evaluation B

$C_5H_{11}NO_2$ (c) 63HUT/COL
2-Amino-3-methylbutanoic acid(L); Valine(L); α-Aminoisovaleric acid
Heat Capacity 298.15 K, C_p=168.82 J·mol^{-1}·K^{-1}
Temperature range 11 to 310 K.
Entropy 298.15 K, S=178.87 J·mol^{-1}·K^{-1}
Molecular Weight 117.1474
Wiswesser Line Notation QVYZY1&1 -L
Evaluation A

$C_5H_{11}NO_2$ (c) 75SPI/WAD
2-Amino-3-methylbutanoic acid(L); Valine(L); α-Aminoisovaleric acid
Heat Capacity 298.15 K, C_p=168.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 117.1474
Wiswesser Line Notation QVYZY1&1 -L
Evaluation B

$C_5H_{11}NO_2$ (c) 89KUL/KOZ
2-Amino-3-methylbutanoic acid(D); Valine(D); α-Aminoisovaleric acid(D)
Heat Capacity 298 K, C_p=158.2 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 117.1474
Wiswesser Line Notation ZVYZY1&1 -D
Evaluation C

$C_5H_{11}NO_2$ (c) 90BAD/KUL
2-Amino-3-methylbutanoic acid(D); Valine(D); α-Aminoisovaleric acid(D)
Heat Capacity 298 K, C_p=158 J· mol^{-1}· K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 117.1474
Wiswesser Line Notation QVYZY1&1 -D
Evaluation D

$C_5H_{11}NO_2$ (c) 89KUL/KOZ
2-Amino-3-methylbutanoic acid(DL); Valine(DL); α-Aminoisovaleric acid(DL)
Heat Capacity 298 K, C_p=164.5 J·mol^{-1}· K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 117.1474
Wiswesser Line Notation QVYZY1&1
Evaluation C

$C_5H_{11}NO_2$ (c) 90BAD/KUL
2-Amino-3-methylbutanoic acid(DL); Valine(DL); α-Aminoisovaleric acid(DL)
Heat Capacity 298 K, C_p=165 J· mol^{-1}· K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 117.1474
Wiswesser Line Notation QVYZY1&1
Evaluation D

$C_5H_{11}NO_2$ (c) 83SKO/SAB
5-Aminopentanoic acid
Heat Capacity 298 K, C_p=163.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 117.1474
Wiswesser Line Notation Z4VQ
Evaluation B

$C_5H_{11}NO_2$ (c) 91BAR/FON
2-Amino-2-methyl-1,3-propanediol
Heat Capacity
Temperature range 273 to 423 K. Data given graphically.
Phase Changes
c,II/c,I 351.25 K, ΔH = 24680 J· mol^{-1}
c,I/liq 383.55 K, ΔH=2731 J· mol^{-1}
Molecular Weight 101.1480
Wiswesser Line Notation ZX1&1&1Q1Q
Evaluation B

$C_5H_{11}NO_2S$ (c) 84GRU/BOU
Methionine (DL)
Phase Changes
c,III/c,II 326 K, ΔH=820 J· mol^{-1}
ΔS=2.51 J·mol^{-1}·K^{-1}
c,II/c,I 380 K
Molecular Weight 149.2074
Wiswesser Line Notation QVYZ2S1
Evaluation B

$C_5H_{11}NO_2S$ (c) 64HUT/COL
Methionine (L)
Heat Capacity 298.15 K, C_p=290.03 J·mol^{-1}·K^{-1}
Temperature range 11 to 348 K.
Entropy 298.15 K, S=231.46 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 305.5 K, ΔH=5440 J·mol^{-1}
ΔS=17.6 J·mol^{-1}·K^{-1}
Lambda transition over the temperature range 250 to 350 K with a maximum at 305.5 K.
Molecular Weight 149.2074
Wiswesser Line Notation QVYZ2S1
Evaluation A

$C_5H_{11}NO_2S$ (c) 84GRU/BOU
Methionine (L)
Phase Changes
c,III/c,II 307 K, ΔH=1980 J·mol^{-1}
ΔS=6.45 J·mol^{-1}·K^{-1}
c,II/c,I 393 K, ΔH=150 J·mol^{-1}
ΔS=0.38 J·mol^{-1}·K^{-1}
Molecular Weight 149.2074
Wiswesser Line Notation QVYZ2S1 -L
Evaluation B

$C_5H_{11}NO_4$ (c) 39SAT/SOG
Ammonium acid pyrotartrate; Ammonium acid 2- methylsuccinate
Heat Capacity 323 K, C_p=234.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100°C. Mean value.
Molecular Weight 149.1462
Wiswesser Line Notation QVY1&1VQ&ZH
Evaluation C

C_5H_{12} (liq) 36AST/MES
2,2-Dimethylpropane; Neopentane
Heat Capacity 278.92 K, C_p=163.89 J·mol^{-1}·K^{-1}
Temperature range 13 to 283 K. Value is unsmoothed experimental datum.
Entropy 282.61 K, S=218.8 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 140.0 K, ΔH=2577 J·mol^{-1}
ΔS=18.41 J·mol^{-1}·K^{-1}
c,I/liq 256.53 K, ΔH=3255 J·mol^{-1}
ΔS=12.68 J·mol^{-1}·K^{-1}
liq/g 282.61 K, ΔH=22753 J·mol^{-1}
ΔS=80.50 J·mol^{-1}·K^{-1}
P=101.325 kPa
Molecular Weight 72.1498
Wiswesser Line Notation 1X1&1&1
Evaluation A

C_5H_{12} (liq) 69ENO/SHI
2.2-Dimethylpropane: Neopentane
Heat Capacity 259.93 K, C_p=153.09 J·mol^{-1}·K^{-1}
Temperature range 4 to 260 K. Value is unsmoothed experimental datum.
Entropy 282.61 K, S=216.81 J·mol^{-1}·K^{-1}
At normal boiling point.
Phase Changes
c,II/c,I 140-142 K, ΔH=2630.5 J·mol^{-1}
ΔS=18.70 J·mol^{-1}·K^{-1}
Second-order transition, 140 to 142 K. ΔS for total change between 140 and 142 K. c,I/liq 256.76 K, ΔH=3096.2 J·mol^{-1}
ΔS=12.06 J·mol^{-1}·K^{-1}
Molecular Weight 72.1498
Wiswesser Line Notation 1X1&1&1
Evaluation A

C_5H_{12} (liq) 70CHA/WES
2,2-Dimethylpropane; Neopentane
Phase Changes
c,II/c,I 140.5 K, ΔH=2630 J·mol^{-1}
ΔS=18.70 J·mol^{-1}·K^{-1}
c,I/liq 256.76 K, ΔH=3096 J·mol^{-1}
ΔS=12.05 J·mol^{-1}·K^{-1}
Molecular Weight 72.1498
Wiswesser Line Notation 1X1&1&1
Evaluation A

C_5H_{12} (liq) 30PAR/HUF
2-Methylbutane; Isopentane
Heat Capacity 275.8 K, C_p=157.3 J·mol^{-1}·K^{-1}
Temperature range 80 to 276 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=254.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 57.49 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 112.6 K, ΔH=5113 J·mol^{-1}
ΔS=45.41 J·mol^{-1}·K^{-1}
Molecular Weight 72.1498
Wiswesser Line Notation 2Y1&1
Evaluation B (C_p),C(S)

C_5H_{12} (liq) 42SCH/AST
2-Methylbutane; Isopentane
Heat Capacity 290 K, C_p=169.41 J·mol^{-1}·K^{-1}
Temperature range 20 to 290 K.
Entropy 298.15 K, S=261.04 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 113.39 K, ΔH=5130 J·mol^{-1}
ΔS=45.24 J·mol^{-1}·K^{-1}
liq/g 293.95 K, ΔH=24832 J·mol^{-1}
ΔS=84.48 J·mol^{-1}·K^{-1}
P=79.15 kPa
Molecular Weight 72.1498
Wiswesser Line Notation 2Y1&1
Evaluation A

C_5H_{12} (liq) 43GUT/HUF
2-Methylbutane; Isopentane
Heat Capacity 298.15 K, C_p=164.85 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=260.41 J·mol^{-1}·K^{-1}
Phase Changes Small second order transition 69 to 77 K.
c/liq 113.37 K, ΔH=5155.5 J·mol^{-1}
ΔS=45.48 J·mol^{-1}·K^{-1}
Molecular Weight 72.1498
Wiswesser Line Notation 2Y1&1
Evaluation A

C_5H_{12} (liq) 88CZA
2-Methylbutane; Isopentane
Heat Capacity 298.3 K, C_p=164.5 J·mol^{-1}·K^{-1}
Temperature range 289 to 299 K. p=0.1 MPa. Unsmoothed experimental datum. C_p values provided over the pressure range 0.1 to 820 MPa.
Molecular Weight 72.1498
Wiswesser Line Notation 2Y1&1
Evaluation B

C_5H_{12} (liq) 30PAR/HUF2
n-Pentane
Heat Capacity 290.0 K, C_p=163.2 J·mol^{-1}·K^{-1}
Temperature range 93 to 290 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=259.4 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 56.61 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 143.4 K, ΔH=8376 J· mol^{-1}
ΔS=58.41 J·mol^{-1}·K^{-1}
Molecular Weight 72.1498
Wiswesser Line Notation 5H
Evaluation B (C_p),C(S)

C_5H_{12} (liq) 40MES/KEN
n-Pentane
Heat Capacity 290 K, C_p=167.99 J·mol^{-1}·K^{-1}
Temperature range 12 to 290 K.
Entropy 298.15 K, S=262.67 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 143.46 K, ΔH=8414.9 J· mol^{-1}
ΔS=58.66 J·mol^{-1}·K^{-1}
liq/g 298.15 K, ΔH=26200 J· mol^{-1}
ΔS=87.88 J·mol^{-1}·K^{-1}
P=68.68 kPa
Molecular Weight 72.1498
Wiswesser Line Notation 5H
Evaluation A

C_5H_{12} (liq) 67MES/GUT
n-Pentane
Heat Capacity 298.15 K, C_p=167.19 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=263.47 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 143.47 K, ΔH=8401 J· mol^{-1}
ΔS=58.56 J·mol^{-1}·K^{-1}
Molecular Weight 72.1498
Wiswesser Line Notation 5H
Evaluation A

C_5H_{12} (liq) 75GRI/RAS
n-Pentane
Heat Capacity 298 K, C_p=168.6 J·mol^{-1}·K^{-1}
Temperature range 300 to 463 K.
Molecular Weight 72.1498
Wiswesser Line Notation 5H
Evaluation B

$C_5H_{12}N_2O$ (liq) 88KOZ/KRA
Tetramethylurea; Tetramethylcarbamide
Heat Capacity 320 K, C_p=241.2 J·mol^{-1}·K^{-1}
Temperature range 160 to 425 K. Equation only. C_p(c)=60.22 + 0.520 T J· mol^{-1}· K^{-1} (160 to 240 K); C_p(liq)=153.30 + 0.2748 J· mol^{-1}· K^{-1} (320 to 425 K).
Phase Changes
c/liq 272.2 K, ΔH=13400 J· mol^{-1}
ΔS=49.2 J· mol^{-1}· K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation 1N1&VN1&1
Evaluation A

$C_5H_{12}N_2O$ (liq) 88KOZ/KRA2
Tetramethylurea; Tetramethylcarbamide
Heat Capacity
Temperature range 160 to 425 K. Due to melting temperature of 272.2K, C_p(liq) at 298.15K could not be calculated.
Phase Changes
c/liq 272.2 K, ΔH=13400 J· mol^{-1}
ΔS=49.2 J· mol^{-1}· K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation 1N1&VN1&1
Evaluation B
C_p(c)=60.22+0.5207 T (160 to 240K); C_p(liq)=153.30+0.2748 T (320 to 425 K) J· mol^{-1}· K^{-1}.

$C_5H_{12}N_2O$ (c) 87DEL/FER
1,3-Diethylurea
Phase Changes
c,II/c,I 339.4 K, ΔH=1870 J· mol^{-1}
ΔS= 55.1 J·mol^{-1}·K^{-1}
c/liq 383.4 K, ΔH=12460 J· mol^{-1}
ΔS=32.5 J· mol^{-1}· K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation 2MVM2
Evaluation A

$C_5H_{12}N_2O$ (c) 87DEL/FER
Butylurea; Monobutylurea
Phase Changes
c,III/c,II 313.1 K, ΔH=7020 J· mol^{-1}
c,II/c,I 344.9 K, ΔH=880 J· mol^{-1}
c/liq 369.3 K, ΔH=14550 J· mol^{-1}
ΔS=39.4 J· mol^{-1}· K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation ZVM4
Evaluation A

$C_5H_{12}N_2O$ (c) 87DEL/FER
tert-Butylurea; Mono-tert-butylurea
Phase Changes
c/liq 449.8 K, ΔH=33130 J· mol^{-1}
ΔS=73.6 J· mol^{-1}· K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation ZVMX
Evaluation A

$C_5H_{12}N_2O$ (c) 86KRA/KOZ
N,N-Diethylurea; 1,1-Diethylurea
Heat Capacity 300 K, C_p=185.2 J·mol^{-1}·K^{-1}
Temperature range 140 to 310 K.
Phase Changes
c,II/c,I 195-225 K, ΔH=2000 J· mol^{-1}
ΔS=9.61 J·mol^{-1}· K^{-1}
Reversible transition.
c,I/liq 384.43 K, ΔH=16100 J· mol^{-1}
ΔS=41.9 J· mol^{-1}· K^{-1}
c/g 326 K, ΔH=96800 J· mol^{-1}
ΔS=296.9 J·mol^{-1}·K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation ZVN2&2
Evaluation B

$C_5H_{12}N_2O$ (c) 87DEL/FER
N,N-Diethylurea; 1,1-Diethylurea
Phase Changes
c/liq 342.3 K, $\Delta H = 16780$ J· mol^{-1}
$\Delta S = 49.0$ J· mol^{-1}· K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation ZVN2&2
Evaluation A

$C_5H_{12}N_2O_2$ (c) 40HUF/FOX
Ornithine(DL)
Heat Capacity 298.1 K, $C_p = 191.33$ J·mol^{-1}·K^{-1}
Temperature range 90 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S = 193.3$ J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 55.06 J· mol^{-1}· K^{-1}.
Molecular Weight 132.1620
Wiswesser Line Notation Z3YZVQ -DL
Evaluation C

$C_5H_{12}O$ (liq) 36EVA/EDL
3,3-Dimethyl-2-oxabutane; Methyl tert-butyl ether
Heat Capacity 298 K, $C_p = 188$ J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation 1X1&1&O1
Evaluation C

$C_5H_{12}O$ (liq) 75AND/MAR
3,3-Dimethyl-2-oxabutane; Methyl tert-butyl ether
Heat Capacity 298.15 K, $C_p = 187.5$ J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Entropy 298.15 K, $S = 265.3$ J· mol^{-1}· K^{-1}
Phase Changes
c/liq 164.56 K, $\Delta H = 7600$ J· mol^{-1}
$\Delta S = 46.18$ J·mol^{-1}·K^{-1}
Molecular Weight 88.1492
Wiswesser Line Notation 1X1&1&O1
Evaluation A

$C_5H_{12}O$ (liq) 75FEN/HAR
3,3-Dimethyl-2-oxabutane; Methyl tert-butyl ether
Heat Capacity 298.15 K, $C_p = 187.8$ J·mol^{-1}K^{-1}·
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation 1X1&1&O1
Evaluation B

$C_5H_{12}O$ (liq) 75AND/MAR
3-Oxahexane; Ethyl n-propyl ether
Heat Capacity 298.15 K, $C_p = 197.2$ J·mol^{-1}· K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, $S = 295.0$ J· mol^{-1}· K^{-1}
Phase Changes
c/liq 145.65 K, $\Delta H = 8395$ J· mol^{-1}
$\Delta S = 57.64$ J·mol^{-1}· K^{-1}
Molecular Weight 88.1492
Wiswesser Line Notation 3O2
Evaluation A

$C_5H_{12}O$ (liq) 75FEN/HAR
3-Oxahexane; Ethyl n-propyl ether
Heat Capacity 298.15 K, $C_p = 197.5$ J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation 3O2
Evaluation B

$C_5H_{12}O$ (liq) 75AND/MAR
2-Oxahexane; Methyl n-butyl ether
Heat Capacity 298.15 K, $C_p = 192.7$ J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Entropy 298.15 K, $S = 295.3$ J· mol^{-1}· K^{-1}
Phase Changes
c/liq 157.48 K, $\Delta H = 10850$ J· mol^{-1}
$\Delta S = 68.90$ J·mol^{-1}·K^{-1}
Molecular Weight 88.1492
Wiswesser Line Notation 4O1
Evaluation A

$C_5H_{12}O$ (liq) 75FEN/HAR
2-Oxahexane; Methyl n-butyl ether
Heat Capacity 298.15 K, $C_p = 193.0$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation 4O1
Evaluation B

$C_5H_{12}O$ (liq) 82VIL/CAS
2-Oxahexane
Methyl n-butyl ether
Heat Capacity 298.15 K, $C_p = 192.48$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation 4O1
Evaluation B

$C_5H_{12}O$ (liq) 24WIL/DAN
3-Methyl-1-butanol; Isoamyl alcohol
Heat Capacity 303 K, $C_p = 210.0$ J·mol^{-1}·K^{-1}
Temperature range 303 to 343 K. Equation only.
Molecular Weight 88.1492
Wiswesser Line Notation Q2Y1&1
Evaluation C

$C_5H_{12}O$ (liq) 45ZHI
3-Methyl-1-butanol; Isoamyl alcohol
Heat Capacity 295.52 K, $C_p = 209.52$ J·mol^{-1}·K^{-1}
Temperature range 7 to 47°C. Value is unsmoothed experimental datum.
Molecular Weight 88.1492
Wiswesser Line Notation Q2Y1&1
Evaluation C

$C_5H_{12}O$ (liq) 58SWI/ZIE
3-Methyl-1-butanol; Isoamyl alcohol
Heat Capacity 347 K, $C_p = 257.7$ J·mol^{-1}·K^{-1}
Mean value 22 to 126°C.
Molecular Weight 88.1492
Wiswesser Line Notation Q2Y1&1
Evaluation C

$C_5H_{12}O$ (liq) 1881RE
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 298 K, $C_p = 183.3$ J·mol^{-1}·K^{-1}
Temperature range 298 to 400 K.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation D

$C_5H_{12}O$ (liq) 33PAR/HUF
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 298.0 K, C_p=209.12 J·mol^{-1}·K^{-1}
Temperature range 94 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S−254.8 J mol^{-1}· K^{-1}
Extrapolation below 90 K, 57.66 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 194.2 K, ΔH=9828 J· mol^{-1}
ΔS=50.61 J·mol^{-1}·K^{-1}
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation B (C_p),C(S)

$C_5H_{12}O$ (liq) 39PHI
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 302.4 K, C_p=201.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation C
Isomer not specified; normal assumed.

$C_5H_{12}O$ (liq) 68COU/LEE
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 298.15 K, C_p=208.3 J·mol^{-1}· K^{-1}
Temperature range 10 to 390 K.
Entropy 298.15 K, S=258.9 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 195.56 K, ΔH=10502 J· mol^{-1}
ΔS=53.70 J·mol^{-1}· K^{-1}
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation A

$C_5H_{12}O$ (liq) 70PAZ/PAZ
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 313.2 K, C_p=240.6 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation B

$C_5H_{12}O$ (liq) 76SKO/SUU
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 298.15 K, C_p=208.40 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation A

$C_5H_{12}O$ (liq) 79GRI/YAN
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 301.26 K, C_p=212.3 J·mol^{-1}· K^{-1}
Temperature range 301 to 463 K. p=0.98 bar.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation B

$C_5H_{12}O$ (liq) 81ARU/BAG
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 293.15 K, C_p=205.6 J·mol^{-1}· K^{-1}
Temperature range 293 to 393 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.332 kJ/kg· K. C_p given from 293.15 to 533.15 K for pressure range 10 to 60 MPa.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation B

$C_5H_{12}O$ (liq) 83DAP/DEL
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 298.15 K, C_p=207.4 J·mol^{-1}· K^{-1}
Data given at 288 and 298 K.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation B

$C_5H_{12}O$ (liq) 84ZEG/SOM
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 298.15 K, C_p=208.98 J·mol^{-1}· K^{-1}
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation B

$C_5H_{12}O$ (liq) 86BEN/DAR
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 298.15 K, C_p=207.45 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation B

$C_5H_{12}O$ (liq) 86BEN/DAR2
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 298.15 K, C_p=207.45 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation B

$C_5H_{12}O$ (liq) 86TAN/TOY
1-Pentanol; n-Amyl alcohol; n-Pentyl alcohol
Heat Capacity 298.15 K, C_p=208.19 J·mol^{-1}· K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation A

$C_5H_{12}O$ (c) 70MUR/BRE
2,2-Dimethyl-1-propanol
Phase Changes
c,II/c,I 242 K, ΔH=4463 J· mol^{-1}
ΔS=18.4 J· mol^{-1}· K^{-1}
c,I/liq 325 K, ΔH=4057 J· mol^{-1}
ΔS=12.5 J· mol^{-1}· K^{-1}
Molecular Weight 88.1492
Wiswesser Line Notation Q1X1&1&1
Evaluation A

$C_5H_{12}O$ (liq) 33PAR/HUF
2-Methyl-2-butanol; tert-Amyl alcohol; tert-Pentyl alcohol
Heat Capacity 294.4 K, C_p=244.14 J·mol^{-1}· K^{-1}
Temperature range 92 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=229.3 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 46.78 J· mol^{-1}· K^{-1}.
Phase Changes
c,III/c,II 146.0 K, ΔH=1962 J· mol^{-1}
ΔS=13.44 J·mol^{-1}· K^{-1}
c,II/c,I 213 K, ΔH=167 J· mol^{-1}
ΔS=0.79 J· mol^{-1}· K^{-1}
c,I/liq 264.0 K, ΔH=4456 J· mol^{-1}
ΔS=16.88 J·mol^{-1}· K^{-1}
Molecular Weight 88.1492
Wiswesser Line Notation QX1&1&2
Evaluation B (C_p),C(S)

$C_5H_{12}O$ (liq) 83DAP/DEL
2-Methyl-2-butanol; tert-Amyl alcohol; tert-Pentyl alcohol
Heat Capacity 298.15 K, C_p=247.3 J·mol^{-1}·K^{-1}
Data given at 288 and 298 K.
Molecular Weight 88.1492
Wiswesser Line Notation QX1&1&2
Evaluation B

$C_5H_{12}O$ (liq) 86BEN/DAR
2-Methyl-2-butanol; tert-Amyl alcohol; tert-Pentyl alcohol
Heat Capacity 298.15 K, C_p=248.86 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation QX1&1&2
Evaluation B

$C_5H_{12}O$ (liq) 86BEN/DAR2
2-Methyl-2-butanol; tert-Amyl alcohol; tert-Pentyl alcohol
Heat Capacity 298.15 K, C_p=248.86 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation QX1&1&2
Evaluation B

$C_5H_{12}O$ (liq) 88PIE/SOM
2-Methyl-2-butanol; tert-Amyl alcohol; tert-Pentyl alcohol
Heat Capacity 298.15 K, C_p=247.15 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation QX1&1&2
Evaluation B

$C_5H_{12}O$ (liq) 91ATR/NES
3-Methyl-2-butanol
Heat Capacity 298.15 K, C_p=245.9 J·mol^{-1}·K^{-1}
Temperature range 218 to 373 K. C_p(liq)=4.81853− 3.12708(T/100)+0.182356(T/100)^2+0.484126(T/100)^3−0.0905712(T/100)^4 kJ/kg· K.
Molecular Weight 88.1492
Wiswesser Line Notation QY1&Y1&1
Evaluation B

$C_5H_{12}O$ (liq) 76CON/GIN
3-Pentanol
Heat Capacity 298 K, C_p=239.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation QY2&2
Evaluation B

$C_5H_{12}O_2$ (liq) 84BAG/BAE
2,2-Dimethoxypropane
Heat Capacity 298.15 K, C_p=218.0 J·mol^{-1}·K^{-1}
Temperature range 273 to 334 K. C_p(liq)= 2.75970 - 0.007898T + 1.9 × 10^{-5}T^2 kJ/kg· K (273 to 334 K).
Molecular Weight 104.1486
Wiswesser Line Notation 1OXO1
Evaluation B

$C_5H_{12}O_2$ (liq) 88BAG/GUR
2,2-Dimethoxypropane
Heat Capacity 298.15 K, C_p=217.7 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 104.1486
Wiswesser Line Notation 1OXO1
Evaluation B

$C_5H_{12}O_2$ (liq) 73KUS/SUU
2,5-Dioxaheptane; 1-Ethoxy-2-methoxyethane
Heat Capacity 298.15 K, C_p=224.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 104.1486
Wiswesser Line Notation 2O2O1
Evaluation B

$C_5H_{12}O_2$ (c) 70MUR/BRE
2,2-Dimethyl-1,3-propanediol
Phase Changes

c,II/c,I	314 K,	ΔH=13639 J· mol^{-1}
		ΔS=43.1 J· mol^{-1}· K^{-1}
c,I/liq	398 K,	ΔH=4706 J· mol^{-1}
		ΔS=11.7 J· mol^{-1}· K^{-1}

Molecular Weight 104.1486
Wiswesser Line Notation Q1X1&1&1Q
Evaluation A

$C_5H_{12}O_2$ (c) 88ZHA/HON
2,2-Dimethyl-1,3-propanediol
Heat Capacity 298.15 K, C_p=183.18 J·mol^{-1}·K^{-1}
Temperature range 270 to 440 K. C_p(c)=176.017 + 14.708x +6.114x^2 +6.148^3− 9.805×^4x= (T-290)/20] (270 to 310 K) J · mol^{-1}· K^{-1}.
Phase Changes

c,II/c,I	314.8 K,	ΔH=12410 J· mol^{-1}
		ΔS=39.4 J· mol^{-1}· K^{-1}
c,I/liq	403.3 K,	ΔH=4440 J· mol^{-1}
		ΔS=10.5 J· mol^{-1}· K^{-1}

Molecular Weight 104.1486
Wiswesser Line Notation Q1X1&1&1Q
Evaluation B

$C_5H_{12}O_2$ (c) 88ZHA/ZOU
2,2-Dimethyl-1,3-propanediol
Heat Capacity 298.15 K, C_p=183.18 J·mol^{-1}·K^{-1}
Temperature range 270 to 440 K.
Phase Changes

c,II/c,I	314.8 K,	ΔH=12410 J· mol^{-1}
		ΔS=39.4 J· mol^{-1}· K^{-1}
c,I/liq	403.3 K,	ΔH=4440 J· mol^{-1}
		ΔS=10.5 J· mol^{-1}· K^{-1}

Molecular Weight 104.1486
Wiswesser Line Notation Q1X1Q&1&1
Evaluation B

$C_5H_{12}O_2$ (liq) 73KUS/SUU
3-Oxa-1-hexanol; 2-n-Propoxyethanol
Heat Capacity 298.15 K, C_p=241.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 104.1486
Wiswesser Line Notation Q2O3
Evaluation B

$C_5H_{12}O_2$ (liq) 78ROU/PER
3-Oxa-1-hexanol; 2-n-Propoxyethanol
Heat Capacity 298.15 K, C_p=244.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 104.1486
Wiswesser Line Notation Q2O3
Evaluation C

$C_5H_{12}O_2$ (liq) 73KUS/SUU
4-Methyl-3-oxa-1-pentanol; 2-Isopropoxyethanol
Heat Capacity 298.15 K, C_p=238.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 104.1486
Wiswesser Line Notation Q2OY1&1
Evaluation B

$C_5H_{12}O_2$ (liq) 35MIL
1,5-Pentanediol
Heat Capacity
Temperature range 100 to 298 K. Data in thesis only.
Entropy 298.15 K, S= 321.3 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 78.49 J· mol^{-1}· K^{-1}.
Phase Changes
c/liq 248.0 K, ΔH=15728 J· mol^{-1}
ΔS=63.4 J· mol^{-1}· K^{-1}
Molecular Weight 104.1486
Wiswesser Line Notation Q5Q
Evaluation C

$C_5H_{12}O_3$ (c) 70MUR/BRE
2-Hydroxymethyl-2-methyl-1,3-propanediol; Trimethylolethane
Phase Changes
c,II/c,I 354 K, ΔH=23174 J· mol^{-1}
ΔS=65.3 J· mol^{-1}· K^{-1}
c,I/liq 470 K, ΔH=5379 J· mol^{-1}
ΔS=11.3 J· mol^{-1}· K^{-1}
Molecular Weight 120.1480
Wiswesser Line Notation Q1X1&1Q1Q
Evaluation A

$C_5H_{12}O_3$ (c) 90SUE/MAT
2-Hydroxymethyl-2-methyl-1,3-propanediol; Trimethylolethane
Heat Capacity 299.15 K, C_p=182.6 J·mol^{-1}·K^{-1}
Temperature range 18 to 375 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 358.2 K, ΔH=21240 J· mol^{-1}
ΔS=59.28 J·mol^{-1}·K^{-1}
c,I/liq 474 K, ΔH=4700 J· mol^{-1}
ΔS=9.89 J·mol^{-1}·K^{-1}
Molecular Weight 120.1480
Wiswesser Line Notation Q1X1&1Q1Q
Evaluation A

$C_5H_{12}O_3 \cdot 4H_2O$ (c) 91LAU/TEI
2-Hydroxymethyl-2-methyl-1,3-propanediol tetrahydrate; Trimethylolethane tetrahydrate
Phase Changes
c/liq 302.95 K, ΔH=35559 J· mol^{-1}
Molecular Weight 192.2088
Wiswesser Line Notation Q1X1&1Q1Q &QH 4
Evaluation B

$C_5H_{12}O_4$ (c) 50HOS/NAG
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane; Pentaerythritol
Phase Changes
c,II/c,I 457 K, ΔH=35146 J· mol^{-1}
ΔS=76.9 J·mol^{-1}·K^{-1}
c,I/liq 529 K, ΔH=5439 J· mol^{-1}
ΔS=10.28 J·mol^{-1}·K^{-1}
Molecular Weight 136.1474
Wiswesser Line Notation Q1X1Q1Q1Q
Evaluation B

$C_5H_{12}O_4$ (c) 50NIT/SEK
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane; Pentaerythritol
Heat Capacity 373.2 K, C_p=254.4 J·mol^{-1}·K^{-1}
Temperature range 373 to 567 K.
Phase Changes
c,II/c,I 460.4 K, ΔH=43930 J· mol^{-1}
ΔS=95.4 J· mol^{-1}· K^{-1}
c,I/liq 538.7 K, ΔH=7110 J· mol^{-1}
ΔS=13.2 J· mol^{-1}· K^{-1}
Molecular Weight 136.1474
Wiswesser Line Notation Q1X1Q1Q1Q
Evaluation B

$C_5H_{12}O_4$ (c) 59WES
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane; Pentaerythritol
Heat Capacity 298.15 K, C_p=190.41 J·mol^{-1}·K^{-1}
Based on data 10 to 350 K, to be reported elsewhere.
Entropy 298.15 K, S=198.07 J·mol^{-1}·K^{-1}
Molecular Weight 136.1474
Wiswesser Line Notation Q1X1Q1Q1Q
Evaluation B

$C_5H_{12}O_4$ (c) 70MUR/BRE
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane; Pentaerythritol
Phase Changes
c,II/c,I 455 K, ΔH=41014 J· mol^{-1}
ΔS=90.0 J· mol^{-1}· K^{-1}
c,I/liq 531 K, ΔH=5070 J· mol^{-1}
ΔS=9.6 J· mol^{-1}· K^{-1}
Molecular Weight 136.1474
Wiswesser Line Notation Q1X1Q1Q1Q
Evaluation A

$C_5H_{12}O_4$ (c) 89ZHA/YAN
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane; Pentaerythritol
Heat Capacity 298.98 K, C_p=188.40 J·mol^{-1}·K^{-1}
Temperature range 277 to 510 K.
Phase Changes
c,II/c,I 461.60 K, ΔH=41380 J· mol^{-1}
ΔS=89.64 J·mol^{-1}·K^{-1}
Molecular Weight 136.1474
Wiswesser Line Notation Q1X1Q1Q1Q
Evaluation A

$C_5H_{12}O_4$ (c) 90BAR/DEL
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane; Pentaerythritol
Phase Changes
c,II/c,I 458.3 K, ΔH=40500 J· mol^{-1}
ΔS=88.4 J· mol^{-1}· K^{-1}
c,I/liq 513.2 K, ΔH=4600 J· mol^{-1}
ΔS=9.0 J· mol^{-1}· K^{-1}
Molecular Weight 136.1474
Wiswesser Line Notation Q1X1Q1Q1Q
Evaluation A

$C_5H_{12}O_5$ (c) 90BAR/DEL
Adonitol; 1,2,3,4,5-Pentahydroxypentane; 1,2,3,4,5-Pentanepentol; Ribitol
Phase Changes
c/liq 374.7 K, $\Delta H = 37600$ J·mol^{-1}
$\Delta S = 100.3$ J·mol^{-1}·K^{-1}
Molecular Weight 152.1468
Wiswesser Line Notation Q1YQYQYQ1Q -AAA
Evaluation A

$C_5H_{12}O_5$ (c) 90BAR/DEL
xylo-1,2,3,4,5-Pentanepentol; Xylitol
Phase Changes
c/liq 365.7 K, $\Delta H = 37400$ J·mol^{-1}
$\Delta S = 102.3$ J·mol^{-1}·K^{-1}
Molecular Weight 152.1468
Wiswesser Line Notation Q1YQYQYQ1Q -ABA
Evaluation A

$C_5H_{12}O_5$ (c) 90BAR/DEL
1,2,3,4,5-Pentahydroxypentane; 1,2,3,4,5-Pentanepentol; Arabinitol(D); Arabitol(D)
Phase Changes
c/liq 379.4 K, $\Delta H = 38900$ J·mol^{-1}
$\Delta S = 102.5$ J·mol^{-1}·K^{-1}
Molecular Weight 152.1468
Wiswesser Line Notation Q1YQYQYQ1Q -BAA
Evaluation A

$C_5H_{12}S$ (liq) 62SCO/GOO
3,3-Dimethyl-2-thiabutane; Methyl tert-butyl sulfide
Heat Capacity 298.15 K, $C_p = 199.95$ J·mol^{-1}·K^{-1}
Temperature range 15 to 364 K.
Entropy 298.15 K, $S = 276.14$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 190.84 K, $\Delta H = 8414$ J·mol^{-1}
$\Delta S = 44.09$ J·mol^{-1}·K^{-1}
Molecular Weight 104.2098
Wiswesser Line Notation 1X1&1&S1
Evaluation A

$C_5H_{12}S$ (liq) 61MCC/FIN
3-Thiahexane; Ethyl n-propyl sulfide
Heat Capacity 298.15 K, $C_p = 198.41$ J·mol^{-1}·K^{-1}
Temperature range 11 to 370 K.
Entropy 298.15 K, $S = 309.53$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 156.10 K, $\Delta H = 10581$ J·mol^{-1}
$\Delta S = 67.78$ J·mol^{-1}·K^{-1}
Molecular Weight 104.2098
Wiswesser Line Notation 3S2
Evaluation A

$C_5H_{12}S$ (liq) 61MCC/FIN
2-Thiahexane; n-Butyl methyl sulfide
Heat Capacity 298.15 K, $C_p = 200.92$ J·mol^{-1}·K^{-1}
Temperature range 11 to 370 K.
Entropy 298.15 K, $S = 307.48$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 175.30 K, $\Delta H = 12452$ J·mol^{-1}
$\Delta S = 71.03$ J·mol^{-1}·K^{-1}
Molecular Weight 104.2098
Wiswesser Line Notation 4S1
Evaluation A

$C_5H_{12}S$ (gls) 74MES/FIN
3-Methyl-1-butanethiol; Isoamyl mercaptan
Heat Capacity 103 K, $C_p = 93.72$ J·mol^{-1}·K^{-1}
Temperature range 10 to 103 K.
Molecular Weight 104.2098
Wiswesser Line Notation SH2Y1&1
Evaluation A

$C_5H_{12}S$ (liq) 74MES/FIN
3-Methyl-1-butanethiol; Isoamyl mercaptan
Heat Capacity 298.15 K, $C_p = 200.33$ J·mol^{-1}·K^{-1}
Temperature range 12 to 370 K.
Entropy 298.15 K, $S = 298.49$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 139.635 K, $\Delta H = 7406$ J·mol^{-1}
$\Delta S = 53.04$ J·mol^{-1}·K^{-1}
Molecular Weight 104.2098
Wiswesser Line Notation SH2Y1&1
Evaluation A

$C_5H_{12}S$ (liq) 52FIN/SCO
1-Pentanethiol; n-Amyl mercaptan
Heat Capacity 296.21 K, $C_p = 201.17$ J·mol^{-1}·K^{-1}
Temperature range 12 to 320 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S = 310.37$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 197.46 K, $\Delta H = 17531$ J·mol^{-1}
$\Delta S = 88.78$ J·mol^{-1}·K^{-1}
Molecular Weight 104.2098
Wiswesser Line Notation SH5
Evaluation A

$C_5H_{12}S$ (liq) 62SCO/DOU
2-Methyl-2-butanethiol; tert-Amyl mercaptan
Heat Capacity 298.15 K, $C_p = 198.15$ J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, $S = 290.12$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 159.1 K, $\Delta H = 7979.3$ J·mol^{-1}
$\Delta S = 50.15$ J·mol^{-1}·K^{-1}
Lambda transition at about 145 K.
c,I/liq 169.3 K, $\Delta H = 608.4$ J·mol^{-1}
$\Delta S = 3.59$ J·mol^{-1}·K^{-1}
Molecular Weight 104.2098
Wiswesser Line Notation SHX1&1&2
Evaluation A

$C_5H_{12}S$ (liq) 74MES/FIN
3-Methyl-2-butanethiol
Heat Capacity 298.15 K, $C_p = 198.95$ J·mol^{-1}·K^{-1}
Temperature range 10 to 390 K.
Entropy 298.15 K, $S = 295.60$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 144.47 K, $\Delta H = 7063$ J·mol^{-1}
$\Delta S = 48.89$ J·mol^{-1}·K^{-1}
c,I/liq 146.05 K, $\Delta H = 607.1$ J·mol^{-1}
$\Delta S = 4.16$ J·mol^{-1}·K^{-1}
Molecular Weight 104.2098
Wiswesser Line Notation SHY1&Y1&1
Evaluation A

$C_5H_{12}S_4$ (c,II) 43BAC/PER
Tetrakis(methylthia)methane
Heat Capacity 307 K,
C_p=146.4 J· mol^{-1}· K^{-1} Mean value 23.2 to 45.5°C. Value for c,III at 23.2°C=133.9 J· mol^{-1}· K^{-1}; c,I, between 45.5 and 65.5°C=197.5 J· mol^{-1}· K^{-1}; liquid at 65.5°C= 216.7 J· mol^{-1}· K^{-1}.
Phase Changes

c,III/c,II	296.4 K,	ΔH=6110 J· mol^{-1}
		ΔS=20.6 J· mol^{-1}· K^{-1}
c,II/c,I	318.7 K,	ΔH=7610 J· mol^{-1}
		ΔS=23.9 J· mol^{-1}· K^{-1}
c,I/liq	338.7 K,	ΔH=4140 J· mol^{-1}
		ΔS=12.2 J· mol^{-1}· K^{-1}

Molecular Weight 200.3898
Wiswesser Line Notation 1SXS1&S1&S1
Evaluation C

$C_5H_{12}Si$ (liq) 75RAB/LEB
Vinyltrimethylsilane
Heat Capacity 300 K, C_p=198.3 J·mol^{-1}·K^{-1}
Temperature range 50 to 300 K.
Entropy 300 K, S=313.4 J· mol^{-1}· K^{-1}
Phase Changes

c/liq	141.65 K,	ΔH=7657 J· mol^{-1}
		ΔS=54.06 J·mol^{-1}·K^{-1}

Molecular Weight 100.2353
Wiswesser Line Notation 1U1-SI-1&1&1
Evaluation A

$C_5H_{12}Si$ (liq) 73LEB/TSV
Vinyltrimethylsilane
Heat Capacity 300 K, C_p=198.3 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 300 K, S=313.4 J· mol^{-1}· K^{-1}
Phase Changes

c/liq	141.57 K,	ΔH=7657 J· mol^{-1}
		ΔS=54.06 J·mol^{-1}·K^{-1}

Molecular Weight 100.2353
Wiswesser Line Notation 1U1-SI-1&1&1
Evaluation A

$C_5H_{12}Si$ (liq) 81LEB/LEB
Vinyltrimethylsilane
Heat Capacity 298.15 K, C_p=198.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=312.2 J· mol^{-1}· K^{-1}
Phase Changes

c/liq	141.57 K,	ΔH=7660 J· mol^{-1}
		ΔS=54.0 J· mol^{-1}· K^{-1}

Molecular Weight 100.2353
Wiswesser Line Notation 1U1-SI-1&1&1
Evaluation A

$C_5H_{12}Si$ (c) 75GUS/KAR
1,1-Dimethyl-1-silacyclobutane
Heat Capacity 298.15 K, C_p=197.53 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K. Data given graphically.
Entropy 298.15 K, S=279.49 J·mol^{-1}·K^{-1}
Phase Changes

c/liq	155.52 K,	ΔH=6761 J· mol^{-1}
		ΔS=43.51 J·mol^{-1}·K^{-1}
liq/g	355.91 K,	ΔH=32141 J· mol^{-1}
		ΔS=90.29 J·mol^{-1}·K^{-1}

Molecular Weight 100.2353
Wiswesser Line Notation T4-SI-TJ A1 A1
Evaluation B

$(C_5H_{12}Si)_n$ (gls) 75RAB/LEB
Polyvinyltrimethylsilane
Heat Capacity 300 K, C_p=179.9 J·mol^{-1}·K^{-1}
Temperature range 50 to 300 K.
Entropy 300 K, S=217.6 J· mol^{-1}· K^{-1}
Molecular Weight 100.2353
Wiswesser Line Notation /*1Y*-SI-1&1&1/
Evaluation A

$(C_5H_{12}Si)_n$ (c) 78LEB/RAB3
Poly-1,1-dimethyl-1-silatrimethylene
Heat Capacity 298.15 K, C_p=170.9 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K. C_p(rubber like elastic state, 298.15 K)=199.5 J/mol· K.
Entropy 298.15 K, S=194.1 J· mol^{-1}· K^{-1}
S(rubber like elastic state, 298.15 K)=217.9 J/mol· K.
Phase Changes

c/liq	325 K,	ΔH=8490 J· mol^{-1}
		ΔS=26.1 J· mol^{-1}· K^{-1}

Molecular Weight 100.2353
Wiswesser Line Notation /*-SI-1&1&3*/
Evaluation A
100% crystallinity. T(glass)=201 K.

$(C_5H_{12}Si)_n$ (gls) 73LEB/TSV
Polyvinyltrimethylsilane
Heat Capacity 300 K, C_p=179.9 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 300 K, S=217.6 J· mol^{-1}· K^{-1}
Molecular Weight 100.2353
Wiswesser Line Notation /*1Y*-SI-1&1&1/
Evaluation A

$(C_5H_{12}Si)_n$ (c) 81LEB/LEB
Polyvinyltrimethylsilane
Heat Capacity 298.15 K, C_p=166.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=189.6 J· mol^{-1}· K^{-1}
Molecular Weight 100.2353
Wiswesser Line Notation /*1Y*-SI-1&1&1/
Evaluation A

$C_5H_{13}N$ (liq) 80ROU/ROB
Diethylmethylamine
Heat Capacity 298.15 K, C_p=200 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 87.1644
Wiswesser Line Notation 2N2&1
Evaluation B

$C_5H_{13}N$ (liq) 01KAH
1-Aminopentane; n-Amylamine; n-Pentylamine
Heat Capacity C_p=223.8 J· mol^{-1}· K^{-1}
Temperature range 294.15 to 403.15 K. Heat capacity is an average value over the temperature range.
Molecular Weight 87.1644
Wiswesser Line Notation Z5
Evaluation D

$C_5H_{13}N$ (liq) 71KON/WAD
1-Aminopentane; n-Amylamine; n-Pentylamine
Heat Capacity 198.15 K, C_p=218 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 87.1644
Wiswesser Line Notation Z5
Evaluation B

$C_5H_{13}NO$ (liq) 81LEB/RYA
Methylethylethanolamine
Heat Capacity C_p= 256.8 J· mol^{-1}· K^{-1}
Temperature range 298 to 343 K. Heat capacity is an average value over the temperature range.
Molecular Weight 103.1638
Wiswesser Line Notation Q2N2&1
Evaluation B

$C_5H_{13}O_2$ (liq) 91SVO/ZAB
2-Propoxyethanol
Heat Capacity 298.15 K, C_p=241.78 J·mol^{-1}·K^{-1}
Temperature range 298 to 330 K. C:(liq)=118.555 + 0.4133(T/K) J· mol^{-1}· K^{-1}. C_p value calculated from equation.
Molecular Weight 105.1565
Wiswesser Line Notation Q2O3
Evaluation B

$C_5H_{14}ClN$ (c,I) 33SOU/MIL
n-Amylammonium chloride; n-Pentylammonium chloride
Heat Capacity 278.19 K, C_p=213.38 J·mol^{-1}·K^{-1}
Temperature range 20 to 280 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=266.69 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 221.5 K, ΔH=1184 J· mol^{-1}
ΔS=5.35 J· mol^{-1}· K^{-1}
c,II/c,I 246.5 K, ΔH=134 J· mol^{-1}
ΔS=0.54 J· mol^{-1}· K^{-1}
Molecular Weight 123.6253
Wiswesser Line Notation M5 &GH
Evaluation A

$C_5H_{14}Cl_2N_2O_2$ (c) 40HUF/ELL
Ornithine dihydrochloride
Heat Capacity 292.8 K, C_p=238.36 J·mol^{-1}·K^{-1}
Temperature range 85 to 293 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=293.93 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 89.16 J· mol^{-1}· K^{-1}.
Molecular Weight 205.0838
Wiswesser Line Notation Z3YZVQ &GH2
Evaluation A(C_p),C(S)

$C_5H_{14}NO_6P$ (c) 89MAE/ATA
Betaine phosphate
Heat Capacity
Temperature range 7 to 300 K. Data given graphically over transition region.
Phase Changes
c,III/c,II 82.67 K
c,II/c,I 87.11 K, ΔH=34 J· mol^{-1}
ΔS=0.40 J· mol^{-1}· K^{-1}
Total for both transitions.
Molecular Weight 215.1425
Wiswesser Line Notation OV1N1&1&1 &QPO&QQ
Evaluation B

$C_5H_{14}N_2$ (liq) 81LEB/RYA
N,N-Dimethyl-1,3-propanediamine
Heat Capacity 295.96 K, C_p=249.0 J·mol^{-1}·K^{-1}
Temperature range 296 to 359 K.
Molecular Weight 102.1790
Wiswesser Line Notation Z3N1&1
Evaluation B

$C_5H_{14}N_2$ (liq) 82DZH/KAR
N,N-Dimethyl-1,3-propanediamine
Heat Capacity 298.15 K, C_p=255.7 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=323.0 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 194.43 K, ΔH=12385 J· mol^{-1}
ΔS=63.70 J·mol^{-1}·K^{-1}
Glass to crystal transition at 135 K shown graphically.
Molecular Weight 102.1790
Wiswesser Line Notation Z3N1&1
Evaluation A

$C_5H_{14}N_2$ (liq) 84LEB/GU
N,N-Dimethyl-1,3-propanediamine
Heat Capacity 298 K, C_p=248.71 J·mol^{-1}·K^{-1}
Temperature range 295 to 360 K.
Phase Changes
liq/g 406 K P=9.972×10^4 kPa.
Molecular Weight 102.1790
Wiswesser Line Notation Z3N1&1
Evaluation B
ΔH vaporization=44100 J·mol^{-1}, temperature range=290 to 317 K

$C_5H_{16}Cl_4MnN_2$ (c) 87CHH/AB
Pentyldiamine manganese tetrachloride
Heat Capacity
Temperature range 10 to 300 K. Data given graphically.
Phase Changes
c,II/c,I 299.5 K, ΔS=8.24 J·mol^{-1}· K^{-1}
Molecular Weight 300.9448
Wiswesser Line Notation Z5Z &GH 2 .MN G2
Evaluation A
Second order transition at 210 to 327 K, with a maximum at 299.5 K

$C_5H_{16}Cl_4MnN_2$ (c) 88CHH/AB
Pentyldiamine manganese tetrachloride
Heat Capacity 298.15 K, C_p=424.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 330 K.
Entropy 298.15 K, S=407.6 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 299.6 K, ΔH=2240 J· mol^{-1}
ΔS=8.3 J· mol^{-1}· K^{-1}
Molecular Weight 300.9448
Wiswesser Line Notation Z5Z &GH 2 .MN G2
Evaluation A
C_p data is high due to c,II/c,I transition at 210 to 327 K.

$C_5H_{30}Bi_2Br_{11}N_5$ (c) 92PAW/JAK
Methylammonium bismuth bromide; Pentakis(methylammonium) undecabromodibismuthate
Heat Capacity
Temperature range 273 to 333 K. Data given graphically.
Molecular Weight 1457.2303
Wiswesser Line Notation ZH&1 5 -BI- 2 E 11
Evaluation C

$C_5H_{30}Bi_2Br_{11}N_5$ (c) 92STR/TAR
Methylammonium bismuth bromide; Pentakis(methylammonium) undecabromodibismuthate
Heat Capacity 300 K, C_p=960 J·mol^{-1}·K^{-1}
Temperature range 74 to 340 K. Data given graphically. C_p value is a graphical estimate.
Phase Changes Anom 75 K
c,II/c,I 309 K, ΔH=5140 J·mol^{-1}
ΔS=17.61 J·mol^{-1}·K^{-1}
Molecular Weight 1457.2303
Wiswesser Line Notation ZH&1 5 -BI- 2 E 11
Evaluation B

C_6BRF_5 (liq) 75PAU2
Bromopentafluorobenzene
Entropy 298.15 K, S=311.9 J·mol^{-1}·K^{-1}
Molecular Weight 246.9620
Wiswesser Line Notation FR BE CF DF EF FF
Evaluation A

$C_6Br_2Cl_3F_9$ (liq) 88SVO/VES
1,6-Dibromo-2,3,5-trichlorononafluorohexane
Heat Capacity 298.16 K, C_p=418.6 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K. C_p (J·mol^{-1}·K^{-1})=335.6+0.278 (T/K) (298–318 K).
Molecular Weight 509.2186
Wiswesser Line Notation FXFEXGFXGFXFFXGFXFFE
Evaluation A

C_6ClF_5 (liq) 68AND/COU2
Pentafluorochlorobenzene
Heat Capacity 298.15 K, C_p=221.4 J·mol^{-1}·K^{-1}
Temperature range 12 to 395 K.
Entropy 298.15 K, S=300.7 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 191 K, ΔH=3636 J·mol^{-1}
ΔS=19.04 J·mol^{-1}·K^{-1}
Entropy change reported as 17.91 J·mol^{-1}·K^{-1} from integration of excess heat capacity. Value given assumes isothermal transition.
c,II/c,I 245 K, ΔH=983 J·mol^{-1}
ΔS=4.01 J·mol^{-1}·K^{-1}
c,I/liq 257.49 K, ΔH=8355 J·mol^{-1}
ΔS=32.45 J·mol^{-1}·K^{-1}
Molecular Weight 202.5110
Wiswesser Line Notation GR BF CF DF EF FF
Evaluation A

C_6ClF_5 (liq) 69PAU/GLU2
Pentafluorochlorobenzene
Heat Capacity 298.15 K, C_p=223.17 J·mol^{-1}·K^{-1}
Temperature range 13 to 303 K.
Entropy 298.15 K, S=303.59 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 191.2 K, ΔH=1243 J·mol^{-1}
ΔS=6.50 J·mol^{-1}·K^{-1}
c,I/liq 257.29 K, ΔH=8397 J·mol^{-1}
ΔS=32.64 J·mol^{-1}·K^{-1}
Molecular Weight 202.5110
Wiswesser Line Notation GR BF CF DF EF FF
Evaluation A

$C_6Cl_3F_3$ (c) 69PAU/GLU
1,3,5-Trichloro-2,4,6-trichlorobenzene
Heat Capacity 298.15 K, C_p=197.95 J·mol^{-1}·K^{-1}
Temperature range 13 to 355 K.
Entropy 298.15 K, S=245.35 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 334.16 K, ΔH=19849 J·mol^{-1}
ΔS=59.40 J·mol^{-1}·K^{-1}
Smoothed table gives ΔH=4712 cal·mol^{-1}, ΔS=14.12 cal·mol^{-1}·K^{-1}.
Molecular Weight 235.4202
Wiswesser Line Notation GR CG EF BF DF FF
Evaluation B

$C_6Cl_3F_3$ (c) 73AND/MAR2
1,3,5-Trichloro-2,4,6-trichlorobenzene
Heat Capacity 298.15 K, C_p=197.0 J·mol^{-1}·K^{-1}
Temperature range 14 to 347 K.
Entropy 298.15 K, S=243.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 335.01 K, ΔH=19830 J·mol^{-1}
ΔS=59.19 J·mol^{-1}·K^{-1}
Anomalous heat capacity between 285 and 305 K. Enthalpy of transition 18.1 J·mol^{-1} (excess over extrapolated heat capacities).
Molecular Weight 235.4202
Wiswesser Line Notation GR CG EF BF DF FF
Evaluation A

$C_6Cl_4KO_2$ (c,I) 77KOS/SOR
p-Chloranil potassium
Heat Capacity 300 K, C_p=239.67 J·mol^{-1}·K^{-1}
Temperature range 14 to 331 K.
Entropy 300 K, S=313.97 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 260.01 K, ΔH=2796 J·mol^{-1}
ΔS=11.06 J·mol^{-1}·K^{-1}
ΔS obtained by summation of experimental C_p/T data.
Molecular Weight 284.9751
Wiswesser Line Notation L6V DVJ BG CG EG FG .KA
Evaluation A

$C_6Cl_4O_2$ (c,I) 73CHI/MAS
Chloranil; Tetrachloro-p-benzoquinone
Heat Capacity 298.15 K, C_p=193.8 J·mol^{-1}·K^{-1}
Temperature range 11 to 300 K.
Entropy 298.15 K, S=258.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 92 K, ΔH=38 J·mol^{-1}
ΔS=0.4 J·mol^{-1}·K^{-1}
Lambda transition, 70 to 100 K.
Molecular Weight 245.8768
Wiswesser Line Notation L6V DVJ BG CG EG FG
Evaluation A

C_6Cl_6 (c) 28AND/HAW
Hexachlorobenzene; Perchlorobenzene
Heat Capacity 299.8 K, C_p=257.7 J·mol^{-1}·K^{-1}
Temperature range 101 to 336 K. Value is unsmoothed experimental datum.
Molecular Weight 284.7840
Wiswesser Line Notation GR BG CG DG EG FG
Evaluation C

C_6Cl_6 (c) 58HIL/KRA
Hexachlorobenzene; Perchlorobenzene
Heat Capacity 298.15 K, C_p=201.29 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=260.24 J·mol^{-1}·K^{-1}
Molecular Weight 284.7840
Wiswesser Line Notation GR BG CG DG EG FG
Evaluation A

C_6Cl_6 (c) 91SAB/AN2
Hexachlorobenzene; Perchlorobenzene
Phase Changes
c/liq 502.02 K, ΔH=25180 J·mol^{-1}
ΔS=50.2 J·mol^{-1}·K^{-1}
Molecular Weight 284.7840
Wiswesser Line Notation GR BG CG DG EG FG
Evaluation B

C_6Cl_6 (c) 92SAB/ELW3
Hexachlorobenzene; Perchlorobenzene
Phase Changes
c/liq 501.87 K, ΔH=24960 J·mol^{-1}
Molecular Weight 284.7840
Wiswesser Line Notation GR BG CG DG EG FG
Evaluation A

C_6D_6 (liq) 42ZIE/AND
Benzene-d_6
Heat Capacity 298.5 K, C_p=149.4 J·mol^{-1}·K^{-1}
Temperature range 100 to 320 K. Value is unsmoothed experimental datum.
Phase Changes
c/liq 279.85 K, ΔH=9791 J·mol^{-1}
ΔS=34.99 J·mol^{-1}·K^{-1}
Molecular Weight 84.1506
Wiswesser Line Notation R &1A-F/H-2 6
Evaluation B

C_6D_6 (liq) 62RAB/NIK
Benzene-d_6
Heat Capacity 298 K, C_p=152.46 J·mol^{-1}·K^{-1}
Temperature range 10 to 35 °C.
Molecular Weight 84.1506
Wiswesser Line Notation R &1A-F/H-2 6
Evaluation B

C_6D_{12} (liq) 66NIK/RAB
Cyclohexane-d_{12}
Heat Capacity 298 K, C_p=183.84 J·mol^{-1}·K^{-1}
Temperature range 10 to 50 °C.
Molecular Weight 96.2556
Wiswesser Line Notation L6TJ &1A-F/H-2 12
Evaluation B

C_6D_{12} (liq) 80MRA/NAI
Cyclohexane-d_{12}
Heat Capacity 298.15 K, C_p=188.7 J·mol^{-1}·K^{-1}
Temperature range 120 to 323.15 K.
Entropy 298.15 K, S=228.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 186.0 K, ΔH=6810 J·mol^{-1}
ΔS=36.61 J·mol^{-1}·K^{-1}
c,I/liq 277.2 K, ΔH=2620 J·mol^{-1}
ΔS=9.452 J·mol^{-1}·K^{-1}
Molecular Weight 96.2556
Wiswesser Line Notation *L6TJ &1A-F/H-2 12*
Evaluation A

$C_6D_{17}BeF_4N_3O_6$ (c) 79LOI/OSI
Triglycine fluoroberyllate, deuterated
Heat Capacity 300 K, C_p=447.4 J·mol^{-1}·K^{-1}
Temperature range 294 to 340 K. C_p=0.326 cal·g^{-1}·K^{-1}, 92% deuterated.
Phase Changes
c,II/c,I ΔH=1153 J·mol^{-1}
No temperature given.
Molecular Weight 324.2166
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4 &1/H-2 2 &2/H-2 2 &4/H-2 1 &9/H-2 2
Evaluation B

$C_6D_{17}BeF_4N_3O_6$ (c) 81LOI/KO
Triglycine fluoroberyllate, deuterated
Heat Capacity 308 K, C_p=448 J·mol^{-1}·K^{-1}
One temperature. C_p(35 °C)=0.33 cal·g^{-1}·°C^{-1}.
Molecular Weight 324.2166
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4 &1/H-2 2 &2/H-2 2 &4/H-2 1 &9/H-2 2
Evaluation B
70% deuterated.

$C_6D_{17}BeF_4N_3O_6$ (c) 81LOI/KOS
Triglycine fluoroberyllate, deuterated
Heat Capacity 298 K, C_p=430 J·mol^{-1}·K^{-1}
Temperature range 294 to 375 K. C_p given at "room temperature" as 0.317 cal·K^{-1}·g^{-1}. Data given graphically.
Phase Changes
c,II/c,I 345 K, ΔH=813 J·mol^{-1}
ΔS=2.36 J·mol^{-1}·K^{-1}
Ferroelectric transition.
Molecular Weight 324.2166
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4 &1/H-2 2 &2/H-2 2 &4/H-2 1 &9/H-2 2
Evaluation C
Sample is 70% deuterated.

$C_6D_{17}N_3O_{10}S$ (c) 75CAM/GO
Triglycine sulfate, deuterated
Heat Capacity 300 K, C_p=390 J·mol^{-1}·K^{-1}
Temperature range 100 to 400 K. Data given graphically; C estimated from graph.
Phase Changes
c,II/c,I 331.75 K, ΔH=571 J·mol^{-1}
ΔS=1.72 J·mol^{-1}·K^{-1}
Molecular Weight 338.7013
Wiswesser Line Notation Z1VQ 3 &WSQQ &1/H-2 2 &1/H-2 2 &4/H-2 1 &11/H-2 1 &12/H-2 1
Evaluation D(C_p); B(Phase changes)
Degree of deuteration not indicated, assumed 90%.

$C_6D_{17}N_3O_{10}S$ (c) 79LOI/OSB
Triglycine sulfate, deuterated
Heat Capacity 300 K, C_p=438 J·mol^{-1}·K^{-1}
Temperature range 294 to 340 K. C_p=0.309 cal·g^{-1}·K^{-1}. 90% deuterated.
Molecular Weight 338.7013
Wiswesser Line Notation Z1VQ 3 &WSQQ &1/H-2 2 &1/H-2 2 &4/H-2 1 &11/H-2 1 &12/H-2 1
Evaluation B

$C_6D_{17}N_3O_{10}S$ (c) 81LOI/KOS
Triglycine sulfate, deuterated
Heat Capacity 308 K, C_p=468 J·mol^{-1}·K^{-1}
One temperature. C_p(35 °C)=0.33 cal·g^{-1}·°C^{-1}.
Molecular Weight 338.7013
Wiswesser Line Notation Z1VQ 3 &WSQQ &1/H-2 2 &1/H-2 2 &4/H-2 1 &11/H-2 1 &12/H-2 1
Evaluation B
90% deuterated.

$C_6F_5NO_2$ (liq) 71PAU2
Pentafluoronitrobenzene
Heat Capacity 298.15 K, C_p=272.96 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=323.13 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 250.5 K, ΔH=11807 J·mol^{-1}
ΔS=47.13 J·mol^{-1}·K^{-1}
Molecular Weight 213.0635
Wiswesser Line Notation WNR BF CF DF EF FF
Evaluation A

C_6F_6 (liq) 65COU/GRE
Hexafluorobenzene; Perfluorobenzene
Heat Capacity 298.15 K, C_p=221.58 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S=279.91 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 278.25 K, ΔH=11590 J·mol^{-1}
ΔS=41.65 J·mol^{-1}·K^{-1}
Molecular Weight 186.0564
Wiswesser Line Notation FR BF CF DF EF FF
Evaluation A

C_6F_6 (liq) 70MES/FIN
Hexafluorobenzene; Perfluorobenzene
Heat Capacity 298.15 K, C_p=221.58 J·mol^{-1}·K^{-1}
Temperature range 13 to 342 K.
Entropy 298.15 K, S=280.79 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 278.30 K, ΔH=11585 J·mol^{-1}
ΔS=41.63 J·mol^{-1}·K^{-1}
Molecular Weight 186.0564
Wiswesser Line Notation FR BF CF DF EF FF
Evaluation A

C_6F_6 (liq) 82GOR/GRI
Hexafluorobenzene; Perfluorobenzene
Heat Capacity 300 K, C_p=222.0 J·mol^{-1}·K^{-1}
Temperature range 280 to 353 K. Data also given by equation.
Molecular Weight 186.0564
Wiswesser Line Notation FR BF CF DF EF FF
Evaluation B

C_6F_6 (liq) 82GOR/SIM
Hexafluorobenzene; Perfluorobenzene
Heat Capacity 298.76 K, C_p=221.3 J·mol^{-1}·K^{-1}
Temperature range 284 to 350 K. Value is unsmoothed experimental datum. C_p (298.76 K) given as 1.1892 J·K^{-1}·g^{-1}.
Molecular Weight 186.0564
Wiswesser Line Notation FR BF CF DF EF FF
Evaluation B
C_p(liq) (kJ·kg^{-1}·K^{-1})=1.19132−1.0716×10^{-3}T+3.59×10^{-6}T^2
J·K^{-1}·g^{-1} (325 to 728 K).

C_6F_6 (liq) 82GOR/SIM2
Hexafluorobenzene; Perfluorobenzene
Heat Capacity 298.15 K, C_p=221.6 J·mol^{-1}·K^{-1}
Temperature range 280 to 680 K. Data calculated from the equation: C_p(liq) (kJ·kg^{-1}·K^{-1})=1.19132−1.0716×10^{-3}T+3.59×10^{-6}T^2.
Molecular Weight 186.0564
Wiswesser Line Notation FR BF CF DF EF FF
Evaluation A

C_6F_6 (liq) 87WIL/LAI
Hexafluorobenzene; Perfluorobenzene
Heat Capacity 298.15 K, C_p=225.03 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 186.0564
Wiswesser Line Notation FR BF CF DF EF FF
Evaluation B

C_6F_{14} (liq) 74COC/NOR
n-Perfluorohexane
Heat Capacity 273 K, C_p=248 J·mol^{-1}·K^{-1}
Temperature range 233 to 273 K.
Molecular Weight 338.0436
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFF
Evaluation C

C_6F_{14} (liq) 82CAM/REY
n-Perfluorohexane
Heat Capacity
C_p data is given graphically only. Temperature range 4.2 to 300 K.
Phase Changes
c,II/c,I 103 K, ΔH=967 J·mol^{-1}
ΔS=10.00 J·mol^{-1}·K^{-1}
Transition between 90 and 130 K.
c,I/liq 185 K, ΔH=6837 J·mol^{-1}
ΔS=36.8 J·mol^{-1}·K^{-1}
Molecular Weight 338.0436
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFF
Evaluation A

C_6F_{14} (liq) 83CAM/DIA
n-Perfluorohexane
Heat Capacity 273 K, C_p=240.2 J·mol^{-1}·K^{-1}
Data from 82CAM/REY.
Molecular Weight 338.0436
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFF
Evaluation C
C_p given as 248.1 J·mol^{-1}·K^{-1} at 273 K from Cochran, M.A. *et al.*, J. Chem. Soc. Faraday Trans. II 70, 1274 (1974).

$C_6F_{15}N$ (liq) 79ZHO/KOS
Perfluorotriethylamine
Heat Capacity 298.15 K, C_p=379.49 J·mol^{-1}·K^{-1}
Temperature range 9 to 300 K.
Entropy 298.15 K, S=527.10 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 126.0 K, ΔH=−3749.7 J·mol^{-1}
Glassy (G type) transition at 108.7 K. Monotropic transition at 126.0 K with the liberation of heat.
c,II/c,I 146.4 K, ΔH=1364 J·mol^{-1}
ΔS=10.67 J·mol^{-1}·K^{-1}
Enantiotropic transition at 146.4 K.
c,I/liq 156.2 K, ΔH=5560.1 J·mol^{-1}
ΔS=35.61 J·mol^{-1}·K^{-1}
Molecular Weight 371.0487
Wiswesser Line Notation FXFFXFF 3N
Evaluation A

$C_6F_{15}N$ (liq) 84GOL/KOL
Perfluorotriethylamine
Phase Changes
c/liq 156.1 K, ΔH=4650 J·mol^{-1}
ΔS=29.8 J·mol^{-1}·K^{-1}
Molecular Weight 371.0487
Wiswesser Line Notation FXFFXFF 3N
Evaluation A

C_6HCl_5 (c) 91SAB/AN2
Pentachlorobenzene
Phase Changes
c/liq 357.00 K, ΔH=20100 J·mol^{-1}
ΔS=56.3 J·mol^{-1}·K^{-1}
Molecular Weight 250.3389
Wiswesser Line Notation GR BG CG DG EG
Evaluation B

C_6HCl_5O (c) 58HIL/KRA
Pentachlorophenol; Perchlorophenol
Heat Capacity 298.15 K, C_p=201.96 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=253.17 J·mol^{-1}·K^{-1}
Molecular Weight 266.3383
Wiswesser Line Notation QR BG CG DG EG FG
Evaluation A

C_6HF_5 (liq) 68COU/HAL
Pentafluorobenzene
Heat Capacity 298.15 K, C_p=204.7 J·mol^{-1}·K^{-1}
Temperature range 12 to 324 K.
Entropy 298.15 K, S=275.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 225.83 K, ΔH=10853 J·mol^{-1}
ΔS=48.06 J·mol^{-1}·K^{-1}
Molecular Weight 168.0659
Wiswesser Line Notation FR BF CF DF EF
Evaluation A

C_6HF_5 (liq) 69PAU/LAV
Pentafluorobenzene
Heat Capacity 298.15 K, C_p=210.79 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=279.49 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 225.67 K, ΔH=10883 J·mol^{-1}
ΔS=48.22 J·mol^{-1}·K^{-1}
Molecular Weight 168.0659
Wiswesser Line Notation FR BF CF DF EF
Evaluation A

C_6HF_5O (c,I) 68AND/COU2
Pentafluorophenol
Heat Capacity 298.15 K, C_p=201.3 J·mol^{-1}·K^{-1}
Temperature range 12 to 377 K.
Entropy 298.15 K, S=227.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 287 K, ΔH=1134 J·mol^{-1}
ΔS=3.95 J·mol^{-1}·K^{-1}
c,I/liq 310.62 K, ΔH=16410 J·mol^{-1}
ΔS=52.82 J·mol^{-1}·K^{-1}
Molecular Weight 184.0653
Wiswesser Line Notation QR BF CF DF EF FF
Evaluation A

C_6HF_5O (c,I) 69PAU/LAV
Pentafluorophenol
Heat Capacity 298.15 K, C_p=260.66 J·mol^{-1}·K^{-1}
Temperature range 12 to 329 K.
Entropy 298.15 K, S=242.84 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 248.15 K, ΔH=1485.3 J·mol^{-1}
ΔS=5.99 J·mol^{-1}·K^{-1}
c/liq 305.18 K, ΔH=12845 J·mol^{-1}
ΔS=42.09 J·mol^{-1}·K^{-1}
Molecular Weight 184.0653
Wiswesser Line Notation QR BF CF DF EF FF
Evaluation A

$C_6H_2Br_4$ (c) 87MON/HOU
1,2,4,5-Tetrabromobenzene
Phase Changes
c,II/c,I 306.8 K, ΔH=335 J·mol^{-1}
β to γ transition.
c,I/liq 453.0 K, ΔH=27880 J·mol^{-1}
Molecular Weight 393.6978
Wiswesser Line Notation ER BE DE EE
Evaluation B

$C_6H_2Br_4$ (c) 89MON/CU
1,2,4,5-Tetrabromobenzene
Phase Changes
c,II/c,I 306.8 K, ΔH=335 J·mol^{-1}
c,I/liq 453.1 K, ΔH=27880 J·mol^{-1}
Molecular Weight 393.6978
Wiswesser Line Notation ER BE DE EE
Evaluation A

$C_6H_2Cl_4$ (c) 91SAB/AN
1,2,3,4-Tetrachlorobenzene
Phase Changes
c/liq 319.68 K, ΔH=16960 J·mol^{-1}
ΔS=53.1 J·mol^{-1}·K^{-1}
Molecular Weight 215.8938
Wiswesser Line Notation GR BR CR DR
Evaluation B

$C_6H_2Cl_4$ (c) 91SAB/AN
1,2,3,5-Tetrachlorobenzene
Phase Changes
c/liq 323.77 K, ΔH=18320 J·mol^{-1}
ΔS=56.6 J·mol^{-1}·K^{-1}
Molecular Weight 215.8938
Wiswesser Line Notation GR BG CG EG
Evaluation B

$C_6H_2Cl_4$ (c) 28AND/HAW
1,2,4,5-Tetrachlorobenzene
Heat Capacity 299.8 K, C_p=202.5 J·mol^{-1}·K^{-1}
Temperature range 101 to 336 K. Value is unsmoothed experimental datum.
Molecular Weight 215.8938
Wiswesser Line Notation GR BG DG EG
Evaluation C

$C_6H_2Cl_4$ (c) 82MAR
1,2,4,5-Tetrachlorobenzene
Phase Changes
c,II/c,I 187.5 K, ΔH=34 J·mol^{-1}
ΔS=0.18 J·mol^{-1}·K^{-1}
Molecular Weight 215.8938
Wiswesser Line Notation GR BG DG EG
Evaluation C

$C_6H_2Cl_4$ (c) 87MON/HOU
1,2,4,5-Tetrachlorobenzene
Phase Changes
c,II/c,I 185.6 K, ΔH=95 J·mol^{-1}
α to β transition.
c,I/liq 412.9 K, ΔH=26340 J·mol^{-1}
Molecular Weight 215.8938
Wiswesser Line Notation GR BG DG EG
Evaluation B

$C_6H_2Cl_4$ (c) 89MON/CUE
1,2,4,5-Tetrachlorobenzene
Phase Changes
c,II/c,I 185.6 K, ΔH=95 J·mol^{-1}
c,I/liq 412.8 K, ΔH=26340 J·mol^{-1}
Molecular Weight 215.8938
Wiswesser Line Notation GR BG DG EG
Evaluation A

$C_6H_2Cl_4$ (c) 91SAB/AN2
1,2,4,5-Tetrachlorobenzene
Phase Changes
c/liq 412.59 K, ΔH=24940 J·mol^{-1}
ΔS=60.4 J·mol^{-1}·K^{-1}
Molecular Weight 215.8938
Wiswesser Line Notation GR BG DG EG
Evaluation B

$C_6H_2F_4$ (liq) 73AND/MAR
1,2,3,4-Tetrafluorobenzene
Heat Capacity 298.15 K, C_p=189.9 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=256.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 221 K, ΔH=4900 J·mol^{-1}
ΔS=22.2 J·mol^{-1}·K^{-1}
c,II/liq 231.25 K, ΔH=6180 J·mol^{-1}
ΔS=26.7 J·mol^{-1}·K^{-1}
c,I/liq 233.26 K, ΔH=10930 J·mol^{-1}
ΔS=46.9 J·mol^{-1}·K^{-1}
Molecular Weight 150.0754
Wiswesser Line Notation FR BF CF DF
Evaluation A

$C_6H_2F_4$ (liq) 73AND/MAR
1,2,3,5-Tetrafluorobenzene
Heat Capacity 298.15 K, C_p=190.3 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S=257.3 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 224.2 K, ΔH=4300 J·mol^{-1}
ΔS=19.2 J·mol^{-1}·K^{-1}
c,I/liq 226.90 K, ΔH=6360 J·mol^{-1}
ΔS=28.0 J·mol^{-1}·K^{-1}
Molecular Weight 150.0754
Wiswesser Line Notation FR BF CF EF
Evaluation A

$C_6H_2F_4$ (liq) 73AND/MAR
1,2,4,5-Tetrafluorobenzene
Heat Capacity 298.15 K, C_p=192.2 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S=250.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 277.03 K, ΔH=15050 J·mol^{-1}
ΔS=54.33 J·mol^{-1}·K^{-1}
Molecular Weight 150.0754
Wiswesser Line Notation FR BF DF EF
Evaluation A

$C_6H_2F_5N$ (c,I) 69PAU/LAV3
Pentafluoroaniline
Heat Capacity 298.15 K, C_p=230.79 J·mol^{-1}·K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=246.23 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 287.4 K, ΔH=3941 J·mol^{-1}
ΔS=13.71 J·mol^{-1}·K^{-1}
c,I/liq 306.75 K, ΔH=14267 J·mol^{-1}
ΔS=46.51 J·mol^{-1}·K^{-1}
Molecular Weight 183.0805
Wiswesser Line Notation ZR BF CF DF EF FF
Evaluation A

$C_6H_3Br_3O$ (c) 87ALL/FIN
2,4,6-Tribromophenol
Heat Capacity 298.15 K, C_p=172.0 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.52 J K^{-1} g^{-1}.
Molecular Weight 330.8011
Wiswesser Line Notation QR BE DE FE
Evaluation B

$C_6H_3Cl_3$ (liq) 74PET/TER
1,2,4-Trichlorobenzene
Heat Capacity 297.95 K, C_p=188 J·mol^{-1}·K^{-1}
Temperature range 297 to 454 K. Value is unsmoothed experimental datum.
Molecular Weight 181.4487
Wiswesser Line Notation GR BG DG
Evaluation B

$C_6H_3Cl_3$ (liq) 82WIL/ING
1,2,4-Trichlorobenzene
Heat Capacity 298.15 K, C_p=194.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 181.4487
Wiswesser Line Notation GR BG DG
Evaluation A

$C_6H_3Cl_3$ (liq) 86WIL/LAI
1,2,4-Trichlorobenzene
Heat Capacity 298.15 K, C_p=194.90 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 181.4487
Wiswesser Line Notation GR BG DG
Evaluation B

$C_6H_3Cl_4N$ (c) 87TAN/YE
2-Chloro-6-(trichloromethyl)pyridine
Heat Capacity 297.13 K, C_p=192.09 J·mol^{-1}·K^{-1}
Temperature range 78 to 322 K. Value is unsmoothed experimental datum. C_p (c,70 to 330 K)=146.438+57.0749X−1.31699x^2 +16.2918x^3−11.3899x^4−26.7611x^5+5.59976X^6+21.3037X^7 (J·mol^{-1}·K^{-1}).
Phase Changes
c/liq 337.242 K, ΔH=20298.8 J·mol^{-1}
ΔS=60.190 J·mol^{-1}·K^{-1}
Molecular Weight 230.9084
Wiswesser Line Notation T6NJ BXGGG FG
Evaluation B

$C_6H_3Cl_4N$ (c) 89TAN/SOR
2-Chloro-6-(trichloromethyl)pyridine
Heat Capacity 298.15 K, C_p=189.35 J·mol^{-1}·K^{-1}
Temperature range 2 to 400 K.
Entropy 298.15 K, S=244.596 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 337.242 K, ΔH=20300 J·mol^{-1}
ΔS=60.19 J·mol^{-1}·K^{-1}
Molecular Weight 230.9084
Wiswesser Line Notation T6NJ BXGGG FG
Evaluation A
C_p(c)=144.153+57.0749X−1.31699X^2+16.2918X^3−11.3899X^4 −26.7611X^5+5.59976X^6+21.3037X^7 [X=(T/K−200)/122] J·K^{-1} mol^{-1}; C_p(liq)=261.247+2.6029Y−0.288921Y^2 [Y=(T/K−354.5)/16.5] J·K^{-1}mol^{-1}.

$C_6H_3N_3O_6$ (c) 80RAD/RAD
1,3,5-Trinitrobenzene
Heat Capacity 298.15 K, C_p=214.6 J·mol^{-1}·K^{-1}
Temperature range 180 to 400 K. Data given graphically; C_p calculated from equation. Thermodynamically stable modification I.
Phase Changes
c,I/liq 398.4 K, ΔH=15000 J·mol^{-1}
ΔS=37.7 J·mol^{-1}·K^{-1}
Molecular Weight 213.1064
Wiswesser Line Notation WNR CNW ENW
Evaluation B

$C_6H_3N_3O_6$ (c) 80RAD/RAD
1,3,5-Trinitrobenzene
Heat Capacity 298.15 K, C_p=222.7 J·mol^{-1}·K^{-1}
Temperature range 180 to 380 K. Data given graphically; C_p calculated from equation. Metastable modification II.
Phase Changes
c,II/c,I 370 K, ΔH=1900 J·mol^{-1}
ΔS=5.13 J·mol^{-1}·K^{-1}
c,I/liq 380.3 K, ΔH=14800 J·mol^{-1}
ΔS=38.9 J·mol^{-1}·K^{-1}
Molecular Weight 213.1064
Wiswesser Line Notation WNR CNW ENW
Evaluation B

$C_6H_3N_3O_6$ (c) 80RAD/RAD
1,3,5-Trinitrobenzene
Phase Changes
c,I/liq 383.0 K, ΔH=13200 J·mol^{-1}
ΔS=34.5 J·mol^{-1}·K^{-1}
Metastable modification III.
Molecular Weight 213.1064
Wiswesser Line Notation WNR CNW ENW
Evaluation B

$C_6H_3N_3O_7$ (c) 24TAY/RI
Picric acid; 2,4,6-Trinitrophenol
Heat Capacity 293 K, C_p=239.7 J·mol^{-1}·K^{-1}
Temperature range 90 to 395 K.
Molecular Weight 229.1056
Wiswesser Line Notation WNR BQ CNW ENW
Evaluation C

$C_6H_3N_3O_7$ (c) 79FAR/SH
Picric acid; 2,4,6-Trinitrophenol
Phase Changes
c/liq 394.1 K, ΔH=17100 J·mol^{-1}
ΔS=43.4 J·mol^{-1}·K^{-1}
Molecular Weight 229.1056
Wiswesser Line Notation WNR BQ CNW ENW
Evaluation B

$C_6H_3N_3O_8$ (c) 79FAR/SH
Styphnic acid; 2,4,6-Trinitroresorcinol
Phase Changes
c/liq 454.9 K, ΔH=33500 J·mol^{-1}
ΔS=73.6 J·mol^{-1}·K^{-1}
Molecular Weight 245.1050
Wiswesser Line Notation WNR BQ CNW DQ ENW
Evaluation B

$(C_6H_4)_n$ (liq) 71RAB/SA
Poly-p-phenylene
Heat Capacity 300 K, C_p=89.96 J·mol^{-1}·K^{-1}
Temperature range 10 to 600 K.
Entropy 300 K, S=87.19 J·mol^{-1}·K^{-1}
Molecular Weight 76.0976
Wiswesser Line Notation /*R*/
Evaluation A

C_6H_4BrCl (liq) 18NA
2-Chlorobromobenzene
Heat Capacity 298.15 K, C_p=176.9 J·mol^{-1}·K^{-1}
Temperature range 198 to 374 K. C_p=0.21497+0.0002348t cal g^{-1}·K^{-1}. C_p value calculated from equation.
Phase Changes
c/liq 260.55 K, ΔH=12368 J·mol^{-1}
ΔS=47.5 J·mol^{-1}·K^{-1}
Molecular Weight 191.4546
Wiswesser Line Notation GR BE
Evaluation D

C_6H_4BrCl (liq) 18NAR
3-Chlorobromobenzene
Heat Capacity 298.15 K, C_p=181.9 J·mol^{-1}·K^{-1}
Temperature range 197 to 375 K. C_p=0.221224+0.0002348t cal·g^{-1}·K^{-1}. C_p value calculated from equation.
Phase Changes
c/liq 251.95 K, ΔH=12288 J·mol^{-1}
ΔS=48.8 J·mol^{-1}·K^{-1}
Molecular Weight 191.4546
Wiswesser Line Notation GR CE
Evaluation D

C_6H_4BrCl (c) 18NAR
4-Chlorobromobenzene
Heat Capacity
Temperature range 194 to 336 K.
Phase Changes
c/liq 337.75 K, ΔH=18760 J·mol^{-1}
ΔS=55.5 J·mol^{-1}·K^{-1}
Molecular Weight 191.4546
Wiswesser Line Notation GR DE
Evaluation D

C_6H_4BrI (liq) 18NAR
2-Bromoiodobenzene
Heat Capacity 298.15 K, C_p=179.9 J·mol^{-1}·K^{-1}
Temperature range 195 to 373 K. C_p=0.15285+0.0001332t. C_p value calculated from equation.
Phase Changes
c/liq 275.25 K, ΔH=14441 J·mol^{-1}
ΔS=52.5 J·mol^{-1}·K^{-1}
Molecular Weight 282.9061
Wiswesser Line Notation IR BE
Evaluation D

C_6H_4BrI (liq) 18NAR
3-Bromoiodobenzene
Heat Capacity 298.15 K, C_p=183.1 J·mol^{-1}·K^{-1}
Temperature range 198 to 373 K. C_p=0.15134+0.0001332t. C_p value calculated from equation.
Phase Changes
c/liq 263.85 K, ΔH=12192 J·mol^{-1}
ΔS=46.2 J·mol^{-1}·K^{-1}
Molecular Weight 282.9061
Wiswesser Line Notation IR CE
Evaluation D

C_6H_4BrI (c) 18NAR
4-Bromoiodobenzene
Heat Capacity
Temperature range 270 to 361 K.
Phase Changes
c/liq 363.25 K, ΔH=19614 J·mol^{-1}
ΔS=54.0 J·mol^{-1}·K^{-1}
Molecular Weight 282.9061
Wiswesser Line Notation IR DE
Evaluation D

$C_6H_4Br_2$ (liq) 18NAR
1,2-Dibromobenzene
Heat Capacity 298.15 K, C_p=196.8 J·mol^{-1}·K^{-1}
Temperature range 200 to 375 K. C_p=0.17994+0.0002140t. C_p value calculated from equation.
Phase Changes
c/liq 274.95 K, ΔH=13587 J·mol^{-1}
ΔS=49.4 J·mol^{-1}·K^{-1}
Molecular Weight 235.9056
Wiswesser Line Notation ER BE
Evaluation D

$C_6H_4Br_2$ (liq) 18NAR
1,3-Dibromobenzene
Heat Capacity 298.15 K, C_p=192.0 J·mol^{-1}·K^{-1}
Temperature range 197 to 375 K. C_p=0.17535+0.0002140t. C_p value calculated from equation.
Phase Changes
c/liq 266.25 K, ΔH=14225 J·mol^{-1}
ΔS=53.4 J·mol^{-1}·K^{-1}
Molecular Weight 235.9056
Wiswesser Line Notation ER CE
Evaluation D

$C_6H_4Br_2$ (c) 18NAR
1,4-Dibromobenzene; p-Dibromobenzene
Heat Capacity
Temperature range 194 to 353 K.
Phase Changes
c/liq 360.05 K, ΔH=20530 J·mol^{-1}
ΔS=57.0 J·mol^{-1}·K^{-1}
Molecular Weight 235.9056
Wiswesser Line Notation ER DE
Evaluation D

$C_6H_4Br_2$ (c) 28AND/HAW
1,4-Dibromobenzene; p-Dibromobenzene
Heat Capacity 299.8 K, C_p=174.5 J·mol^{-1}·K^{-1}
Temperature range 101 to 336 K. Value is unsmoothed experimental datum.
Molecular Weight 235.9056
Wiswesser Line Notation ER DE
Evaluation C

$C_6H_4Br_2$ (c) 50UEB/ORT
1,4-Dibromobenzene; p-Dibromobenzene
Heat Capacity 198.15 K, C_p=145.6 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Phase Changes
c/liq 360 K, ΔH=20040 J·mol^{-1}
ΔS=55.7 J·mol^{-1}·K^{-1}
Molecular Weight 235.9056
Wiswesser Line Notation ER DE
Evaluation C

$C_6H_4Br_2O$ (liq) 1884WER
2,4-Dibromophenol
Heat Capacity ~313 K, C_p=260 J·mol^{-1}·K^{-1}
Temperature range 18.5–73 °C, mean value for supercooled liquid.
Phase Changes
c/liq 313 K, ΔH=15000 J·mol^{-1}
ΔS=46 J·mol^{-1}·K^{-1}
Molecular Weight 252.4990
Wiswesser Line Notation QR BE DE
Evaluation D

$C_6H_4Br_3N$ (c) 87ALL/FIN
2,4,6-Tribromoaniline
Heat Capacity 298.15 K, C_p=181.4 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.55 J·K^{-1}·g^{-1}.
Molecular Weight 329.8163
Wiswesser Line Notation ZR BE DE FE
Evaluation B

$C_6H_4ClNO_2$ (c) 81LEB/RYA
1-Chloro-2-nitrobenzene
Heat Capacity C_p=247.8 J·mol^{-1}·K^{-1}
Temperature range 298 to 303 K. Data given over temperature range.
Molecular Weight 157.5561
Wiswesser Line Notation WNR BG
Evaluation B

$C_6H_4ClNO_2$ (c) 78MAR/CIO
4-Nitrochlorobenzene
Heat Capacity 298 K, C_p=250.2 J·mol^{-1}·K^{-1}
Temperature range 298 to 467 K.
Phase Changes
c/liq 354.6 K, ΔH=11850 J·mol^{-1}
ΔS=33.4 J·mol^{-1}·K^{-1}
Molecular Weight 157.5561
Wiswesser Line Notation WNR DG
Evaluation C

$C_6H_4ClNO_2$ (c) 81LEB/RYA
4-Nitrochlorobenzene
Heat Capacity C_p=182.6 J·mol^{-1}·K^{-1}
Temperature range 298 to 353 K. Data given over temperature range.
Molecular Weight 157.5561
Wiswesser Line Notation WNR DG
Evaluation B

$C_6H_4ClNO_2$ (c) 81VOR/BOR
4-Nitrochlorobenzene
Phase Changes
c/liq 358 K, ΔH=18030 J·mol^{-1}
ΔS=69.9 J·mol^{-1}·K^{-1}
liq/g 518 K, ΔH=36900 J·mol^{-1}
ΔS=71.2 J·mol^{-1}·K^{-1}
Molecular Weight 157.5561
Wiswesser Line Notation WNR DG
Evaluation C

$C_6H_4Cl_2$ (liq) 18NAl
1,2-Dichlorobenzene; o-Dichlorobenzene
Heat Capacity 298.15 K, C_p=170.9 J·mol^{-1}·K^{-1}
Temperature range 197 to 375 K. C_p=0.27022+0.0003024t cal g^{-1}·K^{-1}. C_p value calculated from equation.
Phase Changes
c/liq 255.65 K, ΔH=12922 J·mol^{-1}
ΔS=50.5 J·mol^{-1}·K^{-1}
Molecular Weight 147.0036
Wiswesser Line Notation GR BG
Evaluation D

$C_6H_4Cl_2$ (liq) 18NA
1,3-Dichlorobenzene; m-Dichlorobenzene
Heat Capacity 298.15 K, C_p=170.9 J·mol^{-1}·K^{-}
Temperature range 197 to 377 K. C_p=0.27022+0.0003024t ca g^{-1}·K^{-1}. C_p value calculated from equation.
Phase Changes
c/liq 248.75 K, ΔH=12590 J·mol^{-1}
ΔS=50.6 J·mol^{-1}·K^{-1}
Molecular Weight 147.0036
Wiswesser Line Notation GR CG
Evaluation D

$C_6H_4Cl_2$ (c) 18NA
1,4-Dichlorobenzene; p-Dichlorobenzene
Heat Capacity 298 K, C_p=147.6 J·mol^{-1}·K^{-}
Temperature range 194 to 372 K. Average specific heat over t temperature range 2.6 to 51.6 °C is 0.2400 cal·g^{-1}·K^{-1}.
Phase Changes
c/liq 326.05 K, ΔH=18144 J·mol^{-1}
ΔS=55.6 J·mol^{-1}·K^{-1}
Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation D

$C_6H_4Cl_2$ (c) 28AND/HA
1,4-Dichlorobenzene; p-Dichlorobenzene
Heat Capacity 299.8 K, C_p=172.0 J·mol^{-1}·K^{-}
Temperature range 101 to 336 K. Value is unsmooth experimental datum.
Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation C

$C_6H_4Cl_2$ (c) 50UEB/O
1,4-Dichlorobenzene; p-Dichlorobenzene
Heat Capacity 298.15 K, C_p=142.7 J·mol^{-1}·K^{-}
Temperature range 293 to 368 K. Equation only.
Phase Changes
c/liq 326 K, ΔH=18160 J·mol^{-1}
ΔS=55.7 J·mol^{-1}·K^{-}
Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation C

$C_6H_4Cl_2$ (c) 72BOO/H
1,4-Dichlorobenzene; p-Dichlorobenzene
Phase Changes
c/liq 326.15 K, ΔH=18050 J·mol^{-1}
ΔS=55.3 J·mol^{-1}·K^{-}
Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation C

$C_6H_4Cl_2$ (c,II) 75DWO/FIG
1,4-Dichlorobenzene; p-Dichlorobenzene
Heat Capacity
Temperature range 18 to 322 K. Data given graphically.
Phase Changes

c,III/c,II	271.77 K,	$\Delta H = 1256\ J \cdot mol^{-1}$
		$\Delta S = 4.62\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I	304.35 K,	$\Delta H = 214.5\ J \cdot mol^{-1}$
		$\Delta S = 0.705\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq	326.14 K,	$\Delta H = 18187\ J \cdot mol^{-1}$
		$\Delta S = 55.76\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation A
See also 76DWO/FIG.

$C_6H_4Cl_2$ (c,II) 76DWO/FIG
1,4-Dichlorobenzene; p-Dichlorobenzene

Heat Capacity	298.15 K,	$C_p = 147.76\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 20 to 330 K.

Entropy	298.15 K,	$S = 175.41\ J \cdot mol^{-1} \cdot K^{-1}$

Phase Changes

c,III/c,II	271.77 K,	$\Delta H = 1256\ J \cdot mol^{-1}$
		$\Delta S = 4.62\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I	304.35 K,	$\Delta H = 214.5\ J \cdot mol^{-1}$
		$\Delta S = 0.705\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq	326.14 K,	$\Delta H = 18187\ J \cdot mol^{-1}$
		$\Delta S = 55.76\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation A

$C_6H_4Cl_2$ (c) 88MAR/MON2
1,4-Dichlorobenzene; p-Dichlorobenzene

Heat Capacity	180 K,	$C_p = 98\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 30 to 180 K. Data given graphically, and estimated from graph.
Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation A

$C_6H_4Cl_2$ (c) 88PET/TSY
1,4-Dichlorobenzene; p-Dichlorobenzene
Phase Changes

c,II/c,I	304.0 K,	$\Delta H = 200\ J \cdot mol^{-1}$
		$\Delta S = 0.6\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation A

$C_6H_4Cl_2O$ (c) 82POE/FAN
2,3-Dichlorophenol
Phase Changes

c/liq	330.0 K,	$\Delta H = 21363\ J \cdot mol^{-1}$
		$\Delta S = 64.74\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 163.0030
Wiswesser Line Notation QR BG CG
Evaluation A

$C_6H_4Cl_2O$ (c) 81VOR/BOR
2,4-Dichlorophenol
Phase Changes

c/liq	323 K,	$\Delta H = 28410\ J \cdot mol^{-1}$
		$\Delta S = 88.0\ J \cdot mol^{-1} \cdot K^{-1}$
liq/g	491 K,	$\Delta H = 36780\ J \cdot mol^{-1}$
		$\Delta S = 74.9\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 163.0030
Wiswesser Line Notation QR BG DG
Evaluation C

$C_6H_4Cl_2O$ (c) 82POE/FAN
2,4-Dichlorophenol
Phase Changes

c/liq	318.0 K,	$\Delta H = 20090\ J \cdot mol^{-1}$
		$\Delta S = 63.18\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 163.0030
Wiswesser Line Notation QR BG DG
Evaluation A

$C_6H_4Cl_2O$ (c) 82POE/FAN
2,5-Dichlorophenol
Phase Changes

c/liq	331.0 K,	$\Delta H = 22434\ J \cdot mol^{-1}$
		$\Delta S = 67.78\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 163.0030
Wiswesser Line Notation QR BG EG
Evaluation A

$C_6H_4Cl_2O$ (c) 82POE/FAN
2,6-Dichlorophenol
Phase Changes

c/liq	340.0 K,	$\Delta H = 22141\ J \cdot mol^{-1}$
		$\Delta S = 65.12\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 163.0030
Wiswesser Line Notation QR BG FG
Evaluation A

$C_6H_4Cl_2O$ (c) 82POE/FAN
3,4-Dichlorophenol
Phase Changes

c/liq	341.0 K,	$\Delta H = 20927\ J \cdot mol^{-1}$
		$\Delta S = 61.37\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 163.0030
Wiswesser Line Notation QR CG DG
Evaluation A

$C_6H_4Cl_2O$ (c) 82POE/FAN
3,5-Dichlorophenol
Phase Changes

c/liq	341.0 K,	$\Delta H = 20509\ J \cdot mol^{-1}$
		$\Delta S = 60.14\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 163.0030
Wiswesser Line Notation QR CG EG
Evaluation A

$C_6H_4F_2$ (liq) 62GOO/LAC
1,2-Difluorobenzene

Heat Capacity	298.15 K,	$C_p = 159.4\ J \cdot mol^{-1} \cdot K^{-1}$

One temperature.
Molecular Weight 114.0944
Wiswesser Line Notation FR BF
Evaluation B

$C_6H_4F_2$ (liq) 63SCO/MES
1,2-Difluorobenzene
Heat Capacity 298.15 K, C_p=159.03 J·mol^{-1}·K^{-1}
Temperature range 14 to 357 K.
Entropy 298.15 K, S=222.59 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 226.01 K, ΔH=11046 J·mol^{-1}
ΔS=48.87 J·mol^{-1}·K^{-1}
Molecular Weight 114.0944
Wiswesser Line Notation FR BF
Evaluation A

$C_6H_4F_2$ (liq) 62GOO/LAC
1,3-Difluorobenzene
Heat Capacity 298.15 K, C_p=157.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.0944
Wiswesser Line Notation FR CF
Evaluation B

$C_6H_4F_2$ (liq) 70MES/FIN
1,3-Difluorobenzene
Heat Capacity 298.15 K, C_p=159.11 J·mol^{-1}·K^{-1}
Temperature range 11 to 355 K.
Entropy 298.15 K, S=223.84 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 186.77 K, ΔH=827.05 J·mol^{-1}
ΔS=4.428 J·mol^{-1}·K^{-1}
c,I/liq 204.03 K, ΔH=8581.0 J·mol^{-1}
ΔS=42.06 J·mol^{-1}·K^{-1}
Molecular Weight 114.0944
Wiswesser Line Notation FR CF
Evaluation A

$C_6H_4F_2$ (liq) 62GOO/LAC
1,4-Difluorobenzene
Heat Capacity 298.15 K, C_p=157.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.0944
Wiswesser Line Notation FR DF
Evaluation B

$C_6H_4F_2$ (liq) 91LIC
1,4-Difluorobenzene
Heat Capacity 298.15 K, C_p=159.1 J·mol^{-1}·K^{-1}
Temperature range 186 to 324 K. C_p(liq)=155.192+0.158T(°C) J·mol^{-1}·K^{-1} (−35 to 51 °C). C_p value calculated from equation.
Phase Changes
c,II/c,I 198 K, ΔH=0.00 J·mol^{-1}
Allotropic transformation.
c,I/liq 249.45 K
Molecular Weight 114.0944
Wiswesser Line Notation FR DF
Evaluation A

$C_6H_4I_2$ (liq) 18NAR
1,2-Diiodobenzene
Heat Capacity 298.15 K, C_p=190.0 J·mol^{-1}·K^{-1}
Temperature range 196 to 373 K. C_p=0.13574+0.0000776t. C_p value calculated from equation.
Phase Changes
c/liq 296.55 K, ΔH=14079 J·mol^{-1}
ΔS=47.5 J·mol^{-1}·K^{-1}
Molecular Weight 329.9066
Wiswesser Line Notation IR BI
Evaluation D

$C_6H_4I_2$ (c) 18NAF
1,3-Diiodobenzene
Heat Capacity
Temperature range 196 to 306 K.
Phase Changes
c/liq 307.35 K, ΔH=15943 J·mol^{-1}
ΔS=51.9 J·mol^{-1}·K^{-1}
Molecular Weight 329.9066
Wiswesser Line Notation IR CI
Evaluation D

$C_6H_4I_2$ (c) 18NA
1,4-Diiodobenzene
Heat Capacity
Temperature range 198 to 400 K.
Phase Changes
c/liq 402.15 K, ΔH=22375 J·mol^{-1}
ΔS=55.6 J·mol^{-1}·K^{-1}
Molecular Weight 329.9066
Wiswesser Line Notation IR DI
Evaluation D

$C_6H_4I_2$ (c) 50UEB/OR
1,4-Diiodobenzene
Heat Capacity 298.15 K, C_p=160.77 J·mol^{-1}·K
Temperature range 293 to 368 K. Equation only.
Phase Changes
c/liq 402 K, ΔH=22340 J·mol^{-1}
ΔS=55.6 J·mol^{-1}·K^{-1}
Molecular Weight 329.9066
Wiswesser Line Notation IR DI
Evaluation C

$C_6H_4NNaO_3 \cdot 2H_2O$ (c) 78MAR/CI
Sodium p-nitrophenoxide dihydrate
Heat Capacity 310 K, C_p=290.4 J·mol^{-1}·K
Temperature range 309 to 393 K.
Molecular Weight 197.1227
Wiswesser Line Notation WNR DO .NA &QH 2
Evaluation D

$C_6H_4N_2O_4$ (c) 26AN
1,2-Dinitrobenzene
Heat Capacity 297.9 K, C_p=186.2 J·mol^{-1}·K
Temperature range 110 to 344 K. Value is unsmooth experimental datum.
Molecular Weight 168.1086
Wiswesser Line Notation WNR BNW
Evaluation C

$C_6H_4N_2O_4$ (c) 26AND/LY
1,2-Dinitrobenzene
Heat Capacity 298 K, C_p=195.0 J·mol^{-1}·K
Temperature range 22 to 240248C.
Phase Changes
c/liq 396.1 K, ΔH=22840 J·mol^{-1}
ΔS=58.6 J·mol^{-1}·K^{-1}
Molecular Weight 168.1086
Wiswesser Line Notation WNR BNW
Evaluation C

$C_6H_4N_2O_4$ (c) 50UEB/ORT
1,2-Dinitrobenzene
Heat Capacity 298.15 K, C_p=200.4 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Molecular Weight 168.1086
Wiswesser Line Notation WNR BNW
Evaluation C

$C_6H_4N_2O_4$ (c) 72BOO/HAU
1,2-Dinitrobenzene
Phase Changes
c/liq 390.05 K, ΔH=22750 J·mol^{-1}
ΔS=58.3 J·mol^{-1}·K^{-1}
Molecular Weight 168.1086
Wiswesser Line Notation WNR BNW
Evaluation C

$C_6H_4N_2O_4$ (c) 26AND
1,3-Dinitrobenzene
Heat Capacity 297.9 K, C_p=188.3 J·mol^{-1}·K^{-1}
Temperature range 110 to 332 K. Value is unsmoothed experimental datum.
Molecular Weight 168.1086
Wiswesser Line Notation WNR CNW
Evaluation C

$C_6H_4N_2O_4$ (c) 26AND/LYN
1,3-Dinitrobenzene
Heat Capacity 298 K, C_p=180.3 J·mol^{-1}·K^{-1}
Temperature range 22 to 245 °C.
Phase Changes
c/liq 363.2 K, ΔH=17360 J·mol^{-1}
ΔS=47.8 J·mol^{-1}·K^{-1}
Molecular Weight 168.1086
Wiswesser Line Notation WNR CNW
Evaluation C

$C_6H_4N_2O_4$ (c) 50UEB/ORT
1,3-Dinitrobenzene
Heat Capacity 298.15 K, C_p=197.5 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Molecular Weight 168.1086
Wiswesser Line Notation WNR CNW
Evaluation C

$C_6H_4N_2O_4$ (c) 72BOO/HAU
1,3-Dinitrobenzene
Phase Changes
c/liq 363.23 K, ΔH=17350 J·mol^{-1}
ΔS=47.8 J·mol^{-1}·K^{-1}
Molecular Weight 168.1086
Wiswesser Line Notation WNR CNW
Evaluation C

$C_6H_4N_2O_4$ (c) 26AND/LYN
1,4-Dinitrobenzene
Heat Capacity 298 K, C_p=192.0 J·mol^{-1}·K^{-1}
Temperature range 22 to 210 °C.
Phase Changes
c/liq 446.7 K, ΔH=28120 J·mol^{-1}
ΔS=62.9 J·mol^{-1}·K^{-1}
Molecular Weight 168.1086
Wiswesser Line Notation WNR DNW
Evaluation C

$C_6H_4N_2O_4$ (c) 50UEB/ORT
1,4-Dinitrobenzene
Heat Capacity 298.15 K, C_p=200.0 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Molecular Weight 168.1086
Wiswesser Line Notation WNR DNW
Evaluation C

$C_6H_4N_2O_4$ (c) 64DAV
1,4-Dinitrobenzene
Heat Capacity 325 K, C_p=167 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K. Mean value. Temperature range uncertain.
Molecular Weight 168.1086
Wiswesser Line Notation WNR DNW
Evaluation D

$C_6H_4N_2O_4$ (c) 72BOO/HAU
1,4-Dinitrobenzene
Phase Changes
c/liq 446.65 K, ΔH=28100 J·mol^{-1}
ΔS=62.9 J·mol^{-1}·K^{-1}
Molecular Weight 168.1086
Wiswesser Line Notation WNR DNW
Evaluation C

$C_6H_4N_2O_5$ (c) 82POE/FAN
2,3-Dinitrophenol
Phase Changes
c/liq 417.0 K, ΔH=26239 J·mol^{-1}
ΔS=62.92 J·mol^{-1}·K^{-1}
Molecular Weight 184.1080
Wiswesser Line Notation WNR BNW CQ
Evaluation A

$C_6H_4N_2O_5$ (c) 82POE/FAN
3,4-Dinitrophenol
Phase Changes
c/liq 407.0 K, ΔH=25376 J·mol^{-1}
ΔS=62.35 J·mol^{-1}·K^{-1}
Molecular Weight 184.1080
Wiswesser Line Notation WNR BNW DQ
Evaluation A

$C_6H_4N_2O_5$ (c) 82POE/FAN
2,6-Dinitrophenol
Phase Changes
c/liq 336.0 K, ΔH=19577 J·mol^{-1}
ΔS=58.26 J·mol^{-1}·K^{-1}
Molecular Weight 184.1080
Wiswesser Line Notation WNR BQ CNW
Evaluation A

$C_6H_4N_2O_5$ (c) 82POE/FAN
2,4-Dinitrophenol
Phase Changes
c/liq 388.0 K, ΔH=24174 J·mol^{-1}
ΔS=62.30 J·mol^{-1}·K^{-1}
Molecular Weight 184.1080
Wiswesser Line Notation WNR CNW DQ
Evaluation A

$C_6H_4N_2O_5$ (c) 82POE/FAN
3,5-Dinitrophenol
Phase Changes
c/liq 399.1 K

Molecular Weight 184.1080
Wiswesser Line Notation WNR CNW EQ
Evaluation A

$C_6H_4N_2O_5$ (c) 82POE/FAN
2,5-Dinitrophenol
Phase Changes
c/liq 381.0 K, ΔH=23730 J·mol^{-1}
ΔS=62.28 J·mol^{-1}·K^{-1}

Molecular Weight 184.1080
Wiswesser Line Notation WNR CQ DNW
Evaluation A

$C_6H_4O_2$ (c) 24LAN
Quinone; p-Benzoquinone
Heat Capacity 291.2 K, C_p=129.7 J·mol^{-1}·K^{-1}
Temperature range 22 to 291 K. Value is unsmoothed experimental datum.
Molecular Weight 108.0964
Wiswesser Line Notation L6V DVJ
Evaluation B

$C_6H_4O_2$ (c) 26AND/LYN
Quinone; p-Benzoquinone
Heat Capacity 298 K, C_p=132.2 J·mol^{-1}·K^{-1}
Temperature range 22 to 160 °C.
Phase Changes
c/liq 386.0 K, ΔH=18450 J·mol^{-1}
ΔS=47.8 J·mol^{-1}·K^{-1}

Molecular Weight 108.0964
Wiswesser Line Notation L6V DVJ
Evaluation C

$C_6H_4O_2$ (c) 50UEB/ORT
Quinone; p-Benzoquinone
Heat Capacity 298.15 K, C_p=126.4 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Molecular Weight 108.0964
Wiswesser Line Notation L6V DVJ
Evaluation C

$(C_6H_4O_2S)_n$ (c) 92VAR/JIN
Poly(sulfonyl-1,4-phenylene)
Heat Capacity 300 K, C_p=141.4 J·mol^{-1}·K^{-1}
Temperature range 150 to 620 K. C_p(c)=esp[14.03310 −6.633458(lnT)+1.356265(lnT)^2−0.08282718(lnT)^3] (150 to 470 K); C_p(liq)=179.007985+0.082375T (510 to 620 K).
Molecular Weight 140.1564
Wiswesser Line Notation /*WSR D*/
Evaluation A
T(glass)=492.6 K.

C_6H_5Br (liq) 1881REI
Bromobenzene
Heat Capacity 298 K, C_p=151.0 J·mol^{-1}·K^{-1}
Temperature range 291 to 444 K.
Molecular Weight 157.0095
Wiswesser Line Notation ER
Evaluation D

C_6H_5Br (liq) 25WIL/DAI
Bromobenzene
Heat Capacity 293.2 K, C_p=151.5 J·mol^{-1}·K^{-1}
Temperature range 20 to 80 °C.
Molecular Weight 157.0095
Wiswesser Line Notation ER
Evaluation B

C_6H_5Br (liq) 28AND/HA
Bromobenzene
Heat Capacity 231.7 K, C_p=127.6 J·mol^{-1}·K^{-1}
Temperature range 101 to 232 K. Value is unsmoothe experimental datum.
Molecular Weight 157.0095
Wiswesser Line Notation ER
Evaluation C

C_6H_5Br (liq) 34KOL/UD
Bromobenzene
Heat Capacity 302.6 K, C_p=145.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 157.0095
Wiswesser Line Notation ER
Evaluation C

C_6H_5Br (liq) 34KOL/UD
Bromobenzene
Heat Capacity 302.6 K, C_p=145.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 157.0095
Wiswesser Line Notation ER
Evaluation C

C_6H_5Br (liq) 37ST
Bromobenzene
Heat Capacity 298.1 K, C_p=155.39 J·mol^{-1}·K
Temperature range 90 to 320 K.
Entropy 298.1 K. S=207.9 J·mol^{-1}·K^{-1}
Extrapolation below 91 K, 55.86 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 242.43 K, ΔH=10627 J·mol^{-1}
ΔS=43.84 J·mol^{-1}·K
Molecular Weight 157.0095
Wiswesser Line Notation ER
Evaluation B(C_p),C(S)

C_6H_5Br (liq) 75MAS/S
Bromobenzene
Heat Capacity 298.15 K. C_p=154.29 J·mol^{-1}·K
Temperature range 11 to 300 K.
Entropy 298.15 K, S=21922 J·mol^{-1}·K
Phase Changes
c/liq 242.40 K, ΔH=10702 J·mol^{-1}
ΔS=44.15 J·mol^{-1}·K
Molecular Weight 157.0095
Wiswesser Line Notation ER
Evaluation A

C_6H_5Br (liq) 86RED
Bromobenzene
Heat Capacity 303.15 K, $C_p = 155.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 303.15, 313.15 K.
Molecular Weight 157.0095
Wiswesser Line Notation ER
Evaluation B

C_6H_5BrO (liq) 1884WER
4-Bromophenol
Heat Capacity ~337 K, $C_p = 230\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 18 to 77 °C, mean value for supercooled liquid.
Phase Changes
c/liq 3367 K, $\Delta H = 13000\ J \cdot mol^{-1}$
$\Delta S = 39\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 173.0091
Wiswesser Line Notation QR DE
Evaluation D

C_6H_5BrO (c) 1884WER
4-Bromophenol
Heat Capacity ~300 K, $C_p = 192\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 13.5 to 51.5 °C, mean value.
Molecular Weight 173.0091
Wiswesser Line Notation QR DE
Evaluation D

C_6H_5BrO (c) 1889EYK
4-Bromophenol
Phase Changes
c/liq 336 K, $\Delta H = 16573\ J \cdot mol^{-1}$
$\Delta S = 49.3\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 173.0091
Wiswesser Line Notation QR DE
Evaluation C

C_6H_5Cl (liq) 1881REI
Chlorobenzene
Heat Capacity 298 K, $C_p = 141.0\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 294 to 425 K.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation D

C_6H_5Cl (liq) 25WIL/DAN
Chlorobenzene
Heat Capacity 293.2 K, $C_p = 145.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 20 to 80 °C.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation B

C_6H_5Cl (c) 28AND/HAW
Chlorobenzene
Heat Capacity 216.8 K, $C_p = 106.3\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 101 to 217 K. Value is unsmoothed experimental datum.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation C

C_6H_5Cl (liq) 37STU
Chlorobenzene
Heat Capacity 298.1 K, $C_p = 150.08\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 320 K.
Entropy 298.1 K, $S = 197.5\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 91 K, 44.02 $J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 227.89 K, $\Delta H = 9556\ J \cdot mol^{-1}$
$\Delta S = 41.93\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation B(C_p),C(S)

C_6H_5Cl (liq) 39PHI
Chlorobenzene
Heat Capacity 305.6 K, $C_p = 157.3\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation C

C_6H_5Cl (liq) 71DES/BHA
Chlorobenzene
Heat Capacity 298 K, $C_p = 147.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 298 to 318 K.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation B

C_6H_5Cl (liq) 77FOR/BEN
Chlorobenzene
Heat Capacity 298.15 K, $C_p = 150.787\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation B

C_6H_5Cl (liq) 86RED
Chlorobenzene
Heat Capacity 303.15 K, $C_p = 150.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 303.15, 313.15 K.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation B

C_6H_5Cl (liq) 88PER/AIC
Chlorobenzene
Heat Capacity 298.15 K, $C_p = 153.78\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation A

C_6H_5Cl (liq) 93SHE
Chlorobenzene
Heat Capacity 298.15 K, $C_p = 152.1\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation B

C_6H_5ClO (liq) 16BRA
2-Chlorophenol
Heat Capacity 283 K, $C_p = 188.7\ J \cdot mol^{-1} \cdot K^{-1}$
Mean value, 0 to 20 °C.
Molecular Weight 128.5579
Wiswesser Line Notation QR BG
Evaluation C

C_6H_5ClO (liq) 82POE/FAN
2-Chlorophenol
Phase Changes
c/liq 283.0 K, $\Delta H = 12523\ J \cdot mol^{-1}$
$\Delta S = 44.25\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 128.5579
Wiswesser Line Notation QR BG
Evaluation A

C_6H_5ClO (c) 82POE/FAN
3-Chlorophenol
Phase Changes
c/liq 305.8 K, $\Delta H = 14905\ J \cdot mol^{-1}$
$\Delta S = 48.74\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 128.5579
Wiswesser Line Notation QR CG
Evaluation A

C_6H_5ClO (c) 82POE/FAN
4-Chlorophenol
Phase Changes
c/liq 316.0 K, $\Delta H = 14067\ J \cdot mol^{-1}$
$\Delta S = 44.51\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 128.5579
Wiswesser Line Notation QR DG
Evaluation A

$C_6H_5Cl_3Ge$ (c) 69NUR/KOS
Phenyltrichlorogermane
Entropy 298.15 K, $S = 339.9\ J \cdot mol^{-1} \cdot K^{-1}$
Deposited in VINITI, No 540-69, 11 March 1969.
Molecular Weight 256.0545
Wiswesser Line Notation G-GE-GGR
Evaluation A

$C_6H_5Cl_3Si$ (liq) 65GUM/KOS
Phenyltrichlorosilane
Heat Capacity 298.15 K, $C_p = 220.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 14 to 289 K.
Entropy 298.15 K, $S = 314.7\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 233.4 K, $\Delta H = 11660\ J \cdot mol^{-1}$
$\Delta S = 49.96\ J \cdot mol^{-1} \cdot K^{-1}$
Smoothed table gives $\Delta H = 11650\ J \cdot mol^{-1}$.
Molecular Weight 211.5500
Wiswesser Line Notation G-SI-GGR
Evaluation A

$C_6H_5Cl_3Sn$ (c) 69NUR/KOS
Phenyltrichlorostannane
Entropy 298.15 K, $S = 347.5\ J \cdot mol^{-1} \cdot K^{-1}$
Deposited in VINITI, No 540-69, 11 March 1969.
Molecular Weight 302.1545
Wiswesser Line Notation G-SN-GGR
Evaluation A

C_6H_5F (liq) 37ST
Fluorobenzene
Heat Capacity 298.1 K, $C_p = 146.57\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 320 K.
Entropy 298.1 K, $S = 195.0\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 91 K, 42.55 $J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 231.10 K, $\Delta H = 10397\ J \cdot mol^{-1}$
$\Delta S = 44.99\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 96.1039
Wiswesser Line Notation FR
Evaluation B(C_p),C(S)

C_6H_5F (liq) 56SCO/MC
Fluorobenzene
Heat Capacity 298.15 K, $C_p = 146.36\ J \cdot mol^{-1} \cdot K$
Temperature range 14 to 350 K.
Entropy 298.15 K, $S = 205.94\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 230.94 K, $\Delta H = 11305\ J \cdot mol^{-1}$
$\Delta S = 48.95\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 96.1039
Wiswesser Line Notation FR
Evaluation A

C_6H_5F (liq) 84ROU/GF
Fluorobenzene
Heat Capacity 298.15 K, $C_p = 146.29\ J \cdot mol^{-1} \cdot K$
One temperature.
Molecular Weight 96.1039
Wiswesser Line Notation FR
Evaluation B

C_6H_5FO (c) 91L
p-Fluorophenol
Heat Capacity 298.15 K, $C_p = 144.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 183 to 354 K. C_p(c) = 123.0 $-0.579T + 9.573 \times 10^{-3}T^2 + 7.243 \times 10^{-5}T^3$ (T in °C) $J \cdot mol^{-1} \cdot K^{-1}$ (−90 to 34 °C). C_p value calculated from equation.
Phase Changes
c/liq 321.15 K
Molecular Weight 112.1033
Wiswesser Line Notation QR DF
Evaluation A

C_6H_5I (c) 35AOY/K.
Iodobenzene
Heat Capacity 226.1 K, $C_p = 112.1\ J \cdot mol^{-1} \cdot K$
Temperature range 81 to 226 K. Value is unsmoothed experimer datum.
Molecular Weight 204.0100
Wiswesser Line Notation IR
Evaluation B

C_6H_5I (liq) 37S
Iodobenzene
Heat Capacity 298.1 K, $C_p = 158.70\ J \cdot mol^{-1} \cdot K$
Temperature range 90 to 320 K.
Entropy 298.1 K, $S = 205.4\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 91 K, 53.14 $J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 241.83 K, $\Delta H = 9749\ J \cdot mol^{-1}$
$\Delta S = 40.31\ J \cdot mol^{-1} \cdot K$
Molecular Weight 204.0100
Wiswesser Line Notation IR
Evaluation B(C_p),C(S)

C_6H_5I (liq) 93SHE
Iodobenzene
Heat Capacity 298.15 K, C_p=158.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 204.0100
Wiswesser Line Notation IR
Evaluation B

$C_6H_5NO_2$ (c) 89ALL/GED
Picolinic acid
Phase Changes
c/liq 411 K, ΔH=30000 J·mol^{-1}
Molecular Weight 123.1110
Wiswesser Line Notation T6NJ BVQ
Evaluation A

$C_6H_5NO_2$ (c) 89ALL/GED
Nicotinic acid
Phase Changes
c/liq 510 K, ΔH=30000 J·mol^{-1}
Molecular Weight 123.1110
Wiswesser Line Notation T6NJ CVQ
Evaluation A

$C_6H_5NO_2$ (c) 93ELM/CHA
Nicotinic acid
Phase Changes
c,II/c,I 451.95 K, ΔH=780 J·mol^{-1}
c,I/liq 509.75 K, ΔH=26700 J·mol^{-1}
Molecular Weight 123.1110
Wiswesser Line Notation T6NJ CVQ
Evaluation A

$C_6H_5NO_2$ (c) 89ALL/GED
Isonicotinic acid
Phase Changes
c/liq 593 K, ΔH=135000 J·mol^{-1}
Molecular Weight 123.1110
Wiswesser Line Notation T6NJ DVQ
Evaluation A

$C_6H_5NO_2$ (liq) 1881REI
Nitrobenzene
Heat Capacity 298 K, C_p=177.8 J·mol^{-1}·K^{-1}
Temperature range 291 to 486 K.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation D

$C_6H_5NO_2$ (liq) 02LOU
Nitrobenzene
Heat Capacity 380 K, C_p=205 J·mol^{-1}·K^{-1}
Mean value 21 to 199 °C.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation D

$C_6H_5NO_2$ (liq) 07WAL
Nitrobenzene
Heat Capacity 293 K, C_p=201 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation D

$C_6H_5NO_2$ (liq) 24WIL/DAN
Nitrobenzene
Heat Capacity 303 K, C_p=177.4 J·mol^{-1}·K^{-1}
Temperature range 303 to 358 K. Equation only.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation C

$C_6H_5NO_2$ (liq) 34PAR/TOD
Nitrobenzene
Heat Capacity 298 K, C_p=186.73 J·mol^{-1}·K^{-1}
Temperature range 273 to 299 K.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation B

$C_6H_5NO_2$ (liq) 36PAR/TOD
Nitrobenzene
Heat Capacity 298.1 K, C_p=186.69 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 298.1 K, S=224.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 62.13 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 278.8 K, ΔH=12121 J·mol^{-1}
ΔS=43.48 J·mol^{-1}·K^{-1}
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation B(C_p),C(S)

$C_6H_5NO_2$ (liq) 39MAZ
Nitrobenzene
Heat Capacity 293.15 K, C_p=179.95 J·mol^{-1}·K^{-1}
Temperature range 5 to 20 °C.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation B

$C_6H_5NO_2$ (liq) 39MAZ3
Nitrobenzene
Heat Capacity 293 K, C_p=179.9 J·mol^{-1}·K^{-1}
Temperature range 5 to 20 °C.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation B

$C_6H_5NO_2$ (liq) 58LUT/PAN
Nitrobenzene
Heat Capacity 335.5 K, C_p=188.7 J·mol^{-1}·K^{-1}
Temperature range 62 to 141 °C. Value is unsmoothed experimental datum.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation B

$C_6H_5NO_2$ (liq) 67PAC
Nitrobenzene
Heat Capacity 303 K, C_p=176 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 278.9 K, ΔH=10815 J·mol^{-1}
ΔS=38.8 J·mol^{-1}·K^{-1}
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation C

$C_6H_5NO_2$ (liq) 67RAS/GAN
Nitrobenzene
Heat Capacity 293 K, C_p=180.2 J·mol^{-1}·K^{-1}
Temperature range 293 to 373 K.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation C

$C_6H_5NO_2$ (liq) 85LAI/ROD
Nitrobenzene
Heat Capacity 298.15 K, C_p=181.13 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation B

$C_6H_5NO_2$ (liq) 86RED
Nitrobenzene
Heat Capacity 303.15 K, C_p=177.3 J·mol^{-1}·K^{-1}
Temperature range 303.15, 313.15 K.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation B

$C_6H_5NO_3$ (c) 82POE/FAN
2-Nitrophenol
Phase Changes
c/liq 318.0 K, ΔH=17446 J·mol^{-1}
ΔS=54.86 J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR BQ
Evaluation A

$C_6H_5NO_3$ (c) 72BOO/HAU
3-Nitrophenol
Phase Changes
c/liq 369.95 K, ΔH=21300 J·mol^{-1}
ΔS=57.6 J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR CQ
Evaluation C

$C_6H_5NO_3$ (c) 82POE/FAN
3-Nitrophenol
Phase Changes
c/liq 370.0 K, ΔH=19196 J·mol^{-1}
ΔS=51.88 J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR CQ
Evaluation A

$C_6H_5NO_3$ (c) 89WOJ/MAR
3-Nitrophenol
Phase Changes
c,II/c,I 356 K, ΔH=167 J·mol^{-1}
ΔS=0.47 J·mol^{-1}·K^{-1}
c,I/liq 370 K, ΔH=19960 J·mol^{-1}
ΔS=54 J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR CQ
Evaluation A

$C_6H_5NO_3$ (c) 41CAM/CAM
4-Nitrophenol
Heat Capacity 283 K, C_p=144 J·mol^{-1}·K^{-1}
Temperature range 273 to 293 K. Value given as C_p=0.248 cal·g^{-1} over temperature range 0 to 20 °C.
Phase Changes
c/liq 387 K, ΔH=24271 J·mol^{-1}
ΔS=62.7 J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR DQ
Evaluation C

$C_6H_5NO_3$ (c) 72BOO/HAU
4-Nitrophenol
Phase Changes
c/liq 368.75 K, ΔH=19300 J·mol^{-1}
ΔS=52.3 J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR DQ
Evaluation C

$C_6H_5NO_3$ (c) 82POE/FAN
4-Nitrophenol
Phase Changes
c/liq 387.0 K, ΔH=18254 J·mol^{-1}
ΔS=47.17 J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR DQ
Evaluation A

$C_6H_5NO_3$ (c) 86SIN/KUN
4-Nitrophenol
Phase Changes
c/liq 385.15 K, ΔH=30118 J·mol^{-1}
ΔS=78.2 J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR DQ
Evaluation A

$C_6H_5N_3$ (c) 89JIM/ROU
Benzotriazole
Heat Capacity 298.15 K, C_p=178.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 119.1256
Wiswesser Line Notation T56 BMNNJ
Evaluation A

C_6H_6 (c) 82BAT/MR
2,4-Hexadiyne
Heat Capacity 298.15 K, C_p=133.57 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, S=178.14 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 117.9 K, ΔH=996.6 J·mol^{-1}
ΔS=8.42 J·mol^{-1}·K^{-1}
Molecular Weight 78.1134
Wiswesser Line Notation 2UU2UU2
Evaluation A

C_6H_6 (liq) 1881REI
Benzene
Heat Capacity 298 K, $C_p = 133.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 292 to 364 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation D

C_6H_6 (liq) 19DEJ
Benzene
Heat Capacity 298 K, $C_p = 137.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 24 to 50 °C.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 24WIL/DAN
Benzene
Heat Capacity 303 K, $C_p = 133.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 303 to 333 K. Equation only.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (c) 25MAA/WAL
Benzene
Heat Capacity 273 K, $C_p = 118.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 93 to 273 K.
Phase Changes
c/liq 278.64 K, $\Delta H = 10000\ J \cdot mol^{-1}$
$\Delta S = 35.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 25WIL/DAN
Benzene
Heat Capacity 293.2 K, $C_p = 133.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 20 to 60 °C.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 26AND/LYN
Benzene
Heat Capacity 298 K, $C_p = 132.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range −18 to 110 °C.
Phase Changes
c/liq 278.55 K, $\Delta H = 9875\ J \cdot mol^{-1}$
$\Delta S = 35.5\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 30HUF/PAR
Benzene
Heat Capacity 300.0 K, $C_p = 135.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 93 to 300 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, $S = 175.3\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, 47.49 $J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 278.6 K, $\Delta H = 9803\ J \cdot mol^{-1}$
$\Delta S = 35.19\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B(C_p).C(S)

C_6H_6 (liq) 31FIO/GIN
Benzene
Heat Capacity 323.15 K, $C_p = 143.57\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 50 to 110 °C.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 32RIC/WAL
Benzene
Heat Capacity 298.1 K, $C_p = 135.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 333 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 33FER/MIL
Benzene
Heat Capacity 298.15 K, $C_p = 131.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 323 K. Data calculated from equation.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 33KOL/UDO
Benzene
Heat Capacity 287.8 K, $C_p = 131.4\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 34KOL/UDO2
Benzene
Heat Capacity 287.8 K, $C_p = 131.4\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (c) 35AOY/KAN
Benzene
Heat Capacity 223.9 K, $C_p = 97.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 82 to 224 K. Value is unsmoothed experimental datum.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (c) 37AHL/BLA
Benzene
Heat Capacity 90 K, $C_p = 47.86\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 4 to 93 K.
Entropy 90 K, $S = 45.56\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 40BUR
Benzene
Heat Capacity 298.2 K, $C_p = 135.44\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 281 to 353 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 41ZHD
Benzene
Heat Capacity 298.1 K, $C_p = 136.0\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 8 to 46 °C.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 42ZIE/AND
Benzene
Phase Changes
c/liq 278.65 K, $\Delta H = 9916\ J \cdot mol^{-1}$
$\Delta S = 35.59\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 48TSC
Benzene
Heat Capacity 295 K, $C_p = 119\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Phase Changes
c/liq 278.6 K, $\Delta H = 9937\ J \cdot mol^{-1}$
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 47KUR
Benzene
Heat Capacity 298 K, $C_p = 133.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 9 to 80 °C, mean C_p, five temperatures.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation D

C_6H_6 (liq) 48OLI/EAT
Benzene
Heat Capacity 298.15 K. $C_p = 136.06\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 13 to 337 K.
Entropy 298.15 K, $S = 173.26\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 278.69 K, $\Delta H = 9866.3\ J \cdot mol^{-1}$
$\Delta S = 35.40\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 51SIE/CRU
Benzene
Heat Capacity 293 K, $C_p = 31.8\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 55STA/TUP
Benzene
Heat Capacity 298 K, $C_p = 135.23\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 288 to 347 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 56DUF/EVE
Benzene
Heat Capacity 303 K, $C_p = 136.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 303 to 353 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 60SWI/ZIE
Benzene
Heat Capacity 316 K, $C_p = 135.1\ J \cdot mol^{-1} \cdot K^{-1}$
Mean value 21 to 66 °C.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 62RAB/NIK
Benzene
Heat Capacity 298 K, $C_p = 134.98\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 35 °C.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 65FIN/GRU
Benzene
Heat Capacity 300 K, $C_p = 135.30\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 67PAC
Benzene
Heat Capacity 298 K, $C_p = 130\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Phase Changes
c/liq 278.8 K, $\Delta H = 8950\ J \cdot mol^{-1}$
$\Delta S = 32.1\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 67RAS/GAN
Benzene
Heat Capacity 293 K, $C_p = 134.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 353 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 68REC
Benzene
Heat Capacity 298 K, $C_p = 135.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 24 to 40 °C, equation only.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 69SUB/KHA
Benzene
Heat Capacity 298 K, C_p=135.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 71DES/BHA
Benzene
Heat Capacity 298 K, C_p=134.3 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 71HYD/SUB
Benzene
Heat Capacity 298.15 K, C_p=135.9 J·mol^{-1}·K^{-1}
Temperature range 298; 313 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 74RAJ/SUB
Benzene
Heat Capacity 298.15 K, C_p=135.7 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 323.15 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 76FOR/BEN
Benzene
Heat Capacity 298.15 K, C_p=135.76 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 76FOR/BEN2
Benzene
Heat Capacity 298.15 K, C_p=135.760 J·mol^{-1}·K^{-1}
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A
Data from 76FOR/BEN.

C_6H_6 (liq) 77VES/SVO
Benzene
Heat Capacity 298.15 K, C_p=135.90 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 77WIL/GRO
Benzene
Heat Capacity 298.15 K, C_p=135.60 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 78GRO/WIL
Benzene
Heat Capacity 298.15 K, C_p=135.61 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 79SMI
Benzene
Phase Changes
c/liq 279.1 K, ΔH=9300 J·mol^{-1}
ΔS=33.3 J·mol^{-1}·K^{-1}
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 79VES/ZAB
Benzene
Heat Capacity 298.15 K, C_p=135.90 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 81ATA/ELS
Benzene
Heat Capacity 293.15 K, C_p=133.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 82GOR/GRI
Benzene
Heat Capacity 300 K, C_p=136.5 J·mol^{-1}·K^{-1}
Temperature range 280 to 353 K. Data also given by equation.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 82GOR/SIM2
Benzene
Heat Capacity
Temperature range 280 to 680 K. Data at atmospheric pressure given by the equation: C_p=1.5194−1.299×10^{-3}T+6.927×10^{-6} T^2 kJ·kg^{-1}·K^{-1}.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 82GRO/ING
Benzene
Heat Capacity 298.15 K, C_p=135.7 J·mol^{-1}·K^{-1}
Temperature range 298.15 K. One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 82TAN
Benzene
Heat Capacity 298.15 K, C_p=135.74 J·mol^{-1}·K^{-1}
Temperatures 293.15, 298.15, 303.15 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 82WIL/FAR
Benzene
Heat Capacity 298.15 K, C_p=135.60 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 83GOR/SIM
Benzene
Heat Capacity 298.15 K, C_p=136.24 J·mol^{-1}·K^{-1}
Temperature range 283.78 to 348.47 K. C_p=1.3943−5.857 ×10^{-4}T+5.89×10^{-6}T^2 kJ·kg^{-1}·K^{-1}. C_p value calculated from equation.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 85OGA/MUR
Benzene
Heat Capacity 298.15 K, C_p=136.06 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 85TAN
Benzene
Heat Capacity 298.15 K, C_p=135.718 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 86NAZ/BAS
Benzene
Heat Capacity 322.05 K, C_p=139.9 J·mol^{-1}·K^{-1}
Temperature range 322.05, 351.15 K. p=0.1 MPa. Unsmoothed experimental datum given as 1.7915 kJ/kg·K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 86RED
Benzene
Heat Capacity 303.15 K, C_p=137.4 J·mol^{-1}·K^{-1}
Temperature range 303.15, 313.15 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 87GRO/ROU
Benzene
Heat Capacity 298.15 K, C_p=135.75 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 87KAL/KOH
Benzene
Heat Capacity 293.15 K, C_p=134.61 J·mol^{-1}·K^{-1}
Temperature range 293.15, 313.15 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 87TAN
Benzene
Heat Capacity 298.15 K, C_p=135.707 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 88SHI/OGA
Benzene
Heat Capacity 298.15 K, C_p=134.63 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 89LAI/ROI
Benzene
Heat Capacity 298.15 K, C_p=135.62 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 91CZ
Benzene
Heat Capacity 298.5 K, C_p=135.9 J·mol^{-1}·K^{-1}
One temperature. p=0.1 MPa. C_p values given for the pressur range 0.1 to 68.1 MPa.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 93GRO/ROU
Benzene
Heat Capacity 298.15 K, C_p=135.69 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1334
Wiswesser Line Notation R
Evaluation B

C_6H_6ClN (liq) 65ZAL/KO
m-Chloroaniline
Heat Capacity 294.7 K, C_p=198.7 J·mol^{-1}·K^{-1}
Temperature range 295, 323 K.
Molecular Weight 127.5731
Wiswesser Line Notation ZR CG
Evaluation C

C_6H_6ClN (c) 65ZAL/KOC
p-Chloroaniline
Heat Capacity 305 K, C_p=147.3 J·mol^{-1}·K^{-1}
Temperature range 292 to 323 K. Mean value.
Molecular Weight 127.5731
Wiswesser Line Notation ZR DG
Evaluation C

$C_6H_6Cl_6$ (c) 91SAB/AN
γ-Hexachlorocyclohexane
Phase Changes
c/liq 386.38 K, ΔH=25930 J·mol^{-1}
Molecular Weight 290.8314
Wiswesser Line Notation L6TJ AG BG CG DG EG FG
Evaluation A

C_6H_6FN (liq) 91LIC
p-Fluoroaniline
Heat Capacity 298.15 K, C_p=195.2 J·mol^{-1}·K^{-1}
Temperature range 175 to 333 K. C_p(liq)=192.943+0.092T(°C) J·mol^{-1}·K^{-1} (−49 to 60 °C). C_p value calculated from equation.
Phase Changes
c/liq 271.25 K
Molecular Weight 111.1185
Wiswesser Line Notation ZR DF
Evaluation A

$C_6H_6N_2O_2$ (c) 26AND
2-Nitroaniline
Heat Capacity 297.9 K, C_p=168.2 J·mol^{-1}·K^{-1}
Temperature range 110 to 332 K. Value is unsmoothed experimental datum.
Molecular Weight 138.1256
Wiswesser Line Notation ZR BNW
Evaluation C

$C_6H_6N_2O_2$ (c) 26AND/LYN
2-Nitroaniline
Heat Capacity 298 K, C_p=164.4 J·mol^{-1}·K^{-1}
Temperature range 22 to 150 °C.
Phase Changes
c/liq 342.5 K, ΔH=16110 J·mol^{-1}
ΔS=47.0 J·mol^{-1}·K^{-1}
Molecular Weight 138.1256
Wiswesser Line Notation ZR BNW
Evaluation C

$C_6H_6N_2O_2$ (c) 26AND
3-Nitroaniline
Heat Capacity 297.9 K, C_p=167.4 J·mol^{-1}·K^{-1}
Temperature range 110 to 344 K. Value is unsmoothed experimental datum.
Molecular Weight 138.1256
Wiswesser Line Notation ZR CNW
Evaluation C

$C_6H_6N_2O_2$ (c) 26AND/LYN
3-Nitroaniline
Heat Capacity 298 K, C_p=168.2 J·mol^{-1}·K^{-1}
Temperature range 22 to 210 °C.
Phase Changes
c/liq 385.0 K, ΔH=23680 J·mol^{-1}
ΔS=61.5 J·mol^{-1}·K^{-1}
Molecular Weight 138.1256
Wiswesser Line Notation ZR CNW
Evaluation C

$C_6H_6N_2O_2$ (c) 41SAT/SOG3
3-Nitroaniline
Heat Capacity 323 K, C_p=186.6 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 138.1256
Wiswesser Line Notation ZR CNW
Evaluation C
Same data as 40SAT/SOG4.

$C_6H_6N_2O_2$ (c) 72BOO/HAU
3-Nitroaniline
Phase Changes
c/liq 384.95 K, ΔH=23600 J·mol^{-1}
ΔS=61.3 J·mol^{-1}·K^{-1}
Molecular Weight 138.1256
Wiswesser Line Notation ZR CNW
Evaluation C

$C_6H_6N_2O_2$ (c) 83NIS/SAK
3-Nitroaniline
Heat Capacity 298.15 K, C_p=158.84 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.15 J·K^{-1}·g^{-1}.
Molecular Weight 138.1256
Wiswesser Line Notation ZR CNW
Evaluation B

$C_6H_6N_2O_2$ (c) 90SIN/GUP
3-Nitroaniline
Phase Changes
c/liq 387 K, ΔH=23689 J·mol^{-1}
Molecular Weight 138.1256
Wiswesser Line Notation ZR CNW
Evaluation A

$C_6H_6N_2O_2$ (c) 26AND
4-Nitroaniline
Heat Capacity 297.9 K, C_p=165.7 J·mol^{-1}·K^{-1}
Temperature range 110 to 344 K. Value is unsmoothed experimental datum.
Molecular Weight 138.1256
Wiswesser Line Notation ZR DNW
Evaluation C

$C_6H_6N_2O_2$ (c) 26AND/LYN
4-Nitroaniline
Heat Capacity 298 K, C_p=169.0 J·mol^{-1}·K^{-1}
Temperature range 22 to 195 °C.
Phase Changes
c/liq 420.7 K, ΔH=21090 J·mol^{-1}
ΔS=50.1 J·mol^{-1}·K^{-1}
Molecular Weight 138.1256
Wiswesser Line Notation ZR DNW
Evaluation C

$C_6H_6N_2O_2$ (c) 41SAT/SOG3
4-Nitroaniline
Heat Capacity 323 K, C_p=184.9 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 138.1256
Wiswesser Line Notation ZR DNW
Evaluation C
Same data as 40SAT/SOG4.

$C_6H_6N_2O_2$ (c) 72BOO/HAU
4-Nitroaniline
Phase Changes
c/liq 420.65 K, $\Delta H = 21150$ J·mol^{-1}
$\Delta S = 50.3$ J·mol^{-1}·K^{-1}
Molecular Weight 138.1256
Wiswesser Line Notation ZR DNW
Evaluation C

$C_6H_6N_2O_2$ (c) 83NIS/SAK
4-Nitroaniline
Heat Capacity 298.15 K, $C_p = 154.2$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.116 J·K^{-1}·g^{-1}.
Molecular Weight 138.1256
Wiswesser Line Notation ZR DNW
Evaluation B

C_6H_6O (c) 1889EYK
Phenol; Hydroxybenzene
Phase Changes
c/liq 312.7 K, $\Delta H = 10581$ J·mol^{-1}
$\Delta S = 33.8$ J·mol^{-1}·K^{-1}
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation C

C_6H_6O (liq) 03MAG
Phenol; Hydroxybenzene
Heat Capacity 298 K, $C_p = 220.9$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.561 cal·g^{-1}·K^{-1}.
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation D

C_6H_6O (c) 33PAR/HUF
Phenol; Hydroxybenzene
Heat Capacity 295.8 K, $C_p = 133.09$ J·mol^{-1}·K^{-1}
Temperature range 93 to 296 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, $S = 142.7$ J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 49.04 J·mol^{-1}·K^{-1}.
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation B(C_p),C(S)

C_6H_6O (c) 35AOY/KAN
Phenol; Hydroxybenzene
Heat Capacity 229.3 K, $C_p = 103.8$ J·mol^{-1}·K^{-1}
Temperature range 78 to 229 K. Value is unsmoothed experimental datum.
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation B

C_6H_6O (c) 40CAM/CAM
Phenol; Hydroxybenzene
Heat Capacity 293 K, $C_p = 93.7$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation C

C_6H_6O (c) 57MAS
Phenol; Hydroxybenzene
Phase Changes
c/liq 314.13 K, $\Delta H = 12125$ J·mol^{-1}
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation A

C_6H_6O (c) 63AND/COU
Phenol; Hydroxybenzene
Heat Capacity 298.15 K, $C_p = 127.44$ J·mol^{-1}·K^{-1}
Temperature range 13 to 336 K.
Entropy 298.15 K, $S = 144.01$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 314.06 K, $\Delta H = 11514$ J·mol^{-1}
$\Delta S = 36.66$ J·mol^{-1}·K^{-1}
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation A

C_6H_6O (c) 67RAS/GAN
Phenol; Hydroxybenzene
Heat Capacity 313 K, $C_p = 199.8$ J·mol^{-1}·K^{-1}
Temperature range 313 to 373 K.
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation C

C_6H_6O (c) 75NIC/WAL
Phenol; Hydroxybenzene
Heat Capacity 298.15 K, $C_p = 127.21$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation B

$C_6H_6O_2$ (c) 03MAC
1,2-Dihydroxybenzene; Pyrocatechin; Catechol
Heat Capacity 298 K, $C_p = 144.2$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.313 cal·g^{-1}·K^{-1}.
Molecular Weight 110.1122
Wiswesser Line Notation QR BQ
Evaluation D

$C_6H_6O_2$ (c) 26ANL
1,2-Dihydroxybenzene; Pyrocatechin; Catechol
Heat Capacity 297.9 K, $C_p = 139.3$ J·mol^{-1}·K^{-1}
Temperature range 110 to 344 K. Value is unsmoothed experimental datum.
Molecular Weight 110.1122
Wiswesser Line Notation QR BQ
Evaluation C

$C_6H_6O_2$ (c) 26AND/LYS
1,2-Dihydroxybenzene; Pyrocatechin; Catechol
Heat Capacity 298 K, $C_p = 132.2$ J·mol^{-1}·K^{-1}
Temperature range 22 to 200 °C.
Phase Changes
c/liq 337.5 K, $\Delta H = 22760$ J·mol^{-1}
$\Delta S = 60.3$ J·mol^{-1}·K^{-1}
Molecular Weight 110.1122
Wiswesser Line Notation QR BQ
Evaluation C

$C_6H_6O_2$ (c) 41SAT/SOG3
1,2-Dihydroxybenzene; Pyrocatechin; Catechol
Heat Capacity 323 K, C_p=156.9 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 110.1122
Wiswesser Line Notation QR BQ
Evaluation C
Same data as 40SAT/SOG4.

$C_6H_6O_2$ (c) 50UEB/ORT
1,2-Dihydroxybenzene; Pyrocatechin; Catechol
Heat Capacity 298.15 K, C_p=140.6 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Molecular Weight 110.1122
Wiswesser Line Notation QR BQ
Evaluation C

$C_6H_6O_2$ (c) 89BRI/LIC
1,2-Dihydroxybenzene; Pyrocatechin; Catechol
Heat Capacity 298.15 K, C_p=140.17 J·mol^{-1}·K^{-1}
Temperature range 200 to 500 K. C_p(c)=132.494+0.2808t +5.4046
×10-4t2+2.0581×10^{-5} J·mol^{-1}·K^{-1} (t/°C). C_p value calculated from equation.
Phase Changes
c/liq 376.85 K, ΔH=22000 J·mol^{-1}
ΔS=58 J·mol^{-1}·K^{-1}
Molecular Weight 110.1122
Wiswesser Line Notation QR BQ
Evaluation B

$C_6H_6O_2$ (c) 03MAG
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Heat Capacity 298 K, C_p=122.5 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.266 cal·g^{-1}·K^{-1}.
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation D

$C_6H_6O_2$ (c) 26AND
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Heat Capacity 297.9 K, C_p=131.4 J·mol^{-1}·K^{-1}
Temperature range 110 to 344 K. Value is unsmoothed experimental datum.
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation C

$C_6H_6O_2$ (c) 26AND/LYN
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Heat Capacity 298 K, C_p=131.0 J·mol^{-1}·K^{-1}
Temperature range 22 to 200 °C.
Phase Changes
c/liq 382.8 K, ΔH=21300 J·mol^{-1}
ΔS=55.6 J·mol^{-1}·K^{-1}
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation C

$C_6H_6O_2$ (c) 41SAT/SOG3
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Heat Capacity 323 K, C_p=151.0 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation C
Same data as 40SAT/SOG4.

$C_6H_6O_2$ (c) 50UEB/ORT
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Heat Capacity 298.15 K, C_p=139.3 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation C

$C_6H_6O_2$ (c) 82VII/GAM
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Phase Changes
c/liq 381 K, ΔH=20500 J·mol^{-1}
ΔS=53.8 J·mol^{-1}·K^{-1}
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation B

$C_6H_6O_2$ (c) 87EBI/ASK
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Phase Changes
c,II/c,I 369 K, ΔH=1370 J·mol^{-1}
ΔS=3.71 J·mol^{-1}·K^{-1}
α-β phase transition.
c,I/liq 382.7 K, ΔH=20890 J·mol^{-1}
ΔS=54.59 J·mol^{-1}·K^{-1}
Fusion of β-resorcinol.
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation A

$C_6H_6O_2$ (c) 89BRI/LIC
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Heat Capacity 298.15 K, C_p=135.53 J·mol^{-1}·K^{-1}
Temperature range 200 to 500 K. C_p(c)=126.876+0.3316t +5.6228×10-4t2+9.5321×10-6t3 J·mol^{-1}·K^{-1} (t/°C). C_p value calculated from equation.
Phase Changes
c,II/c,I 366.75 K, ΔH=1200 J·mol^{-1}
ΔS=3.3 J·mol^{-1}·K^{-1}
c,I/liq 382.55 K, ΔH=18900 J·mol^{-1}
ΔS=59 J·mol^{-1}·K^{-1}
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation B

$C_6H_6O_2$ (c) 03MAG
1,4-Dihydroxybenzene; Hydroquinone
Heat Capacity 298 K, C_p=118.9 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.258 cal·g^{-1}·K^{-1}.
Molecular Weight 110.1122
Wiswesser Line Notation QR DQ
Evaluation D

$C_6H_6O_2$ (c) 24LAN
1,4-Dihydroxybenzene; Hydroquinone
Heat Capacity 274.3 K, C_p=130.5 J·mol^{-1}·K^{-1}
Temperature range 28 to 275 K. Value is unsmoothed experimental datum.
Molecular Weight 110.1122
Wiswesser Line Notation QR DQ
Evaluation B

$C_6H_6O_2$ (c) 26AND
1,4-Dihydroxybenzene; Hydroquinone
Heat Capacity 297.9 K, C_p=133.5 J·mol^{-1}·K^{-1}
Temperature range 110 to 344 K. Value is unsmoothed experimental datum.
Molecular Weight 110.1122
Wiswesser Line Notation QR DQ
Evaluation C

$C_6H_6O_2$ (c) 26AND/LYN
1,4-Dihydroxybenzene; Hydroquinone
Heat Capacity 298 K, C_p=139.7 J·mol^{-1}·K^{-1}
Temperature range 22 to 200 °C.
Phase Changes
c/liq 445.5 K, ΔH=27110 J·mol^{-1}
ΔS=60.9 J·mol^{-1}·K^{-1}
Molecular Weight 110.1122
Wiswesser Line Notation QR DQ
Evaluation C

$C_6H_6O_2$ (c) 41SAT/SOG3
1,4-Dihydroxybenzene; Hydroquinone
Heat Capacity 323 K, C_p=150.2 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 110.1122
Wiswesser Line Notation QR DQ
Evaluation C
Same data as 40SAT/SOG4.

$C_6H_6O_2$ (c) 50UEB/ORT
1,4-Dihydroxybenzene; Hydroquinone
Heat Capacity 298.15 K, C_p=136.4 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Molecular Weight 110.1122
Wiswesser Line Notation QR DQ
Evaluation C

$C_6H_6O_2$ (c) 89BRI/LIC
1,4-Dihydroxybenzene; Hydroquinone
Heat Capacity 298.15 K, C_p=131.90 J·mol^{-1}·K^{-1}
Temperature range 200 to 500 K. C_p(c)=125.328+0.2791t −1.0329×10-3t2+1.5075×10-5t3 J·mol^{-1}·K^{-1} (t/°C). C_p value calculated from equation.
Phase Changes
c/liq 444.95 K. ΔH=26500 J·mol^{-1}
ΔS=59 J·mol^{-1}·K^{-1}
Molecular Weight 110.1122
Wiswesser Line Notation QR DQ
Evaluation B

C_6H_6S (liq) 36PAR/TOD
Thiophenol; Phenyl mercaptan
Heat Capacity 298.1 K, C_p=176.56 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 298.1 K, S=220.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 54.68 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 258.2 K, ΔH=11478 J·mol^{-1}
ΔS=44.45 J·mol^{-1}·K^{-1}
Molecular Weight 110.1734
Wiswesser Line Notation SHR
Evaluation B(C_p),C(S)

C_6H_6S (liq) 56SCO/MCC2
Thiophenol; Phenyl mercaptan
Heat Capacity 298.15 K, C_p=173.22 J·mol^{-1}·K^{-1}
Temperature range 10 to 380 K.
Entropy 298.15 K, S=222.80 J·mol^{-1}·K^{-1}
Phase Changes
Lambda transition of about 167 J·mol^{-1} excess enthalpy at 110 to 135 K.
c/liq 258.27 K, ΔH=11447 J·mol^{-1}
ΔS=44.32 J·mol^{-1}·K^{-1}
Molecular Weight 110.1734
Wiswesser Line Notation SHR
Evaluation A

C_6H_7N (liq) 71HAL/BAL
1-Bicyclo[2.1.0]pentyl cyanide; 1-Cyanobicyclo[2.1.0]pentane
Heat Capacity 297 K, C_p=163.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 93.1280
Wiswesser Line Notation L34TJ ACN
Evaluation C

C_6H_7N (liq) 71HAL/BAL
3-Methylenecyclobutyl cyanide; 1-Cyano-3-methylenecyclobutane
Heat Capacity 297 K, C_p=190.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 93.1280
Wiswesser Line Notation L4YTJ AU1 CCN
Evaluation C

C_6H_7N (liq) 01KAH
2-Methylpyridine; α-Picoline
Heat Capacity C_p=169.2 J mol^{-1} K^{-1}
Temperature range 294.15 to 403.15 K. Heat capacity is an average value over the temperature range.
Molecular Weight 93.1280
Wiswesser Line Notation T6NJ B1
Evaluation D

C_6H_7N (liq) 63SCO/HUE
2-Methylpyridine; α-Picoline
Heat Capacity 298.15 K, C_p=158.41 J·mol^{-1}·K^{-1}
Temperature range 12 to 370 K.
Entropy 298.15 K, S=217.86 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 206.45 K. ΔH=9724.0 J·mol^{-1}
ΔS=47.10 J·mol^{-1}·K^{-1}
Molecular Weight 93.1280
Wiswesser Line Notation T6NJ B1
Evaluation A

C_6H_7N (liq) 63SCO/GOO
3-Methylpyridine; β-Picoline
Heat Capacity 298.15 K, C_p=158.69 J·mol^{-1}·K^{-1}
Temperature range 12 to 400 K.
Entropy 298.15 K, S=216.31 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 255.01 K, ΔH=14180 J·mol^{-1}
ΔS=55.61 J·mol^{-1}·K^{-1}
Molecular Weight 93.1280
Wiswesser Line Notation T6NJ C1
Evaluation A

C_6H_7N (liq) 86STE/CHI
4-Methylpyridine
Heat Capacity 298.15 K, C_p=158.99 J·mol^{-1}·K^{-1}
Temperature range 10 to 410 K.
Entropy 298.15 K, S=208.22 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 255.010 K
c,I/liq 276.818 K
Molecular Weight 93.1280
Wiswesser Line Notation T6NJ D1
Evaluation A

C_6H_7N (liq) 87MES/TOD
4-Methylpyridine
Heat Capacity 298.15 K, C_p=158.99 J·mol^{-1}·K^{-1}
Temperature range 10 to 410 K.
Entropy 298.15 K, S=208.22 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 255.010 K, ΔH=0.083 J·mol^{-1}
c,I/liq 276.817 K, ΔH=12577 J·mol^{-1}
ΔS=45.43 J·mol^{-1}·K^{-1}
Molecular Weight 93.1280
Wiswesser Line Notation T6NJ D1
Evaluation A

C_6H_7N (liq) 88MES/TOD
4-Methylpyridine
Heat Capacity 298.150 K, C_p=158.988 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S=209.091 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 255.00 K, ΔH=0.00 J·mol^{-1}
c,I/liq 276.818 K, ΔH=12582.28 J·mol^{-1}
ΔS=45.45 J·mol^{-1}·K^{-1}
Molecular Weight 93.1280
Wiswesser Line Notation T6NJ D1
Evaluation A

C_6H_7N (liq) 1881REI
Aniline
Heat Capacity 298 K, C_p=192.5 J·mol^{-1}·K^{-1}
Temperature range 290 to 465 K.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation D

C_6H_7N (liq) 02LOU
Aniline
Heat Capacity 370 K, C_p=213 J·mol^{-1}·K^{-1}
Mean value 20 to 176 °C.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation D

C_6H_7N (c) 03FOR
Aniline
Heat Capacity 258 K, C_p=87 J·mol^{-1}·K^{-1}
Temperature range 251 to 265 K. C_p=0.223 cal/g·K at −15 °C.
Phase Changes
c/liq 266.12 K, ΔH=15500 J·mol^{-1}
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation D

C_6H_7N (liq) 03FOR
Aniline
Heat Capacity 273 K, C_p=189 J·mol^{-1}·K^{-1}
One temperature. C_p=0.4838 cal/g·K at 0 °C.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation S

C_6H_7N (liq) 28LAN
Aniline
Heat Capacity 298.2 K, C_p=193.38 J·mol^{-1}·K^{-1}
Temperature range 5 to 60 °C.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation B

C_6H_7N (liq) 33FER/MIL
Aniline
Heat Capacity 298.15 K, C_p=178.8 J·mol^{-1}·K^{-1}
Temperature range 293 to 323 K. Data calculated from equation.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation B

C_6H_7N (liq) 33PAR/HUF
Aniline
Heat Capacity 298.2 K, C_p=190.92 J·mol^{-1}·K^{-1}
Temperature range 94 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=191.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 45.27 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 266.8 K, ΔH=10556 J·mol^{-1}
ΔS=39.57 J·mol^{-1}·K^{-1}
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation B(C_p),C(S)

C_6H_7N (liq) 34RAD/JUL
Aniline
Heat Capacity 288 K, C_p=183.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation C

C_6H_7N (liq) 42ZIE/AND
Aniline
Heat Capacity 267.3 K, C_p=109.20 J·mol^{-1}·K^{-1}
Temperature range 40.84 K.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation B

C_6H_7N (liq) 50HOU/MAS
Aniline
Heat Capacity 323 K, C_p=197.5 J·mol^{-1}·K^{-1}
Temperature range 323 to 453 K.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation B

C_6H_7N (liq) 57CRU/JOS
Aniline
Heat Capacity 293 K, C_p=192.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation B

C_6H_7N (liq) 62HAT/HIL
Aniline
Heat Capacity 298.15 K, C_p=192.05 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K. C_p(liq, cal/mol·K)=33.71 +0.0409T (15 to 300 K).
Entropy 298.15 K, S=191.30 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 267.13 K, ΔH=10539 J·mol^{-1}
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation A

C_6H_7N (liq) 71DES/BHA
Aniline
Heat Capacity 298 K, C_p=193.7 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation B

C_6H_7N (liq) 75NIC/WAD
Aniline
Heat Capacity 298.15 K, C_p=191.01 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation B

C_6H_7N (liq) 87LES/LIC
Aniline
Heat Capacity 298 K, C_p=194.1 J·mol^{-1}·K^{-1}
Temperature range 200 to 300 K.
Phase Changes
c/liq 267 K
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation B

C_6H_7NO (c) 89BRI/LIC
2-Aminophenol
Heat Capacity 298.15 K, C_p=139.33 J·mol^{-1}·K^{-1}
Temperature range 200 to 500 K. C_p(c)=129.427+0.4186t −1.1879×10-3t2+1.1367×10-5t3 J·mol^{-1}·K^{-1} (t/°C). C_p value calculated from equation.
Phase Changes
c/liq 447.35 K, ΔH=34000 J·mol^{-1}
ΔS=76 J·mol^{-1}·K^{-1}
Molecular Weight 109.1274
Wiswesser Line Notation ZR BQ
Evaluation B

C_6H_7NO (c) 89BRI/LIC
3-Aminophenol
Heat Capacity 298.15 K, C_p=137.85 J·mol^{-1}·K^{-1}
Temperature range 200 to 500 K. C_p(c) =127.586+0.4029 −2.4963×10-5t2+1.3004×10-5t3 J·mol^{-1}·K^{-1} (t/°C). C_p valu calculated from equation.
Phase Changes
c/liq 394.15 K, ΔH=24700 J·mol^{-1}
ΔS=63 J·mol^{-1}·K^{-1}
Molecular Weight 109.1274
Wiswesser Line Notation ZR CQ
Evaluation B

C_6H_7NO (c) 90SIN/GUI
3-Aminophenol
Phase Changes
c/liq 396 K, ΔH=22967 J·mol^{-1}
Molecular Weight 109.1274
Wiswesser Line Notation ZR CQ
Evaluation A

C_6H_7NO (c) 89BRI/LIC
4-Aminophenol
Heat Capacity 298.15 K, C_p=139.36 J·mol^{-1}·K^{-1}
Temperature range 200 to 500 K. C_p(c)=127.665+0.4447 −4.3675×10-4t2+5.4576×10-5t3J·mol^{-1}·K^{-1} (t/°C). C_p valu calculated from equation.
Phase Changes
c/liq 459.45 K, ΔH=31200 J·mol^{-1}
ΔS=68 J·mol^{-1}·K^{-1}
Molecular Weight 109.1274
Wiswesser Line Notation ZR DQ
Evaluation B

$C_6H_7NO_2S$ (c) 41SAT/SOG
Benzenesulfonamide
Heat Capacity 323 K, C_p=193.3 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 157.1868
Wiswesser Line Notation ZSWR
Evaluation C
Same data as 40SAT/SOG3.

$(C_6H_7N_3O)_n$ (c) 91RO
Poly-L-histidine
Heat Capacity 300 K, C_p=147.9 J·mol^{-1}·K^{-1}
Temperature range 220 to 330 K.
Molecular Weight 137.1408
Wiswesser Line Notation /*VY1- ET5M CNJ &M*/ -L
Evaluation B

$(C_6H_7N_3O)_n$ (c) 93ROL/XE
Poly-L-histidine
Heat Capacity 300 K, C_p=147.9 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 137.1408
Wiswesser Line Notation /*VY1- ET5M CNJ &M*/ -L
Evaluation B

$(C_6H_7N_3O\cdot HCl)_n$ (c) 91ROL
Poly-L-histidine hydrochloride
Heat Capacity 300 K, C_p=177.6 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 173.6017
Wiswesser Line Notation /*VY1- ET5M CNJ A &EH &M*/ -L
Evaluation B

$(C_6H_7N_3O\cdot HCl)_n$ (c) 93ROL/XEN
Poly-L-histidine hydrochloride
Heat Capacity 300 K, C_p=177.6 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 173.6017
Wiswesser Line Notation /*VY1- ET5M CNJ A &EH &M*/ -L
Evaluation B

C_6H_8 (liq) 76GEI/WOL
1,3-Cyclohexadiene
Heat Capacity 298.15 K, C_p=144.56 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=197.28 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 161.0 K, ΔH=4204.5 J·mol^{-1}
ΔS=26.11 J·mol^{-1}·K^{-1}
Molecular Weight 80.1292
Wiswesser Line Notation L6U CUTJ
Evaluation B

C_6H_8 (liq) 89STE/CHI3
1,3-Cyclohexadiene
Heat Capacity 298.15 K, C_p=141.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 80.1292
Wiswesser Line Notation L6U CUTJ
Evaluation B

C_6H_8 (liq) 76GEI/WOL
1,4-Cyclohexadiene
Heat Capacity 298.15 K, C_p=145.94 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=189.37 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 192.0 K, ΔH=816 J·mol^{-1}
ΔS=4.25 J·mol^{-1}·K^{-1}
c,I/liq 224.0 K, ΔH=5715.3 J·mol^{-1}
ΔS=25.51 J·mol^{-1}·K^{-1}
Molecular Weight 80.1292
Wiswesser Line Notation L6U DUTJ
Evaluation B

C_6H_8 (liq) 89STE/CHI3
1,4-Cyclohexadiene
Heat Capacity 298.15 K, C_p=142.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 80.1292
Wiswesser Line Notation L6U DUTJ
Evaluation B

C_6H_8BrN (c) 61SUG
Aniline hydrobromide
Heat Capacity 298.75 K, C_p=159.62 J·mol^{-1}·K^{-1}
Temperature range −74 to 67 °C. Value is unsmoothed experimental datum.
Phase Changes
c,II/c,I 293 K, ΔH=1243 J·mol^{-1}
ΔS=4.60 J·mol^{-1}·K^{-1}
Values obtained by summing excess specific heat between −20 °C and transition temperature.
Molecular Weight 174.0399
Wiswesser Line Notation ZR &EH
Evaluation B

C_6H_8BrN (c) 78KOJ
Aniline hydrobromide
Heat Capacity
Temperature range 200 to 320 K. Data given graphically.
Phase Changes
c,II/c,I 230–300 K, ΔH=1142 J·mol^{-1}
ΔS=3.87 J·mol^{-1}·K^{-1}
Peak at 295 K for order-disorder transition which extends over a 70 K range (230–300 K).
Molecular Weight 174.0399
Wiswesser Line Notation ZR &EH
Evaluation B

$C_6H_8N_2$ (liq) 81LEB/RYA
Phenylhydrazine
Heat Capacity 299.45 K, C_p=217.3 J·mol^{-1}·K^{-1}
Temperature range 293 to 358 K.
Molecular Weight 108.1426
Wiswesser Line Notation ZMR
Evaluation B

$C_6H_8N_2$ (c) 73KUN/KAR
1,2-Phenylenediamine
Heat Capacity 300 K, C_p=162.13 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=152.09 J·mol^{-1}·K^{-1}
Molecular Weight 108.1426
Wiswesser Line Notation ZR BZ
Evaluation A

$C_6H_8N_2$ (c) 89BRE/LIC
1,2-Phenylenediamine
Heat Capacity 298.15 K, C_p=150.82 J·mol^{-1}·K^{-1}
Temperature range 200 to 500 K. C_p(c)=135.620+0.5717t +1.1893×10-3t2+1.0768×10-5t3 J·mol^{-1}·K^{-1} (t/°C). C_p value calculated from equation.
Phase Changes
c/liq 373.85 K, ΔH=23100 J·mol^{-1}
ΔS=62 J·mol^{-1}·K^{-1}
Molecular Weight 108.1426
Wiswesser Line Notation ZR BZ
Evaluation B

$C_6H_8N_2$ (c) 73KUN/KAR
1,3-Phenylenediamine
Heat Capacity 300 K, C_p=161.08 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=149.49 J·mol^{-1}·K^{-1}
Molecular Weight 108.1426
Wiswesser Line Notation ZR CZ
Evaluation A

$C_6H_8N_2$ (c) 84RAB/KAR
1,3-Phenylenediamine
Heat Capacity 298.15 K, C_p=159.6 J·mol^{-1}·K^{-1}
Temperature range 13 to 500 K.
Entropy 298.15 K, S=154.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 339.1 K, ΔH=15570 J·mol^{-1}
ΔS=45.92 J·mol^{-1}·K^{-1}
Molecular Weight 108.1426
Wiswesser Line Notation ZR CZ
Evaluation A

$C_6H_8N_2$ (liq) 87LES/LIC
1,3-Phenylenediamine
Heat Capacity 298 K, C_p=153.7 J·mol^{-1}·K^{-1}
Temperature range 220 to 400 K.
Phase Changes
c/liq 337 K
Molecular Weight 108.1426
Wiswesser Line Notation ZR CZ
Evaluation B

$C_6H_8N_2$ (c) 89BRI/LIC
1,3-Phenylenediamine
Heat Capacity 298.15 K. C_p=152.89 J·mol^{-1}·K^{-1}
Temperature range 200 to 500 K. C_p(c)=136.419+0.5202t +3.9721×10-3t2+6.2879×10-5t3 J·mol^{-1}·K^{-1} (t/°C). C_p value calculated from equation.
Phase Changes
c/liq 335.45 K, ΔH=15400 J·mol^{-1}
ΔS=46 J·mol^{-1}·K^{-1}
Molecular Weight 108.1426
Wiswesser Line Notation ZR CZ
Evaluation B

$C_6H_8N_2$ (c) 73KUN/KAR
1,4-Phenylenediamine
Heat Capacity 300 K, C_p=155.64 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=149.70 J·mol^{-1}·K^{-1}
Molecular Weight 108.1426
Wiswesser Line Notation ZR DZ
Evaluation B

$C_6H_8N_2$ (c) 89BRI/LIC
1,4-Phenylenediamine
Heat Capacity 298.15 K. C_p=152.69 J·mol^{-1}·K^{-1}
Temperature range 200 to 500 K. C_p(c)=139.327 +0.5240t −3.9651×10-5t2+1.8530×10-5t3 J·mol^{-1}·K^{-1} (t/°C). C_p value calculated from equation.
Phase Changes
c/liq 412.25 K. ΔH=21700 J·mol^{-1}
ΔS=52 J·mol^{-1}·K^{-1}
Molecular Weight 108.1426
Wiswesser Line Notation ZR DZ
Evaluation B

$C_6H_8N_2$ (c) 90RAI/MAN
1,4-Phenylenediamine
Phase Changes
c/liq 416 K. ΔH=24900 J·mol^{-1}
ΔS=59.8 J·mol^{-1}·K^{-1}
Temperature from graph.
Molecular Weight 108.1426
Wiswesser Line Notation ZR DZ
Evaluation A

$C_6H_8N_2O_2$ (c) 84ZIE/ZIE
1,3-Dimethyluracil
Phase Changes
c/liq 392.5 K, ΔH=23100 J·mol^{-1}
ΔS=58.9 J·mol^{-1}·K^{-1}
Molecular Weight 140.1414
Wiswesser Line Notation T6NVNVJ A1 C1
Evaluation B

$C_6H_8N_2O_2$ (c) 89IMA/TAK
1,3-Dimethyluracil
Heat Capacity 298.15 K, C_p=170 J·mol^{-1}·K^{-1}
One temperature, estimated.
Phase Changes
c/g 298.15 K, ΔH=96900 J·mol^{-1}
ΔS=325.0 J·mol^{-1}·K^{-1}
Molecular Weight 140.1414
Wiswesser Line Notation T6NVNVJ A1 C1
Evaluation B

$C_6H_8N_2O_2$ (c) 89SAK/IMA
1,3-Dimethyluracil
Phase Changes
c,II/liq 394 K, ΔH=18400 J·mol^{-1}
Melting of the metastable phase.
c,I/liq 398 K, ΔH=14600 J·mol^{-1}
Melting of the stable phase.
Molecular Weight 140.1414
Wiswesser Line Notation T6NVNVJ A1 C1
Evaluation A

$C_6H_8N_2O_2S$ (c) 41SAT/SOG2
p-Aminobenzenesulfonamide
Heat Capacity 323 K, C_p=220.9 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 172.2014
Wiswesser Line Notation ZSWR DZ
Evaluation C
Same data as 40SAT/SOG3.

$(C_6H_8N_2O_9)_n$ (c) 85RAB/KHL
Cellulose nitrate
Heat Capacity 298.15 K, C_p=279.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=318.9 J·mol^{-1}·K^{-1}
Molecular Weight 252.1373
Wiswesser Line Notation /T5OTJ B* CONW DONW EO* FIQ/
Evaluation B
11.9% nitrogen content. Dinitrocellulose has a nitrogen content of 11.11%.

$C_6H_8O_2$ (liq) 71HAL/BAI
Methyl bicyclo[1.1.0]butane-1-carboxylate
Heat Capacity 297 K, C_p=192.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 112.1280
Wiswesser Line Notation L33TJ AVO1
Evaluation C

$C_6H_8O_2$ (c) 92PAJ/LAT
1,3-Cyclohexanedione
Phase Changes
c,II/c,I 287 K, ΔH=493 J·mol^{-1}
Molecular Weight 112.1280
Wiswesser Line Notation L6V CVTJ
Evaluation B

$C_6H_8O_2$ (c) 93PIL/PAR
1,3-Cyclohexanedione
Phase Changes
c/g 298.15 K, ΔH=89800 J·mol^{-1}
Molecular Weight 112.1280
Wiswesser Line Notation L6V CVTJ
Evaluation A

$C_6H_8O_2$ (c) 83DEW/DEK
1,4-Cyclohexanedione
Heat Capacity 300 K, C_p=161.4 J·mol^{-1}·K^{-1}
Temperature range 90 to 310 K. Linearly extrapolated.
Phase Changes
c,III/c,II 319.89 K
c,II/c,I 336.73 K
c,I/liq 351.6 K, ΔH=11325 J·mol^{-1}
Molecular Weight 112.1280
Wiswesser Line Notation L6V DVTJ
Evaluation B(C_p), A(Phase changes).

$C_6H_8O_2$ (c) 93PIL/PAR
1,4-Cyclohexanedione
Phase Changes
c/g 298.15 K, ΔH=75000 J·mol^{-1}
Molecular Weight 112.1280
Wiswesser Line Notation L6V DVTJ
Evaluation A

$C_6H_8O_4$ (liq) 30WAS
Dimethyl maleate
Heat Capacity 298 K, C_p=163.2 J·mol^{-1}·K^{-1}
Temperature range 0 to 99 °C.
Phase Changes
c/liq 254 K, ΔH=14640 J·mol^{-1}
ΔS=58 J·mol^{-1}·K^{-1}
Molecular Weight 144.1268
Wiswesser Line Notation 1OV1U1VO1 -C
Evaluation C

$C_6H_8O_4$ (c) 30WAS
Dimethyl fumarate
Heat Capacity 298 K, C_p=199.2 J·mol^{-1}·K^{-1}
Temperature range 014 to 99 °C.
Phase Changes
c/liq 375 K, ΔH=35150 J·mol^{-1}
ΔS=94 J·mol^{-1}·K^{-1}
Molecular Weight 144.1268
Wiswesser Line Notation 1OV1U1VO1 -T
Evaluation C

$C_6H_8O_4$ (c) 80KUL/LEB
Lactide(DL); 3,6-Dimethyl-1,4-dioxane-2,5-dione
Heat Capacity 298.15 K, C_p=184.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 430 K.
Entropy 298.15 K, S=213.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 397.5 K, ΔH=24700 J·mol^{-1}
ΔS=62.2 J·mol^{-1}·K^{-1}
Molecular Weight 144.1268
Wiswesser Line Notation T6OV DOVTJ C1 F1
Evaluation A

$C_6H_8O_4$ (c) 82KUL/LEB2
Lactide(DL); 3,6-Dimethyl-1,4-dioxane-2,5-dione
Heat Capacity 298.15 K, C_p=184.3 J·mol^{-1}·K^{-1}
Temperature range 8 to 430 K.
Entropy 298.15 K, S=213.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 397 K
Molecular Weight 144.1268
Wiswesser Line Notation T6OV DOVTJ C1 F1
Evaluation A
T(glass)=277 K.

$C_6H_8O_4$ (c) 82LEB/KUL
Lactide(DL); 3,6-Dimethyl-1,4-dioxane-2,5-dione
Heat Capacity 298.15 K, C_p=184.3 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=213.1 J·mol^{-1}·K^{-1}
Molecular Weight 144.1268
Wiswesser Line Notation T6OV DOVTJ C1 F1
Evaluation A

$(C_6H_8O_4)_n$ (gls) 82KUL/LEB2
Polylactide(DL)
Heat Capacity 298.15 K, C_p=264.8 J·mol^{-1}·K^{-1}
Temperature range 8 to 360 K. High-elastic state.
Entropy 298.15 K, S=244.4 J·mol^{-1}·K^{-1}
High-elastic state.
Molecular Weight 144.1268
Wiswesser Line Notation /*VY1&OVY1&O*/
Evaluation A
T(glass)=277 K.

$C_6H_8O_7$ (c) 82DEK/VAN
Citric acid
Heat Capacity 300 K, C_p=226.51 J·mol^{-1}·K^{-1}
Temperature range 90 to 330 K.
Entropy 300 K, S=252.1 J·mol^{-1}·K^{-1}
Molecular Weight 192.1250
Wiswesser Line Notation QV1XQVQ1VQ
Evaluation B(C_p), C(S)

$C_6H_8O_7 \cdot H_2O$ (c) 62EVA/HOA
Citric acid monohydrate
Heat Capacity 298.15 K, C_p=268.1 J·mol^{-1}·K^{-1}
Temperature range 21 to 303 K.
Entropy 298.15 K, S=283.5 J·mol^{-1}·K^{-1}
Molecular Weight 210.1402
Wiswesser Line Notation QV1XQVQ1VQ &QH
Evaluation A

C_6H_8S (liq) 65CAR/WES
2,5-Dimethylthiophene
Heat Capacity 298.15 K, C_p=178.32 J·mol^{-1}·K^{-1}
Temperature range 5 to 305 K.
Entropy 298.15 K, S=244.72 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 210.58 K, ΔH=8191.0 J·mol^{-1}
ΔS=38.90 J·mol^{-1}·K^{-1}
c,II/liq 204.87 K, ΔH=7401.1 J·mol^{-1}
ΔS=36.12 J·mol^{-1}·K^{-1}
Metastable crystals. Note error in table on ΔH_m and T_m.
Molecular Weight 112.1892
Wiswesser Line Notation T5SJ B1 E1
Evaluation A

$C_6H_9ClO_2$ (liq) 85KAR/ABD2
Chloroethyl methacrylate
Phase Changes
c/liq 235.1 K, ΔH=17001 J·mol^{-1}
ΔS=72.3 J·mol^{-1}·K^{-1}
Molecular Weight 148.5889
Wiswesser Line Notation G2OVY1&U1
Evaluation A

C_6H_9Cu (c) 81LEB/BYK
1-Hexynylcopper; Copper butylacetylenide
Heat Capacity 298.15 K, C_p=160.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=180.6 J·mol^{-1}·K^{-1}
Molecular Weight 144.6831
Wiswesser Line Notation -CU-1UU5
Evaluation A

C_6H_9Cu (c) 82BYK/LEB
1-Hexynylcopper; Copper butylacetylenide
Heat Capacity 298.15 K, C_p=160.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=178.3 J·mol^{-1}·K^{-1}
Molecular Weight 144.6831
Wiswesser Line Notation -CU-1UU5
Evaluation A

C_6H_9N (liq) 71HAL/BAL
Cyclopentyl cyanide; Cyanocyclopentane
Heat Capacity 297 K, C_p=167.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 95.1438
Wiswesser Line Notation L5TJ ACN
Evaluation C

C_6H_9N (liq) 86STE/CHI
2,4-Dimethylpyrrole
Heat Capacity 298.15 K, C_p=192.19 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S=222.01 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 268.435 K
Molecular Weight 95.1438
Wiswesser Line Notation T5MJ B1 D1
Evaluation A

C_6H_9N (liq) 86STE/CHI
2,5-Dimethylpyrrole
Heat Capacity 298.15 K, C_p=195.30 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=212.13 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 280.904 K
Molecular Weight 95.1438
Wiswesser Line Notation T5MJ B1 E1
Evaluation A

C_6H_9N (liq) 87MES/TOD
2,5-Dimethylpyrrole
Heat Capacity 298.15 K, C_p=195.30 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=212.13 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 280.904 K, ΔH=9296.0 J·mol^{-1}
ΔS=33.09 J·mol^{-1}·K^{-1}
Molecular Weight 95.1438
Wiswesser Line Notation T5MJ B1 E1
Evaluation A

C_6H_9N (liq) 88MES/TOD
2,5-Dimethylpyrrole
Heat Capacity 298.150 K, C_p=195.297 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S=212.242 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 280.904 K, ΔH=9298.42 J·mol^{-1}
ΔS=33.10 J·mol^{-1}·K^{-1}
Molecular Weight 95.1438
Wiswesser Line Notation T5MJ B1 E1
Evaluation A

$C_6H_9N_3O_3$ (c) 89IMA/TAK
Trimethyl cyanurate
Heat Capacity 298.15 K, C_p=207 J·mol^{-1}·K^{-1}
One temperature, estimated.
Phase Changes
c/g 298.15 K, ΔH=90330 J·mol^{-1}
ΔS=303.0 J·mol^{-1}·K^{-1}
Molecular Weight 171.1554
Wiswesser Line Notation T6N CN ENJ BO1 DO1 FO1
Evaluation B

$C_6H_9O_6Sc$ (c) 92OHT/MAT
Scandium ethanoate
Heat Capacity 298.15 K, C_p=229.89 J·mol^{-1}·K^{-1}
Temperature range 11 to 300 K.
Entropy 298.15 K, S=322.27 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 59.0 K, ΔH=213 J·mol^{-1}
ΔS=3.70 J·mol^{-1}·K^{-1}
First-order transition.
c,II/c,I 167.0 K, ΔH=536 J·mol^{-1}
ΔS=3.81 J·mol^{-1}·K^{-1}
Higher-order transition
Molecular Weight 222.0894
Wiswesser Line Notation OV1 3 &-SC-
Evaluation A

C_6H_{10} (liq) 1881REI
1,5-Hexadiene; Diallyl
Heat Capacity 298 K, C_p=133.1 J·mol^{-1}·K^{-1}
Temperature range 291 to 328 K.
Molecular Weight 82.1450
Wiswesser Line Notation 1U4U1
Evaluation D

C_6H_{10} (liq) 79FUC/PEA
1-Methylcyclopentene
Heat Capacity 298.15 K, C_p=153.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 82.1450
Wiswesser Line Notation L5UTJ A1
Evaluation B

C_6H_{10} (liq) 79FUC/PEA
3-Methylcyclopentene
Heat Capacity 298.15 K, C_p=152.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 82.1450
Wiswesser Line Notation L5UTJ C1
Evaluation B

C_6H_{10} (liq) 30PAR/HUF2
Cyclohexene
Heat Capacity 293.2 K, C_p=145.6 J·mol^{-1}·K^{-1}
Temperature range 92 to 293 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=216.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 49.20 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 138.7 K, ΔH=4075 J·mol^{-1}
ΔS=29.38 J·mol^{-1}·K^{-1}
c,I/liq 169.0 K, ΔH=3289 J·mol^{-1}
ΔS=19.46 J·mol^{-1}·K^{-1}
Molecular Weight 82.1450
Wiswesser Line Notation L6UTJ
Evaluation B(C_p),C(S)

C_6H_{10} (liq) 48HUF/EAT
Cyclohexene
Heat Capacity 298.15 K, C_p=149.16 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=216.19 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 138.7 K, ΔH=4250.5 J·mol^{-1}
ΔS=30.65 J·mol^{-1}·K^{-1}
c,I/liq 169.67 K, ΔH=3293.2 J·mol^{-1}
ΔS=19.41 J·mol^{-1}·K^{-1}
Molecular Weight 82.1450
Wiswesser Line Notation L6UTJ
Evaluation A

C_6H_{10} (liq) 77HAI/SUG2
Cyclohexene
Heat Capacity 298.15 K, C_p=148.35 J·mol^{-1}·K^{-1}
Temperature range 15 to 293 K.
Entropy 298.15 K, S=214.60 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,I 112.3 K, ΔH=1483 J·mol^{-1}
ΔS=13.2 J·mol^{-1}·K^{-1}
c,II/c,I 138.63 K, ΔH=4231 J·mol^{-1}
ΔS=30.52 J·mol^{-1}·K^{-1}
c,I/liq 169.66 K, ΔH=3284 J·mol^{-1}
ΔS=19.36 J·mol^{-1}·K^{-1}
Molecular Weight 82.1450
Wiswesser Line Notation L6UTJ
Evaluation A

C_6H_{10} (liq) 88KAL/WOY
Cyclohexene
Heat Capacity 298.12 K, C_p=152.90 J·mol^{-1}·K^{-1}
Temperature range 183 to 298 K. Unsmoothed experimental datum.
Molecular Weight 82.1450
Wiswesser Line Notation L6UTJ
Evaluation B

C_6H_{10} (liq) 93STE/CHI2
Cyclohexene
Heat Capacity 298.15 K, C_p=148.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 82.1450
Wiswesser Line Notation L6UTJ
Evaluation A

$(C_6H_{10})_n$ (c) 88LEB/SMI
Ethylene-butadiene copolymer
Heat Capacity 298.15 K, C_p=148.8 J·mol^{-1}·K^{-1}
Temperature range 30 to 330 K.
Entropy 298.15 K, S=148.9 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 199 K
Glass transition.
c/liq 333 K
Molecular Weight 82.1450
Wiswesser Line Notation /*2*/ &/*1U2U1*/
Evaluation A

$C_6H_{10}ClN_3O_2$ (c) 63COL/HUT2
Histidine hydrochloride(L)
Heat Capacity 298.15 K, C_p=249.53 J·mol^{-1}·K^{-1}
Temperature range 11 to 305 K.
Entropy 298.15 K, S=276.10 J·mol^{-1}·K^{-1}
Molecular Weight 191.6169
Wiswesser Line Notation T5M DNJ B1YZVQ *GH -L
Evaluation A

$C_6H_{10}N_2O$ (liq) 80BYS
2,3-Diazabicyclo[2.2.2]oct-2-ene N-oxide
Phase Changes
c,III/c,II 359.2 K, ΔH=5020 J·mol^{-1}
ΔS=14.0 J·mol^{-1}·K^{-1}
c,II/c,I 399.3 K, ΔH=8050 J·mol^{-1}
ΔS=20.2 J·mol^{-1}·K^{-1}
c,I/liq 437.9 K, ΔH=3840 J·mol^{-1}
ΔS=8.77 J·mol^{-1}·K^{-1}
Molecular Weight 126.1582
Wiswesser Line Notation T66 A B DNUNTJ DUO
Evaluation A

$C_6H_{10}O$ (liq) 1881REI
4-Methylpenten-3-one-2; Mesityl oxide
Heat Capacity 298 K, C_p=187.9 J·mol^{-1}·K^{-1}
Temperature range 290 to 415 K.
Molecular Weight 98.1444
Wiswesser Line Notation 1Y1&U1V1
Evaluation D

$C_6H_{10}O$ (liq) 24HER/BLO
Cyclohexanone
Heat Capacity 290 K, C_p=177.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.1444
Wiswesser Line Notation L6VTJ
Evaluation C

$C_6H_{10}O$ (liq) 39PHI
Cyclohexanone
Heat Capacity 304.2 K, C_p=200.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.1444
Wiswesser Line Notation L6VTJ
Evaluation C

$C_6H_{10}O$ (liq) 80NAK/SUG
Cyclohexanone
Heat Capacity 300 K, C_p=177.20 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Unsmoothed experimental datum for C_p at 296.40 K is 175.96 J·mol^{-1}·K^{-1}.
Entropy 300 K, S=229.03 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 220.83 K, ΔH=8659.6 J·mol^{-1}
ΔS=39.22 J·mol^{-1}·K^{-1}
c,I/liq 245.21 K, ΔH=1327.6 J·mol^{-1}
ΔS=5.414 J·mol^{-1}·K^{-1}
Molecular Weight 98.1444
Wiswesser Line Notation L6VTJ
Evaluation A

$C_6H_{10}O$ (liq) 92SVO/KUB
Cyclohexanone
Phase Changes
liq/g 428.8 K, ΔH=45130 J·mol^{-1}
Value corrected to 298.15 K.
Molecular Weight 98.1444
Wiswesser Line Notation L6VTJ
Evaluation A

$C_6H_{10}O$ (liq) 90MAY/RAC
Cyclohexanol; Cyclohexyl alcohol
Heat Capacity 298.15 K, C_p=214.06 J·mol^{-1}·K^{-1}
Temperature range 170 to 320 K. C_p(liq)=−2223.2606 +22.0059595T−0.0691686793T^2+0.0000763592T^3 J·mol^{-1}K^{-1} (298 to 320 K). C_p value calculated from equation.
Phase Changes
c,III/c,II 220.9 K, ΔH=378.4 J·mol^{-1}
ΔS=1.713 J·mol^{-1}·K^{-1}
c,III/c,I 244.5 K, ΔH=8620 J·mol^{-1}
ΔS=35.3 J·mol^{-1}·K^{-1}
c,II/c,I 264.86 K, ΔH=8662 J·mol^{-1}
ΔS=32.70 J·mol^{-1}·K^{-1}
c,I/liq 297.92 K, ΔH=1806 J·mol^{-1}
ΔS=6.06 J·mol^{-1}·K^{-1}
Molecular Weight 98.1444
Wiswesser Line Notation L6TJ AQ
Evaluation A

$C_6H_{10}O$ (liq) 80NAK/SU(
Cyclohexene oxide
Heat Capacity 300 K, C_p=166.12 J·mol^{-1}·K^{-}
Temperature range 13 to 300 K. Unsmoothed experimental datur for C_p at 296.96 K is 164.98 J·mol^{-1}·K^{-1}.
Entropy 300 K, S=221.98 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 193.10 K, ΔH=9535.1 J·mol^{-1}
ΔS=49.39 J·mol^{-1}·K^{-1}
c,I/liq 238.14 K, ΔH=1064.5 J·mol^{-1}
ΔS=4.470 J·mol^{-1}·K^{-1}
Molecular Weight 98.1444
Wiswesser Line Notation T36 BOTJ
Evaluation A

$C_6H_{10}O_2$ (liq) 79FU(
Ethyl cyclopropanecarboxylate
Heat Capacity 298.15 K, C_p=213.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.1438
Wiswesser Line Notation L3TJ AVO2
Evaluation B

$C_6H_{10}O_2$ (liq) 71HAL/BAI
Methyl cyclobutanecarboxylate
Heat Capacity 297 K, C_p=190.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.1438
Wiswesser Line Notation L4TJ AVO1
Evaluation D

$C_6H_{10}O_2$ (liq) 78LEB/YEV
ϵ-Caprolactone
Heat Capacity 298.15 K, C_p=196.8 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 350 K.
Entropy 298.15 K, S=235.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 271.83 K, ΔH=13820 J·mol^{-1}
ΔS=50.9 J·mol^{-1}·K^{-1}
Molecular Weight 114.1438
Wiswesser Line Notation T7OVTJ
Evaluation A

$C_6H_{10}O_2$ (liq) 83LEB/YE\
ϵ-Caprolactone
Heat Capacity 298.15 K, C_p=196.8 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 340 K.
Entropy 298.15 K, S=235.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 272.13 K, ΔH=13820 J·mol^{-1}
ΔS=50.9 J·mol^{-1}·K^{-1}
Molecular Weight 114.1438
Wiswesser Line Notation T7OVTJ
Evaluation A

$(C_6H_{10}O_2)_n$ (c) 78LEB/YEV
Poly-ϵ-caprolactone
Heat Capacity 298.15 K, C_p=161.6 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 350 K.
Entropy 298.15 K, S=181.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 336 K, ΔH=16400 J·mol^{-1}
ΔS=48.0 J·mol^{-1}·K^{-1}
Molecular Weight 114.1438
Wiswesser Line Notation /*OV5*/
Evaluation A
T(glass)=209 K.

$C_6H_{10}O_3$ (liq) 1881REI
Ethyl acetoacetate; Acetoacetic ester
Heat Capacity 298 K, C_p=241.8 J·mol^{-1}·K^{-1}
Temperature range 288 to 455 K.
Molecular Weight 130.1432
Wiswesser Line Notation 2OV1V1
Evaluation D

$C_6H_{10}O_3$ (liq) 33KOL/UDO
Ethyl acetoacetate; Acetoacetic ester
Heat Capacity 297.5 K, C_p=246.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.1432
Wiswesser Line Notation 2OV1V1
Evaluation C

$C_6H_{10}O_3$ (liq) 34KOL/UDO2
Ethyl acetoacetate; Acetoacetic ester
Heat Capacity 297.5 K, C_p=250.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.1432
Wiswesser Line Notation 2OV1V1
Evaluation C

$C_6H_{10}O_4$ (liq) 92VER/BEC
Methylmalonic acid dimethyl ester
Heat Capacity 298.15 K, C_p=261.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 146.1426
Wiswesser Line Notation 1OVY1&VO1
Evaluation B

$C_6H_{10}O_4$ (liq) 83SAN/CIO
Ethylene glycol diacetate
Heat Capacity 298.15 K, C_p=310 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K. C_p°(kJ·kg^{-1}·K^{-1}) =0.044175T−11.049.
Molecular Weight 146.1426
Wiswesser Line Notation 1VO2OV1
Evaluation D

$C_6H_{10}O_4$ (liq) 86NIL/WAD
Ethylene glycol diacetate
Heat Capacity 298.15 K, C_p=269.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 146.1426
Wiswesser Line Notation 1VO2OV1
Evaluation A

$C_6H_{10}O_4$ (liq) 1881REI
Diethyl ethanedioate; Diethyl oxalate
Heat Capacity 298 K, C_p=260.7 J·mol^{-1}·K^{-1}
Temperature range 294 to 472 K.
Molecular Weight 146.1426
Wiswesser Line Notation 2OVVO2
Evaluation D

$C_6H_{10}O_4$ (c) 74CIN/BER
Adipic acid; 1,6-Hexanedioic acid
Phase Changes
c/liq 425.5 K, ΔH=34852 J·mol^{-1}
ΔS=81.92 J·mol^{-1}·K^{-1}
Molecular Weight 146.1426
Wiswesser Line Notation QV4VQ
Evaluation B

$C_6H_{10}O_4$ (c) 84VAS/PET
Adipic acid; 1,6-Hexanedioic acid
Heat Capacity 298.15 K, C_p=196.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 450 K.
Entropy 298.15 K, S=219.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 424.7 K
Molecular Weight 146.1426
Wiswesser Line Notation QV4VQ
Evaluation A

$C_6H_{10}O_4S_2$ (c) 35HUF/ELL
4,5-Dithia-1,8-octanedioic acid; β,β'-Dithiodilactic acid
Heat Capacity 296.8 K, C_p=239.3 J·mol^{-1}·K^{-1}
Temperature range 85 to 305 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=274.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 84.43 J·mol^{-1}·K^{-1}.
Molecular Weight 210.2626
Wiswesser Line Notation QV2SS2VQ
Evaluation B(C_p),C(S)

$C_6H_8O_7·H_2O$ (c) 82DEK/VAN
Citric acid monohydrate
Heat Capacity 300 K, C_p=269.52 J·mol^{-1}·K^{-1}
Temperature range 120 to 300 K.
Entropy 300 K, S=285.32 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 312.1 K, ΔH=14980 J·mol^{-1}
ΔS=48.0 J·mol^{-1}·K^{-1}
Molecular Weight 210.1402
Wiswesser Line Notation QV1XQVQ1VQ &QH
Evaluation B

$C_6H_{11}Br$ (liq) 93SHE
Bromocyclohexane; Cyclohexyl bromide
Heat Capacity 298.15 K, C_p=182.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 163.0569
Wiswesser Line Notation L6TJ AE
Evaluation B

$C_6H_{11}LiO_2$ (c) 85FRA/WES
Lithium n-hexanoate
Heat Capacity 298.15 K, C_p=217.01 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=229.81 J·mol^{-1}·K^{-1}
Molecular Weight 122.0927
Wiswesser Line Notation OV5 .LI
Evaluation A
A gradual thermodynamic transformation starts at 120 and 260 K, respectively.

$C_6H_{11}LiO_2$ (c) 86NGE/WES
Lithium n-hexanoate
Heat Capacity 298.15 K, C_p=216.01 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=228.48 J·mol^{-1}·K^{-1}
Molecular Weight 122.0927
Wiswesser Line Notation OV5 .LI
Evaluation A

$C_6H_{11}NO$ (c) 91KOZ/SHE
Cyclohexanone oxime
Heat Capacity 298.15 K, C_p=199.34 J·mol^{-1}·K^{-1}
Temperature range 6 to 430 K. C_p(c,J/mol·K)=−143.81 +1.6984T−1.8334×10^{-3}×T^2 (300 to 340 K); C_p(liq,J/mol·K) =214.30+0.1900T (380 to 430 K).
Entropy 298.15 K, S=185.12 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 240.8 K, ΔH=14.0 J·mol^{-1}
ΔS=0.06 J·mol^{-1}·K^{-1}
c,II/c,I 273.4 K, ΔH=93.7 J·mol^{-1}
ΔS=0.34 J·mol^{-1}·K^{-1}
c,I/liq 362.5 K, ΔH=12700 J·mol^{-1}
Molecular Weight 113.1590
Wiswesser Line Notation L6TJ ANO
Evaluation A

$C_6H_{11}NO$ (c) 92KOZ/KAB
Cyclohexanone oxime
Heat Capacity 298.15 K, C_p=199.38 J·mol^{-1}·K^{-1}
Temperature range 6 to 450 K. C_p(c, 300 to 340 K)= 143.81 +1.6984(T/K)−1.8334×10^{-3}(T/K)^2; CP(liq, 380 to 430 K) =214.30+0.1900(T/K) J/K·mol.
Entropy 298.15 K, S=185.08 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 240.8 K, ΔH=14.0 J·mol^{-1}
ΔS=0.06 J·mol^{-1}·K^{-1}
c,II/c,I 273.4 K, ΔH=93.7 J·mol^{-1}
ΔS=0.34 J·mol^{-1}·K^{-1}
c,I/liq 362.5 K, ΔH=12700 J·mol^{-1}
c,I/g 353.7 K, ΔH=74010 J·mol^{-1}
liq/g 367.8 K, ΔH=58660 J·mol^{-1}
Molecular Weight 113.1590
Wiswesser Line Notation L6YTJ AUNQ
Evaluation A

$C_6H_{11}NO$ (c) 57MAS
ε-Caprolactam; 6-Caprolactam
Phase Changes
c/liq 342.36 K, ΔH=16134 J·mol^{-1}
Molecular Weight 113.1590
Wiswesser Line Notation T7MVTJ
Evaluation A

$C_6H_{11}NO$ (c) 59KOL/PAU
ε-Caprolactam; 6-Caprolactam
Heat Capacity 300 K, C_p=158.1 J·mol^{-1}·K^{-1}
Temperature range 60 to 370 K.
Entropy 298.15 K, S=168.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 342.305 K, ΔH=16096 J·mol^{-1}
ΔS=47.0 J·mol^{-1}·K^{-1}
Molecular Weight 113.1590
Wiswesser Line Notation T7MVTJ
Evaluation B

$C_6H_{11}NO$ (c) 59PAU/KOL
ε-Caprolactam; 6-Caprolactam
Heat Capacity 298.15 K, C_p=156.77 J·mol^{-1}·K^{-1}
Temperature range 60 to 373 K.
Entropy 298.15 K, S=168.6 J·mol^{-1}·K^{-1}
Debye-Einstein extrapolation below 60 K.
Molecular Weight 113.1590
Wiswesser Line Notation T7MVTJ
Evaluation B

$C_6H_{11}NO$ (c) 62KOL/PA
ε-Caprolactam; 6-Caprolactam
Heat Capacity 300.00 K, C_p=156.3 J·mol^{-1}·K^{-1}
Temperature range 60 to 350 K.
Entropy 298.15 K, S=168.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 342.305 K, ΔH=16096 J·mol^{-1}
ΔS=47.0 J·mol^{-1}·K^{-1}
Molecular Weight 113.1590
Wiswesser Line Notation T7MVTJ
Evaluation B

$C_6H_{11}NO$ (liq) 91KOZ/SH
ε-Caprolactam; 6-Caprolactam
Heat Capacity
Temperature range 340 to 520 K. C_p(liq)=323.08+0.0342 −1.1074 ×10^{-7}T^2 J/mol·K (340 to 520 K).
Molecular Weight 113.1590
Wiswesser Line Notation T7MVTJ
Evaluation A

$C_6H_{11}NO$ (c) 92KAB/KO
ε-Caprolactam; 6-Caprolactam
Heat Capacity 298.15 K, C_p=156.78 J·mol^{-1}·K^{-}
Temperature range 5 to 550 K. C_p(liq)=323.08 +0.0342(T K)−1.1074 ×10^{-7}(T/K)^2 J/K·mol (340 to 520 K).
Entropy 298.15 K, S=173.21 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 342.305 K, ΔH=16096 J·mol^{-1}
liq/g 298.15 K, ΔH=87260 J·mol^{-1}
Molecular Weight 113.1590
Wiswesser Line Notation T7MVTJ
Evaluation A

$(C_6H_{11}NO)_n$ (c) 55MAR/SM
Poly-ε-caprolactam
Heat Capacity 298.15 K, C_p=171.6 J·mol^{-1}·K^{-1}
Temperature range 270 to 498 K. C_p(c)=0.325+1.5×10^{-3}T ca ·g^{-1}·deg^{-1} (−10 to 225 °C). C_p value calculated from equation
Phase Changes
c/liq 498 K, ΔH=21220 J·mol^{-1}
ΔS=42.61 J·mol^{-1}·K^{-}
Molecular Weight 113.1567
Wiswesser Line Notation /*MV5*/
Evaluation A
C_p(liq)=0.577+3.36×10^{-3}T cal·g^{-1}deg^{-1} (above 225 °C).

$(C_6H_{11}NO)_n$ (c) 62KOL/PA
Poly-ε-caprolactam
Heat Capacity 298.15 K, C_p=169.7 J·mol^{-1}·K^{-1}
Temperature range 60 to 350 K.
Entropy 298.15 K, S=173.0 J·mol^{-1}·K^{-1}
Molecular Weight 113.1567
Wiswesser Line Notation /*MV5*/
Evaluation B

$(C_6H_{11}NO)_n$ (c) 91RO
Poly-L-leucine
Heat Capacity 300 K, C_p=175.8 J·mol^{-1}·K^{-}
Temperature range 220 to 390 K.
Molecular Weight 113.1590
Wiswesser Line Notation /*VYM*&1Y1&1/ -L
Evaluation B

$(C_6H_{11}NO)_n$ (c) 93ROL/XEN
Poly-L-leucine
Heat Capacity 300 K, C_p=175.8 J·mol^{-1}·K^{-1}
Temperature range 2220 to 390 K.
Molecular Weight 113.1590
Wiswesser Line Notation /*VYM*&1Y1&1/ -L
Evaluation B

$C_6H_{11}NO_2$ (liq) 83GEI/KAR
1,1-Dimethoxy-3-cyanopropane; Dimethyl acetal of β-cyanopropionaldehyde
Heat Capacity 298.15 K, C_p=253.63 J·mol^{-1}·K^{-1}
Temperature range 55 to 300 K.
Entropy 298.15 K, S=295.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 154 K
Glassy (solid) to liquid transition.
Molecular Weight 129.1584
Wiswesser Line Notation NC2YO1&O1
Evaluation A

$C_6H_{11}N_3O_4$ (c) 90BAD/KUL
Triglycine
Heat Capacity 298 K, C_p=216 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 189.1706
Wiswesser Line Notation Z1VM1VM1VQ
Evaluation D

$C_6H_{11}N_3O_4$ (c) 89KUL/KOZ
Diglycylglycine
Heat Capacity 298 K, C_p=215.5 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 189.1706
Wiswesser Line Notation Z1VNV1Z1VQ
Evaluation C

$C_6H_{11}O_2Tl$ (c) 76MEI/SEY
Thallium hexanoate
Phase Changes
c,III/c,II 395 K, ΔH=179 J·mol^{-1}; ΔS=0.46 J·mol^{-1}·K^{-1}
c,II/c,I 412 K, ΔH=1841 J·mol^{-1}; ΔS=1.84 J·mol^{-1}·K^{-1}
c,I/liq 418 K, ΔH=4477 J·mol^{-1}; ΔS=10.9 J·mol^{-1}·K^{-1}
Solid-mesophase.
liq/liq 500 K, ΔH=3035 J·mol^{-1}; ΔS=6.69 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
Molecular Weight 319.5217
Wiswesser Line Notation OV5 .TL
Evaluation B

$C_6H_{11}O_2Tl$ (c) 84FER/LOP
Thallium hexanoate
Heat Capacity 320 K, C_p=235 J·mol^{-1}·K^{-1}
Temperature range 320 to 480 K.
Phase Changes
c,III/c,II 397.9 K, ΔH=208 J·mol^{-1}; ΔS=0.50 J·mol^{-1}·K^{-1}
c,II/c,I 415.0 K, ΔH=657 J·mol^{-1}; ΔS=1.58 J·mol^{-1}·K^{-1}
c,I/liq 425.0 K, ΔH=4598 J·mol^{-1}; ΔS=10.8 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 319.5217
Wiswesser Line Notation OV5 .TL
Evaluation A
Mesophase to isotropic liquid phase change data also given: T=499.8 K; $\Delta\Delta H$=3941 J·mol^{-1}; $\Delta\Delta S$=7.90 J·mol^{-1}·K^{-1}.

$C_6H_{11}O_2Tl$ (c) 85BOE/LOP
Thallium hexanoate
Heat Capacity 298.15 K, C_p=234.96 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S=324.76 J·mol^{-1}·K^{-1}
Phase Changes
c,V/c,IV 203.5 K, ΔH=1734 J·mol^{-1}; ΔS=8.62 J·mol^{-1}·K^{-1}
c,IV/c,III 280.3 K, ΔH=2511 J·mol^{-1}; ΔS=8.88 J·mol^{-1}·K^{-1}
c,III/c,II 397.9 K
c,II/c,I 415.0 K
c,I/liq 425.0 K
Solid-mesomorphic liquid.
Molecular Weight 319.5217
Wiswesser Line Notation OV5 .TL
Evaluation A
Mesomorphic liquid-isotropic liquid transition at 499.8 K. See 84FER/LOP, 81LIN/DIE, and 76MEI/SEY for transition data.

C_6H_{12} (liq) 38KEN/SHO
3,3-Dimethyl-1-butene; tert-Butylethylene
Heat Capacity 295.9 K, C_p=188.28 J·mol^{-1}·K^{-1}
Temperature range 80 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=156.5 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 47.66 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 124.9 K, ΔH=4347 J·mol^{-1}; ΔS=34.80 J·mol^{-1}·K^{-1}
c,II/liq 158.4 K, ΔH=1096 J·mol^{-1}; ΔS=6.92 J·mol^{-1}·K^{-1}
Molecular Weight 84.1608
Wiswesser Line Notation 1X1&1&1U1
Evaluation B(C_p),C(S)

C_6H_{12} (liq) 36PAR/TOD2
2,3-Dimethyl-2-butene; Tetramethylethylene
Heat Capacity 295.5 K, C_p=175.73 J·mol^{-1}·K^{-1}
Temperature range 83 to 296 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=272.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 58.45 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 196.6 K, ΔH=4577 J·mol^{-1}; ΔS=23.28 J·mol^{-1}·K^{-1}
c,I/liq 198.5 K, ΔH=5460 J·mol^{-1}; ΔS=27.51 J·mol^{-1}·K^{-1}
Molecular Weight 84.1608
Wiswesser Line Notation 1Y1&UY1&1
Evaluation B(C_p),C(S)

C_6H_{12} (liq) 55SCO/FIN

2,3-Dimethyl-2-butene; Tetramethylethylene

Heat Capacity	298.15 K,	C_p=174.68 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.		
Entropy	298.15 K,	S=270.20 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/c,I	196.82 K,	ΔH=3531 J·mol^{-1}
		ΔS=17.94 J·mol^{-1}·K^{-1}
c,I/liq	198.92 K,	ΔH=6452 J·mol^{-1}
		ΔS=32.44 J·mol^{-1}·K^{-1}

Enthalpies of transition and fusion calculated from total enthalpy change 196.82 to 198.92 K and assumed C_p of 150 J·mol^{-1}·K^{-1} for c,I.

Molecular Weight 84.1608

Wiswesser Line Notation 1Y1&UY1&1

Evaluation A

C_6H_{12} (liq) 90MES/TOD

cis-2-Hexene

Heat Capacity	298.15 K,	C_p=178.36 J·mol^{-1}·K^{-1}
Temperature range 10 to 330 K.		
Entropy	298.15 K,	S=291.86 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	132.030 K,	ΔH=8878.23 J·mol^{-1}
		ΔS=67.24 J·mol^{-1}·K^{-1}

Molecular Weight 84.1608

Wiswesser Line Notation 4U2 -C

Evaluation A

C_6H_{12} (liq) 57MCC/FIN2

1-Hexene

Heat Capacity	298.15 K,	C_p=183.30 J·mol^{-1}·K^{-1}
Temperature range 11 to 360 K.		
Entropy	298.15 K,	S=295.18 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	133.39 K,	ΔH=9347 J·mol^{-1}
		ΔS=70.07 J·mol^{-1}·K^{-1}

Molecular Weight 84.1608

Wiswesser Line Notation 5U1

Evaluation A

C_6H_{12} (liq) 85KAL/WOY

1-Hexene

Heat Capacity	298.56 K,	C_p=182.77 J·mol^{-1}·K^{-1}
Temperature range 180 to 300 K. Value is unsmoothed experimental datum.		

Molecular Weight 84.1608

Wiswesser Line Notation 5U1

Evaluation B

C_6H_{12} (liq) 31HUF/PAR

Methylcyclopentane

Heat Capacity	295.7 K,	C_p=157.3 J·mol^{-1}·K^{-1}
Temperature range 92 to 294 K. Value is unsmoothed experimental datum.		
Entropy	298.1 K,	S=247.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 57.86 J·mol^{-1}·K^{-1}.		
Phase Changes		
c/liq	130.1 K,	ΔH=6883 J·mol^{-1}
		ΔS=52.9 J·mol^{-1}·K^{-1}

Molecular Weight 84.1608

Wiswesser Line Notation L5TJ A1

Evaluation B(C_p),C(S)

C_6H_{12} (liq) 46DOU/HUF

Methylcyclopentane

Heat Capacity	298.15 K,	C_p=158.70 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.		
Entropy	298.15 K,	S=247.78 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	130.73 K,	ΔH=6928.7 J·mol^{-1}
		ΔS=53.00 J·mol^{-1}·K^{-1}

Molecular Weight 84.1608

Wiswesser Line Notation L5TJ A1

Evaluation A

C_6H_{12} (liq) 51CON/SAC

Methylcyclopentane

Heat Capacity	299.8 K,	C_p=159.12 J·mol^{-1}·K^{-1}
Temperature range 80 to 200 °F.		

Molecular Weight 84.1608

Wiswesser Line Notation L5TJ A1

Evaluation B

C_6H_{12} (liq) 83SID/SVE

Methylcyclopentane

Heat Capacity	293.15 K,	C_p=157.66 J·mol^{-1}·K^{-1}
One temperature.		

Molecular Weight 84.1608

Wiswesser Line Notation L5TJ A1

Evaluation B

C_6H_{12} (liq) 19DEJ

Cyclohexane

Heat Capacity	298 K,	C_p=176.1 J·mol^{-1}·K^{-1}
Temperature range 22 to 50 °C.		

Molecular Weight 84.1608

Wiswesser Line Notation L6TJ

Evaluation B

C_6H_{12} (liq) 30PAR/HUF

Cyclohexane

Heat Capacity	298.9 K,	C_p=143.9 J·mol^{-1}·K^{-1}
Temperature range 92 to 299 K. Value is unsmoothed experimental datum.		
Entropy	298.15 K,	S=205.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 50.54 J·mol^{-1}·K^{-1}.		
Phase Changes		
c,II/c,I	185.9 K,	ΔH=6234 J·mol^{-1}
		ΔS=33.53 J·mol^{-1}·K^{-1}
c,I/liq	279.3 K,	ΔH=2423 J·mol^{-1}
		ΔS=8.68 J·mol^{-1}·K^{-1}

Molecular Weight 84.1608

Wiswesser Line Notation L6TJ

Evaluation B(C_p),C(S)

C_6H_{12} (liq) 39PH

Cyclohexane

Heat Capacity	304.2 K,	C_p=100.4 J·mol^{-1}·K^{-1}

Molecular Weight 84.1608

Wiswesser Line Notation L6TJ

Evaluation C

C_6H_{12} (liq) 42ZIE/AND
Cyclohexane
Phase Changes
c,II/c,I 186.4 K, $\Delta H = 6820$ J·mol^{-1}
$\Delta S = 36.59$ J·mol^{-1}·K^{-1}
c,I/liq 279.4 K, $\Delta H = 2728$ J·mol^{-1}
$\Delta S = 9.76$ J·mol^{-1}·K^{-1}
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 43AST/SZA
Cyclohexane
Heat Capacity 295 K, $C_p = 155.85$ J·mol^{-1}·K^{-1}
Temperature range 12 to 293 K.
Entropy 298.15 K, $S = 203.89$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 186.09 K, $\Delta H = 6686$ J·mol^{-1}
$\Delta S = 35.93$ J·mol^{-1}·K^{-1}
c,I/liq 279.84 K, $\Delta H = 2628$ J·mol^{-1}
$\Delta S = 9.39$ J·mol^{-1}·K^{-1}
liq/g 298.15 K, $\Delta H = 33334$ J·mol^{-1}
$\Delta S = 111.80$ J·mol^{-1}·K^{-1}
P = 13.18 kPa
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation A

C_6H_{12} (liq) 43RUE/HUF
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.31$ J·mol^{-1}·K^{-1}
Temperature range 13 to 302 K.
Entropy 298.15 K, $S = 204.35$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 186.1 K, $\Delta H = 6739.6$ J·mol^{-1}
$\Delta S = 36.21$ J·mol^{-1}·K^{-1}
c,I/liq 279.82 K, $\Delta H = 2676.9$ J·mol^{-1}
$\Delta S = 9.57$ J·mol^{-1}·K^{-1}
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation A

C_6H_{12} (liq) 50AUE/SAG
Cyclohexane
Heat Capacity 300 K, $C_p = 154.2$ J·mol^{-1}·K^{-1}
Temperature range 300 to 366 K. C_p given as 0.4378 Btu(lb)$^{-1}$ (°R)$^{-1}$ at 80 °F.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 60SWI/ZIE
Cyclohexane
Heat Capacity 311 K. $C_p = 155.2$ J·mol^{-1}·K^{-1}
Mean value 20 to 56 °C.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation C

C_6H_{12} (liq) 64MOE/THO
Cyclohexane
Heat Capacity 298.00 K, $C_p = 155.31$ J·mol^{-1}·K^{-1}
Temperature range 297 to 327 K.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 66NIK/RAB
Cyclohexane
Heat Capacity 298 K, $C_p = 152.93$ J·mol^{-1}·K^{-1}
Temperature range 10 to 50 °C.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 68REC
Cyclohexane
Heat Capacity 298 K, $C_p = 155.5$ J·mol^{-1}·K^{-1}
Temperature range 24 to 40 °C, equation only.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation C

C_6H_{12} (liq) 69WIL/SCH
Cyclohexane
Heat Capacity 298.15 K, $C_p = 155.2$ J·mol^{-1}·K^{-1}
Temperature 20, 30, and 40 °C.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 73SUB/RAS
Cyclohexane
Heat Capacity 298.15 K, $C_p = 159.6$ J·mol^{-1}·K^{-1}
Temperature range 298 to 323 K.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 74WIL/ZET
Cyclohexane
Heat Capacity 293.15 K, $C_p = 154.80$ J·mol^{-1}·K^{-1}
Temperature range 273 to 323 K.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 75JOL/BOI
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.20$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 76FOR/BEN
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.07$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 76FOR/BEN2
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.070$ J·mol^{-1}·K^{-1}
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation A
Data from 76FOR/BEN.

C_6H_{12} (liq) 77VES/SVO
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.12$ J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 78GRO/WIL
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.35$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 78SAF
Cyclohexane
Heat Capacity 298 K, $C_p = 156.7$ J·mol^{-1}·K^{-1}
Temperature range 298 to 313 K. Data calculated from equation $C_p = 1.7493 + 0.00452$ T kJ·kg^{-1}·K^{-1}.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 79FOR/DAR
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.149$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 79VES/ZAB
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.12$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 79WIL/GRO
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.4$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 82GRO/ING
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.4$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation A

C_6H_{12} (liq) 82TAI
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.0$ J·mol^{-1}·K^{-1}
Temperature range 293.15, 298.15, 303.15 K. Data at thre temperatures.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation A

C_6H_{12} (liq) 83SID/SV
Cyclohexane
Heat Capacity 293.15 K, $C_p = 154.81$ J·mol^{-1}·K^{-}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 85NKI/CH
Cyclohexane
Heat Capacity 298.15 K, $C_p = 156.5$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 85TAN/NAI
Cyclohexane
Heat Capacity 298.15 K, $C_p = 155.96$ J·mol^{-1}·K^{-}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 86JIM/RO
Cyclohexane
Heat Capacity 298.15 K, $C_p = 157.06$ J·mol^{-1}·K^{-}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 86OR
Cyclohexane
Heat Capacity 298.15 K, $C_p = 155.85$ J·mol^{-1}·K^{-}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 87KAL/KO
Cyclohexane
Heat Capacity 293.15 K, $C_p = 155.13$ J·mol^{-1}·K^{-}
Temperature range 293.15, 313.15 K.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 88SAI/TAN
Cyclohexane
Heat Capacity 298.15 K, C_p=155.96 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 88SHI/OGA2
Cyclohexane
Heat Capacity 298.15 K, C_p=154.32 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation A

C_6H_{12} (liq) 89LAI/ROD
Cyclohexane
Heat Capacity 298.15 K, C_p=156.90 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 89VOS/SLO
Cyclohexane
Heat Capacity 326.5 K, C_p=143.9 J·mol^{-1}·K^{-1}
Temperature range 326.5 to 450.0 K. Unsmoothed experimental datum.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation C

C_6H_{12} (liq) 91TRE/COS
Cyclohexane
Heat Capacity 298.15 K, C_p=156.00 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

$(C_6H_{12})_n$ (c) 67MEL/TYS
Poly(4-methyl-1-pentene)
Heat Capacity 298.15 K, C_p=145.6 J·mol^{-1}·K^{-1}
Temperature range 80 to 310 K. Values per unit formula weight.
Entropy 298.15 K, S=151.5 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 38.2 J·mol^{-1}·K^{-1}. Values do not include zero-point entropy.
Molecular Weight 84.1608
Wiswesser Line Notation /*Y1*1Y1&1/
Evaluation B(C_p),C(S)
65% crystalline, isotactic material.

$(C_6H_{12})_n$ (gls) 74LEB/LEB
1-Polyhexene
Entropy 298.15 K, S=171.3 J·mol^{-1}·K^{-1}
Deposited in VINITI, No 2118-74, 30 July 1974.
Molecular Weight 84.1608
Wiswesser Line Notation /*Y4&1*/
Evaluation A
T(glass)=215.5 K.

$C_6H_{12}BNO_3$ (c) 64CAS/STO
Triethanolamine borate
Heat Capacity 298.15 K, C_p=187.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=183.2 J·mol^{-1}·K^{-1}
Molecular Weight 156.9757
Wiswesser Line Notation T88 A B C AO DN GO HB IOTJ
Evaluation A

$C_6H_{12}BNO_3$ (c) 64CLE/WON
Triethanolamine borate
Heat Capacity 320 K, C_p=226.4 J·mol^{-1}·K^{-1}
Temperature range 320 to 525 K.
Entropy 320 K, S=216.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 466.54 K, ΔH=4774 J·mol^{-1}
ΔS=10.3 J·mol^{-1}·K^{-1}
c,I/liq 511.86 K, ΔH=24100 J·mol^{-1}
ΔS=47.11 J·mol^{-1}·K^{-1}
Molecular Weight 156.9757
Wiswesser Line Notation T88 A B C AO DN GO HB IOTJ
Evaluation A

$C_6H_{12}BrFeN_2S_4$ (c) 89YOS/SOR
Bis(N,N-dimethyldithiocarbamato) iron(III) bromide
Heat Capacity 296.421 K, C_p=294.9 J·mol^{-1}·K^{-1}
Temperature range 0.4 to 300 K. C_p value is unsmoothed experimental datum.
Phase Changes
c,III/c,II 0.837 K
Ferromagnetic/paramagnetic transition.
c,II/c,I 8.8 K, ΔH=5.77 J·mol^{-1}
ΔS=6.05 J·mol^{-1}·K^{-1}
Schottky anomaly.
Molecular Weight 376.1898
Wiswesser Line Notation SUYS&N1&1 2 .FE &E
Evaluation A
The total magnetic entropy and enthalpy in the temperature range 0.4 to 30 K are S=11.74 J·mol^{-1}·K^{-1} and 92.0 J·mol^{-1}, respectively.

$C_6H_{12}ClFeN_2S_4$ (c) 84YOS/SOR
Chlorobis(N,N-dimethyldithiocarbamate)iron(III)
Heat Capacity 300 K, C_p=299 J·mol^{-1}·K^{-1}
Temperature range 0.4 to 300 K. Data graphically only. Value estimated from graph.
Phase Changes
c,III/c,II 0.609 K
Lambda transition.
c,II/c,I 2 K
Schottky-type anomaly.
Molecular Weight 331.7142
Wiswesser Line Notation SUYS&N1&1 2 .FE &G
Evaluation A
Total magnetic entropy is 14.05 J·mol^{-1}·K^{-1}.

$C_6H_{12}Cl_2$ (liq) 85LAI/GRO
1,6-Dichlorohexane
Heat Capacity 298.15 K, C_p=239.57 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 155.0668
Wiswesser Line Notation G6G
Evaluation B

$C_6H_{12}Cl_3O_4P$ (liq) 86FAM/MAS
Tri-(2-chloroethyl) phosphate
Heat Capacity 298.15 K, C_p=396.5 J·mol^{-1}·K^{-1}
Temperature range 15 to 320 K. C_p data given for the glassy state from 0 to 170 K.
Entropy 298.15 K, S=495 J·mol^{-1}·K^{-1}
Phase Changes
gls/liq 185 K, ΔS=38.0 J·mol^{-1}·K^{-1}
Molecular Weight 285.4912
Wiswesser Line Notation OPO2G&O2G&O2G
Evaluation A

$C_6H_{12}FeIN_2S_4$ (c) 83YOS/SOR2
Iodobis(N,N-dimethyldithiocarbamato) iron (III)
Heat Capacity 298.352 K, C_p=301.9 J·mol^{-1}·K^{-1}
Temperature range 0.4 to 300 K. Unsmoothed experimental datum.
Molecular Weight 423.1657
Wiswesser Line Notation SYUS&N1&1 2 .FE &I
Evaluation A
Lambda type anomaly observed at 1.65 K; Schottky type anomaly observed at ca. 0.7 K.

$C_6H_{12}N_2$ (c) 60CHA/WES2
Triethylenediamine; 1,4 Diazabicyclo[2.2.2]octane
Heat Capacity 298.15 K, C_p=152.97 J·mol^{-1}·K^{-1}
Temperature range 5 to 353 K.
Entropy 298.15 K, S=157.61 J·mol^{-1}·K^{-1}
Molecular Weight 112.1742
Wiswesser Line Notation T66 A B CN FNTJ
Evaluation A

$C_6H_{12}N_2$ (c) 61WES
Triethylenediamine; 1,4-Diazabicyclo[2.2.2]octane
Heat Capacity 298.15 K, C_p=153.18 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K. Only value at 298.15 K given.
Entropy 298.15 K, S=157.61 J·mol^{-1}·K^{-1}
Molecular Weight 112.1742
Wiswesser Line Notation T66 A B CN FNTJ
Evaluation A
Details reported in other papers.

$C_6H_{12}N_2$ (c,II) 63TRO/WES
Triethylenediamine; 1,4-Diazabicyclo[2.2.2]octane
Heat Capacity 300 K, C_p=153.97 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c,II/c.I 351.08 K, ΔH=10560 J·mol^{-1}
ΔS=30.08 J·mol^{-1}·K^{-1}
Transformation to plastic crystalline phase.
c,I/liq 432.99 K, ΔH=7431 J·mol^{-1}
ΔS=17.16 J·mol^{-1}·K^{-1}
Molecular Weight 112.1742
Wiswesser Line Notation T66 A B CN FNTJ
Evaluation A

$C_6H_{12}N_2O_2$ (c) 91ABA/DEL
2-(Acetylamino)-N-methylpropanamide(DL);
N-Acetylalanine-N′-methylamide(DL)
Heat Capacity 298 K, C_p=196.47 J·mol^{-1}·K^{-1}
Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 144.1730
Wiswesser Line Notation 1VMYVM1&1 -DL
Evaluation C

$C_6H_{12}N_2O_2$ (c) 91ABA/DE
2-(Acetylamino)-N-methylpropanamide(L);
N-Acetylalanine-N′-methylamide(L)
Heat Capacity 298 K, C_p=201.30 J·mol^{-1}·K^{-1}
Data extrapolated to 298 K from values obtained at high temperatures.
Molecular Weight 144.1730
Wiswesser Line Notation 1VMYVM1&1 -L
Evaluation C

$C_6H_{12}N_2O_3$ (c) 89KUL/KO
β-Alanyl-β-alanine
Heat Capacity 298 K, C_p=196.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 160.1724
Wiswesser Line Notation Z2VM2VQ
Evaluation C

$C_6H_{12}N_2O_3$ (c) 90BAD/KU
β-Alanyl-β-alanine
Heat Capacity 298 K, C_p=196 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Phase Changes
c/liq 480.05 K, ΔH=58300 J·mol^{-1}
Melting with decomposition.
Molecular Weight 160.1724
Wiswesser Line Notation Z2VM2VQ
Evaluation D

$C_6H_{12}N_2O_3$ (c) 89KUL/KC
α,α-Alanylalanine(DL)
Heat Capacity 298 K, C_p=189.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 160.1724
Wiswesser Line Notation ZY1&VMY1&VQ -DL
Evaluation C

$C_6H_{12}N_2O_3$ (c) 90BAD/KU
α,α-Alanylalanine(DL)
Heat Capacity 298 K, C_p=189 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Phase Changes
c/liq 483.15 K, ΔH=33200 J·mol^{-1}
Melting with decomposition.
Temperature range 433 to 483.
Molecular Weight 160.1724
Wiswesser Line Notation ZY1&VMY1&VQ -DL
Evaluation C

$C_6H_{12}N_2O_3$ (c) 89KUL/KC
α,α-Alanylalanine(L)
Heat Capacity 298 K, C_p=194.9 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 160.1724
Wiswesser Line Notation ZY1&VMY1&VQ -L
Evaluation C

$C_6H_{12}N_2O_3$ (c) 90BAD/K
α,α-Alanylalanine(L)
Heat Capacity 298 K, C_p=195 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 160.1724
Wiswesser Line Notation ZY1&VMY1&VQ -L
Evaluation C

$C_6H_{12}N_2O_4S_2$ (c) 35HUF/ELL
Cystine(L)
Heat Capacity 297.3 K, C_p=268.6 J·mol^{-1}·K^{-1}
Temperature range 85 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=286.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 79.45 J·mol^{-1}·K^{-1}.
Molecular Weight 240.2918
Wiswesser Line Notation QVYZ1SS1YZVQ -L
Evaluation B(C_p),C(S)

$C_6H_{12}N_2O_4S_2$ (c) 64HUT/COL
Cystine(L)
Heat Capacity 298.15 K, C_p=261.92 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S=280.58 J·mol^{-1}·K^{-1}
Molecular Weight 240.2918
Wiswesser Line Notation QVYZ1SS1YZVQ -L
Evaluation A

$C_6H_{12}N_2S_3$ (c) 61GOO/LAC
Bis-(dimethylthiocarbamoyl)sulfide; Tetramethylthiuram monosulfide
Heat Capacity 298.15 K, C_p=261.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 208.3542
Wiswesser Line Notation
Evaluation B

$C_6H_{12}N_2S_4$ (c) 61GOO/LAC
Bis-(dimethylthiocarbamoyl)disulfide; Tetramethylthiuram disulfide
Heat Capacity 298.15 K, C_p=301.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 240.4142
Wiswesser Line Notation
Evaluation B

$C_6H_{12}N_4$ (c) 60CHA/WES
Hexamethylenetetramine; 1,3,5,7-Tetraazatricyclo[3.3.1.1^{3,7}]decane
Heat Capacity 298.15 K, C_p=152.29 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=163.38 J·mol^{-1}·K^{-1}
Molecular Weight 140.1876
Wiswesser Line Notation T66 B6/B-H/DI A B- C 1B I BN DN FN HNTJ
Evaluation A

$C_6H_{12}N_4$ (c) 61WES
Hexamethylenetetramine; 1,3,5,7 Tetraazatricyclo[3.3.1.1^{3,7}]decane
Heat Capacity 298.15 K, C_p=152.29 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K. Only value at 298.15 K given.
Entropy 298.15 K, S=163.38 J·mol^{-1}·K^{-1}
Molecular Weight 140.1876
Wiswesser Line Notation T66 B6/B-H/DI A B- C 1B I BN DN FN HNTJ
Evaluation A
Details reported in other papers.

$C_6H_{12}O$ (liq) 70AND/COU
3,3-Dimethyl-2-butanone; Methyl tert-butyl ketone
Heat Capacity 298.15 K, C_p=206.9 J·mol^{-1}·K^{-1}
Temperature range 10 to 360 K.
Entropy 298.15 K, S=282.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 221.74 K, ΔH=11330 J·mol^{-1}
ΔS=51.10 J·mol^{-1}·K^{-1}
Molecular Weight 100.1602
Wiswesser Line Notation 1X1&1&V1
Evaluation A

$C_6H_{12}O$ (liq) 70HAR/HEA
3,3-Dimethyl-2-butanone; Methyl tert-butyl ketone
Heat Capacity 298.15 K, C_p=207.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.1602
Wiswesser Line Notation 1X1&1&V1
Evaluation B

$C_6H_{12}O$ (liq) 92SVO/KUB
3,3-Dimethyl-2-butanone; Methyl tert-butyl ketone
Phase Changes
liq/g 441.4 K, ΔH=50780 J·mol^{-1}
Value corrected to 298.15 K.
Molecular Weight 100.1602
Wiswesser Line Notation 1X1&1&V1
Evaluation A

$C_6H_{12}O$ (liq) 47SCH/ZOS
5-Methyl-3-oxahex-1-ene; Vinyl isobutyl ether
Heat Capacity 298.15 K, C_p=231.8 J·mol^{-1}·K^{-1}
One value, no details.
Molecular Weight 100.1602
Wiswesser Line Notation 1Y1&1O1U1
Evaluation D

$C_6H_{12}O$ (liq) 89VES/BAR
4-Methyl-2-pentanone; Isobutylmethylketone
Heat Capacity 298.15 K, C_p=211.9 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K.
Molecular Weight 100.1602
Wiswesser Line Notation 1Y1&1V1
Evaluation A

$C_6H_{12}O$ (liq) 92SVO/KUB
4-Methyl-2-pentanone; Isobutylmethylketone
Phase Changes
liq/g 388.9 K, ΔH=40610 J·mol^{-1}
Value corrected to 298.15 K.
Molecular Weight 100.1602
Wiswesser Line Notation 1Y1&1V1
Evaluation A

$C_6H_{12}O$ (liq) 70AND/COU
3-Hexanone; Ethyl n-propyl ketone
Heat Capacity 298.15 K, C_p=216.9 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=305.3 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 145 K, ΔH=682 J·mol^{-1}
ΔS=4.73 J·mol^{-1}·K^{-1}
c,I/liq 217.72 K, ΔH=13490 J·mol^{-1}
ΔS=61.98 J·mol^{-1}·K^{-1}
Molecular Weight 100.1602
Wiswesser Line Notation 3V2
Evaluation A

$C_6H_{12}O$ (liq) 70HAR/HEA
3-Hexanone; Ethyl n-propyl ketone
Heat Capacity 298.15 K, C_p=216.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.1602
Wiswesser Line Notation 3V2
Evaluation B

$C_6H_{12}O$ (liq) 47SCH/ZOS
3-Oxahept-1-ene; Vinyl n-butyl ether
Heat Capacity 298.15 K, C_p=231.8 J·mol^{-1}·K^{-1}
One value, no details.
Molecular Weight 100.1602
Wiswesser Line Notation 4O1U1
Evaluation D

$C_6H_{12}O$ (liq) 70AND/COU
2-Hexanone; Methyl n-butyl ketone
Heat Capacity 298.15 K, C_p=213.4 J·mol^{-1}·K^{-1}
Temperature range 10 to 380 K.
Entropy 298.15 K, S=308.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 217.69 K, ΔH=14900 J·mol^{-1}
ΔS=68.44 J·mol^{-1}·K^{-1}
Molecular Weight 100.1602
Wiswesser Line Notation 4V1
Evaluation A

$C_6H_{12}O$ (liq) 70HAR/HEA
2-Hexanone; Methyl n-butyl ketone
Heat Capacity 298.15 K, C_p=213.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.1602
Wiswesser Line Notation 4V1
Evaluation B

$C_6H_{12}O$ (liq) 92SVO/KUB
2-Hexanone; Methyl n-butyl ketone
Phase Changes
liq/g 400.7 K, ΔH=43100 J·mol^{-1}
Value corrected to 298.15 K.
Molecular Weight 100.1602
Wiswesser Line Notation 4V1
Evaluation A

$C_6H_{12}O$ (liq) 24HER/BLO
Cyclohexanol; Cyclohexyl alcohol
Heat Capacity 290 K, C_p=174.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.1602
Wiswesser Line Notation L6TJ AQ
Evaluation C

$C_6H_{12}O$ (liq) 29KEI
Cyclohexanol; Cyclohexyl alcohol
Heat Capacity 298.15 K, C_p=209.03 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Value is unsmoothed experimenta
datum.
Entropy 298.15 K, S=199.6 J·mol^{-1}·K^{-1}
Average of values derived from measurements on both low an
high temperature crystal forms down to 13 K, plus entropy o
transition and fusion. Debye extrapolation below 13.5 K.
Phase Changes
c,II/c,I 263.5 K, ΔH=8205 J·mol^{-1}
ΔS=31.14 J·mol^{-1}·K^{-1}
Excess enthalpy over extrapolated heat capacity curves.
c,I/liq 297.0 K, ΔH=1699 J·mol^{-1}
ΔS=5.72 J·mol^{-1}·K^{-1}
Tm is 23.87 °C from 16RIC/SHI.
Molecular Weight 100.1602
Wiswesser Line Notation L6TJ AQ
Evaluation B
Sample may have contained a trace of water.

$C_6H_{12}O$ (liq) 39PH
Cyclohexanol; Cyclohexyl alcohol
Heat Capacity 305.1 K, C_p=202.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.1602
Wiswesser Line Notation L6TJ AQ
Evaluation C

$C_6H_{12}O$ (liq) 68ADA/SU
Cyclohexanol; Cyclohexyl alcohol
Heat Capacity 300 K, C_p=213.59 J·mol^{-1}·K^{-}
Temperature range 14 to 320 K.
Entropy 300 K, S=203.87 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,I 244.8 K, ΔH=8640 J·mol^{-1}
ΔS=35.29 J·mol^{-1}·K^{-}
c,II/c,I 265.50 K, ΔH=8827 J·mol^{-1}
ΔS=33.25 J·mol^{-1}·K^{-}
c,I/liq 299.09 K, ΔH=1783 J·mol^{-1}
ΔS=5.96 J·mol^{-1}·K^{-1}
Molecular Weight 100.1602
Wiswesser Line Notation L6TJ AQ
Evaluation B

$C_6H_{12}O$ (liq) 74PET/TE
Cyclohexanol; Cyclohexyl alcohol
Heat Capacity 297.95 K, C_p=212 J·mol^{-1}·K^{-1}
Temperature range 297 to 428 K. Value is unsmoothe
experimental datum.
Molecular Weight 100.1602
Wiswesser Line Notation L6TJ AQ
Evaluation B

$C_6H_{12}O$ (liq) 76CON/GI
Cyclohexanol; Cyclohexyl alcohol
Heat Capacity 298 K, C_p=220.1 J·mol^{-1}·K^{-}
One temperature.
Molecular Weight 100.1602
Wiswesser Line Notation L6TJ AQ
Evaluation B

$C_6H_{12}O$ (liq) 88CAC/COS
Cyclohexanol; Cyclohexyl alcohol
Heat Capacity 298.15 K, C_p=209.99 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.1602
Wiswesser Line Notation L6TJ AQ
Evaluation B

$C_6H_{12}O$ (liq) 91VAS/BYK
1-Hexanal
Heat Capacity 298.15 K, C_p=210.4 J·mol^{-1}·K^{-1}
Temperature range 11 to 300 K.
Entropy 298.15 K, S=280.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 214.94 K, ΔH=13330 J·mol^{-1}
ΔS=62.0 J·mol^{-1}·K^{-1}
Molecular Weight 100.1602
Wiswesser Line Notation VH5
Evaluation A

$C_6H_{12}O_2$ (liq) 79FUC
2-Methyl-2-propyl ethanoate; tert-Butyl acetate
Heat Capacity 298.15 K, C_p=231.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 1X1&1&OV1
Evaluation B

$C_6H_{12}O_2$ (liq) 71HAL/BAL
Methyl 2,2-dimethylpropanoate; Methyl pivalate
Heat Capacity 297 K, C_p=223.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 1X1&1&VO1
Evaluation C

$C_6H_{12}O_2$ (liq) 79FUC
Methyl 2,2-dimethylpropanoate; Methyl pivalate
Heat Capacity 298.15 K, C_p=257.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 1X1&1&VO1
Evaluation B

$C_6H_{12}O_2$ (liq) 36KUR/VOS
2-Methyl-1-propyl ethanoate; Isobutyl acetate
Heat Capacity 290 K, C_p=240.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 1Y1&1OV1
Evaluation D

$C_6H_{12}O_2$ (liq) 86JIM/ROM
Propyl propionate; n-Propyl propanoate
Heat Capacity 298.15 K, C_p=226.65 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 30V2
Evaluation B

$C_6H_{12}O_2$ (liq) 87ZAB/HYN
Propyl propionate; n-Propyl propanoate
Heat Capacity 298.38 K, C_p=229.00 J·mol^{-1}·K^{-1}
Temperature range 294 to 367 K. Unsmoothed experimental datum.
Molecular Weight 116.1596
Wiswesser Line Notation 30V2
Evaluation B

$C_6H_{12}O_2$ (liq) 33KOL/UDO
Ethyl butanoate; Ethyl butyrate
Heat Capacity 297.2 K, C_p=220.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 3VO2
Evaluation C

$C_6H_{12}O_2$ (liq) 34KOL/UDO2
Ethyl butanoate; Ethyl butyrate
Heat Capacity 297.2 K, C_p=220.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 3VO2
Evaluation C

$C_6H_{12}O_2$ (liq) 36KUR/VOS
Ethyl butanoate; Ethyl butyrate
Heat Capacity 290 K, C_p=229.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 3VO2
Evaluation D

$C_6H_{12}O_2$ (liq) 79FUC
Ethyl butanoate; Ethyl butyrate
Heat Capacity 298.15 K, C_p=228.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 3VO2
Evaluation B

$C_6H_{12}O_2$ (liq) 33KOL/UDO
n-Butyl acetate; n-Butyl ethanoate
Heat Capacity 292.5 K, C_p=242.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 40V1
Evaluation C

$C_6H_{12}O_2$ (liq) 34KOL/UDO2
n-Butyl acetate; n-Butyl ethanoate
Heat Capacity 292.5 K, C_p=242.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 40V1
Evaluation C

$C_6H_{12}O_2$ (liq) 79FUC
n-Butyl acetate; n-Butyl ethanoate
Heat Capacity 298.15 K, C_p=228.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 40V1
Evaluation B

$C_6H_{12}O_2$ (liq) 86JIM/ROM
n-Butyl acetate; n-Butyl ethanoate
Heat Capacity 298.15 K, C_p=225.11 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 40V1
Evaluation B

$C_6H_{12}O_2$ (liq) 87ZAB/HYN
n-Butyl acetate; n-Butyl ethanoate
Heat Capacity 298.35 K, C_p=228.11 J·mol^{-1}·K^{-1}
Temperature range 294 to 364 K. Unsmoothed experimental datum.
Molecular Weight 116.1596
Wiswesser Line Notation 40V1
Evaluation B

$C_6H_{12}O_2$ (liq) 79FUC
Methyl pentanoate; Methyl valerate
Heat Capacity 298.15 K, C_p=229.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 4VO1
Evaluation B

$C_6H_{12}O_2$ (liq) 88PIN/BRA
Methyl pentanoate; Methyl valerate
Heat Capacity 298.15 K, C_p=226.11 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 4VO1
Evaluation B

$C_6H_{12}O_2$ (liq) 1881REI
Hexanoic acid; n-Caproic acid
Heat Capacity 298 K, C_p=225.1 J·mol^{-1}·K^{-1}
Temperature range 292 to 483 K.
Molecular Weight 116.1596
Wiswesser Line Notation QV5
Evaluation D

$C_6H_{12}O_2$ (liq) 76BON/CER
Tetrahydropyran-2-methanol
Heat Capacity 298.15 K, C_p=222 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation T6OTJ B1Q
Evaluation B

$(C_6H_{12}O_2S)_n$ (c) 62DAI/EVA
1-Hexene polysulphone
Heat Capacity 298.15 K, C_p=221.04 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 298.15 K, S=J·mol^{-1}·K^{-1}
Molecular Weight 148.2196
Wiswesser Line Notation
Evaluation A

$C_6H_{12}O_3$ (liq) 83SAN/CI
2-Ethoxyethanol acetate
Heat Capacity 298.15 K, C_p=376 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K. C_p°(kJ·kg^{-1}·K^{-1} =0.009426T+0.036.
Molecular Weight 132.1590
Wiswesser Line Notation 1VO1O2
Evaluation D

$C_6H_{12}O_3$ (liq) 1881R
2,4,6-Trimethyl-1,3,5-trioxane; Paraldehyde
Heat Capacity 298 K, C_p=250.2 J·mol^{-1}·K^{-1}
Temperature range 293 to 400 K.
Molecular Weight 132.1590
Wiswesser Line Notation T6O CO EOTJ B1 D1 F1
Evaluation D

$C_6H_{12}O_3$ (liq) 39P
2,4,6-Trimethyl-1,3,5-trioxane; Paraldehyde
Heat Capacity 306.6 K, C_p=254.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 132.1590
Wiswesser Line Notation T6O CO EOTJ B1 D1 F1
Evaluation C

$C_6H_{12}O_3$ (liq) 69CLE/MEI
2,4,6-Trimethyl-1,3,5-trioxane; Paraldehyde
Heat Capacity 298.15 K, C_p=257.3 J·mol^{-1}·K^{-1}
Temperature range 80 to 310 K.
Entropy 298.15 K, S=289.4 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 61.1 J·mol^{-1}·K^{-1}.
Phase Changes
c,IV/c,III 142.7 K, ΔH=257.7 J·mol^{-1}
ΔS=1.81 J·mol^{-1}·K^{-1}
c,III/c,II 147.5 K, ΔH=773.1 J·mol^{-1}
ΔS=5.24 J·mol^{-1}·K^{-1}
ΔH and ΔS of transition for c,II/c,I at 230.3 K has been added i
ΔH and ΔS of fusion at 285.7 K.
c,I/liq 285.7 K, ΔH=13520 J·mol^{-1}
ΔS=47.32 J·mol^{-1}·K
Molecular Weight 132.1590
Wiswesser Line Notation T6O CO EOTJ B1 D1 F1
Evaluation B(C_p),C(S)

$C_6H_{12}O_6$ (c) 82LIA/CI
meso-Inositol
Heat Capacity 298.15 K, C_p=218.31 J·mol^{-1}·K
One temperature.
Molecular Weight 180.1572
Wiswesser Line Notation L6TJ AQ BQ CQ DQ EQ FQ
Evaluation B

$C_6H_{12}O_6$ (c) 90BAR/DEL
myo-Inositol
Phase Changes
c/liq 496.9 K, ΔH=47900 J·mol^{-1}
ΔS=96.4 J·mol^{-1}·K^{-1}
Molecular Weight 180.1572
Evaluation A

$C_6H_{12}O_6$ (c) 03MAG
Fructose
Heat Capacity 298 K, C_p=208.0 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.276 cal·g^{-1}·K^{-1}.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ B1Q CQ DQ EQ -A&DE -B&BC
Evaluation D

$C_6H_{12}O_6$ (c) 81KAW/NIS
Fructose(D)
Heat Capacity 300 K, C_p=231 J·mol^{-1}·K^{-1}
Temperature range 270 to 325 K. C_p given as 1.28 J·g^{-1}·K^{-1} at 300 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ B1Q CQ DQ EQ -A&DE -B&BC
Evaluation B

$C_6H_{12}O_6$ (c) 89FIN/FRA
Fructose(D)
Heat Capacity 300 K, C_p=201 J·mol^{-1}·K^{-1}
One temperature. T(glass)=286 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ B1Q CQ DQ EQ -A&DE -B&BC
Evaluation B

$C_6H_{12}O_6$ (c) 03MAG
α-Glucose(D); Dextrose
Heat Capacity 298 K, C_p=235.9 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.313 cal·g^{-1}·K^{-1}.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF
Evaluation D

$C_6H_{12}O_6$ (c) 22SIM
α-Glucose(D); Dextrose
Heat Capacity 300 K, C_p=229.3 J·mol^{-1}·K^{-1}
Temperature range 20 to 287 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF
Evaluation B

$C_6H_{12}O_6$ (c) 29PAR/KEL
α-Glucose(D); Dextrose
Heat Capacity 298.1 K, C_p=211.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K. 55.23 J·mol^{-1}·K^{-1}.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DO EO F1Q -A&BCE -B&DF
Evaluation C

$C_6H_{12}O_6$ (c) 34PAR/THO
α-Glucose(D); Dextrose
Heat Capacity 298 K, C_p=220.9 J·mol^{-1}·K^{-1}
Temperature range 273 to 318 K. Curve given also for undercooled liquid.
Phase Changes
c/liq 414 K, ΔH=31420 J·mol^{-1}
ΔS=75.9 J·mol^{-1}·K^{-1}
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF
Evaluation B

$C_6H_{12}O_6$ (c) 41NEL/NEW
α-Glucose(D); Dextrose
Heat Capacity 298 K, C_p=218.0 J·mol^{-1}·K^{-1}
Temperature range 0 to 60 °C. Equation only.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF
Evaluation B

$C_6H_{12}O_6$ (c) 51DOU/BAL
α-Glucose(D); Dextrose
Heat Capacity 298.15 K, C_p=218.8 J·mol^{-1}·K^{-1}
Temperature range 273 to 368 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF
Evaluation B

$C_6H_{12}O_6$ (c) 81KAW/NIS
α-Glucose(D); Dextrose
Heat Capacity 300 K, C_p=222 J·mol^{-1}·K^{-1}
Temperature range 270 to 325 K. C_p given as 1.23 J·g^{-1}·K^{-1} at 300 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF
Evaluation B

$C_6H_{12}O_6$ (c) 82LIA/CHE
α-Glucose(D); Dextrose
Heat Capacity 298.15 K, C_p=219.79 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF
Evaluation B

$C_6H_{12}O_6$ (c) 89FIN/FRA
α-Glucose(D); Dextrose
Heat Capacity 300 K, C_p=221 J·mol^{-1}·K^{-1}
One temperature. T(glass)=312 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF
Evaluation B

$C_6H_{12}O_6$ (c) 91BOE
α-Glucose(D); Dextrose
Heat Capacity 298.15 K, C_p=219.19 J·mol^{-1}·K^{-1}
Temperature range 7 to 347 K.
Entropy 298.15 K, S=209.19 J·mol^{-1}·K^{-1}
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF
Evaluation A

$C_6H_{12}O_6$ (c) 41JAC/STE
α-Galactose(D)
Heat Capacity 296.9 K, C_p=220.54 J·mol^{-1}·K^{-1}
Temperature range 64 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=205.4 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 48.95 J·mol^{-1}·K^{-1}.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BC -B&DEF
Evaluation B(C_p),C(S)

$C_6H_{12}O_6$ (c) 81KAW/NIS
Galactose(D)
Heat Capacity 300 K, C_p=216 J·mol^{-1}·K^{-1}
Temperature range 270 to 325 K. C_p given as 1.20 J·g^{-1}·K^{-1} at 300 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&BC -B&DEF
Evaluation B

$C_6H_{12}O_6$ (c,I) 41JAC/STE
Sorbose(L)
Heat Capacity 295.9 K, C_p=228.61 J·mol^{-1}·K^{-1}
Temperature range 64 to 296 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=220.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 50.21 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 199.22 K, ΔH=601.2 J·mol^{-1}
ΔS=3.02 J·mol^{-1}·K^{-1}
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&E -B&BCDF
Evaluation B(C_p),C(S)

$C_6H_{12}O_6$ (c) 81KAW/NIS
Mannose(D)
Heat Capacity 300 K, C_p=214 J·mol^{-1}·K^{-1}
Temperature range 270 to 325 K. C_p given as 1.19 J·g^{-1}·K^{-1} at 300 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q -A&E -B&CDF
Evaluation B

$C_6H_{12}S$ (liq) 74MES/FI
Cyclopentyl-1-thiaethane; Cyclopentyl methyl sulfide
Heat Capacity 298.15 K, C_p=192.92 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=285.47 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 165.0 K, ΔH=895 J·mol^{-1}
ΔS=5.42 J·mol^{-1}·K^{-1}
c,I/liq 169.85 K, ΔH=9226 J·mol^{-1}
ΔS=54.32 J·mol^{-1}·K^{-1}
c,II/liq 169.34 K, ΔH=10104 J·mol^{-1}
ΔS=59.67 J·mol^{-1}·K^{-1}
Molecular Weight 116.2208
Wiswesser Line Notation L5TJ AS1
Evaluation A

$C_6H_{12}S$ (liq) 67MES/TO
Cyclohexanethiol; Cyclohexyl mercaptan
Heat Capacity 298.15 K, C_p=192.63 J·mol^{-1}·K
Temperature range 10 to 370 K.
Entropy 298.15 K, S=255.57 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 189.64 K, ΔH=10000 J·mol^{-1}
ΔS=52.73 J·mol^{-1}·K^{-1}
Molecular Weight 116.2208
Wiswesser Line Notation L6TJ ASH
Evaluation A

$C_6H_{13}Br$ (liq) 31DE
1-Bromohexane; n-Hexyl bromide
Heat Capacity 298.8 K, C_p=203.55 J·mol^{-1}·K
Temperature range 95 to 290 K. Value is unsmoothed experimen datum.
Entropy 298.15 K, S=452.92 J·mol^{-1}·K^{-1}
Extrapolation below 100 K, 58.12 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 188.1 K, ΔH=18054 J·mol^{-1}
ΔS=95.98 J·mol^{-1}·K^{-1}
Molecular Weight 165.0727
Wiswesser Line Notation E6
Evaluation B(C_p),C(S)

$C_6H_{13}Br$ (liq) 93SI
1-Bromohexane; n-Hexyl bromide
Heat Capacity 298.15 K, C_p=219.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 165.0727
Wiswesser Line Notation E6
Evaluation B

$(C_6H_{12}N_2O\cdot HBr)_n$ (c) 91R(
Poly-L-lysine hydrobromide
Heat Capacity 300 K, C_p=208.5 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 209.0855
Wiswesser Line Notation /*VY4Z &EH &M*/ -L
Evaluation B

$(C_6H_{12}N_2O\cdot HBr)_n$ (c) 93ROL/XEN
Poly-L-lysine hydrobromide
Heat Capacity 300 K, C_p=208.5 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 209.0855
Wiswesser Line Notation /*VY4Z &EH &M*/ -L
Evaluation B

$C_6H_{13}Cl$ (liq) 93SHE
1-Chlorohexane; n-Hexyl chloride
Heat Capacity 298.15 K, C_p=216.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 120.6217
Wiswesser Line Notation G6
Evaluation B

$(C_6H_{12}N_4O\cdot HCl)_n$ (c) 91ROL
Poly-L-arginine hydrochloride
Heat Capacity 300 K, C_p=236.3 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 192.6479
Wiswesser Line Notation /*VY3MYUM&Z &GH &M*/ -L
Evaluation aB

$(C_6H_{12}N_4O\cdot HCl)_n$ (c) 93ROL/XEN
Poly-L-arginine hydrochloride
Heat Capacity 300 K, C_p=236.3 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 192.6479
Wiswesser Line Notation /*VY3MYUM&Z &GH &M*/ -L
Evaluation B

$C_6H_{13}I$ (liq) 93SHE
1-Iodohexane; n-Hexyl iodide
Heat Capacity 298.15 K, C_p=222.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 212.0732
Wiswesser Line Notation I6
Evaluation B

$C_6H_{13}N$ (liq) 76CON/GIN
2-Methylpiperidine
Heat Capacity 298 K, C_p=205 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 99.1754
Wiswesser Line Notation T6MTJ B1
Evaluation C

$C_6H_{13}N$ (liq) 86STE/CHI
2-Methylpiperidine
Heat Capacity 298.15 K, C_p=212.97 J·mol^{-1}·K^{-1}
Temperature range 10 to 380 K.
Entropy 298.15 K, S=243.75 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.357 K
Molecular Weight 99.1754
Wiswesser Line Notation T6MTJ B1
Evaluation A

$C_6H_{13}N$ (liq) 87MES/TOD
2-Methylpiperidine
Heat Capacity 298.15 K, C_p=212.96 J·mol^{-1}·K^{-1}
Temperature range 10 to 390 K.
Entropy 298.15 K, S=243.75 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.357 K, ΔH=18583.6 J·mol^{-1}
Molecular Weight 99.1754
Wiswesser Line Notation T6MTJ B1
Evaluation A

$C_6H_{13}N$ (liq) 88MES/TOD
2-Methylpiperidine
Heat Capacity 298.150 K, C_p=212.965 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S=243.762 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.357 K, ΔH=18583.87 J·mol^{-1}
Molecular Weight 99.1754
Wiswesser Line Notation T6MTJ B1
Evaluation A

$C_6H_{13}N$ (liq) 76CON/GIN
4-Methylpiperidine
Heat Capacity 298 K, C_p=209 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 99.1754
Wiswesser Line Notation T6MTJ D1
Evaluation C

$C_6H_{13}N$ (liq) 76CON/GIN
N-Methylpiperidine
Heat Capacity 298 K, C_p=184.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 99.1754
Wiswesser Line Notation T6NTJ A1
Evaluation B

$C_6H_{13}N$ (liq) 76CON/GIN
Hexamethyleneimine; Perhydroazepine
Heat Capacity 298 K, C_p=205 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 99.1754
Wiswesser Line Notation T7MTJ
Evaluation C

$C_6H_{13}NO$ (c) 71KON/WAD
2,2,N-Trimethylpropanamide
Heat Capacity 298.15 K, C_p=183 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 115.1748
Wiswesser Line Notation 1X1&1&VM1
Evaluation B

$C_6H_{13}NO$ (c) 71KON/WAD
N-(1,1-Dimethylethyl)ethanamide; N-tert-Butylacetamide
Heat Capacity 298.15 K, C_p=190 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 115.1748
Wiswesser Line Notation 1X1&1&MV1
Evaluation B

$C_6H_{13}NO$ (liq) 71KON/WAD
N-n-Butylethanamide; N-n-Butylacetamide
Heat Capacity 298.15 K, C_p=236 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 115.1748
Wiswesser Line Notation 4MV1
Evaluation B

$C_6H_{13}NO$ (liq) 86ZEG/BOE
N-n-Butylethanamide; N-n-Butylacetamide
Heat Capacity 298.15 K, C_p=236.89 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 115.1748
Wiswesser Line Notation 4MV1
Evaluation B

$C_6H_{13}NO$ (liq) 71KON/WAD
N-Methylpentanamide; N-Methylvaleramide
Heat Capacity 298.15 K, C_p=229 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 115.1748
Wiswesser Line Notation 4VM1
Evaluation B

$C_6H_{13}NO$ (liq) 76SKO/SUU
N-Methylpentanamide; N-Methylvaleramide
Heat Capacity 298.15 K, C_p=238.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 115.1748
Wiswesser Line Notation 4VM1
Evaluation A

$C_6H_{13}NO_2$ (liq) 92VER/BEC
N,N-Dimethyl-L-alanine methyl ester
Heat Capacity 298.15 K, C_p=268.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 131.1742
Wiswesser Line Notation 1OVY1&N1&1
Evaluation B

$C_6H_{13}NO_2$ (liq) 92VER/BEC
N,N-Dimethylglycine ethyl ester
Heat Capacity 298.15 K, C_p=244.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 131.1742
Wiswesser Line Notation 2OV1N1&1
Evaluation B

$C_6H_{13}NO_2$ (c) 37HUF/ELL
Leucine(DL); 2-Amino-4-methylpentanoic acid(DL)
Heat Capacity 296.6 K, C_p=194.30 J·mol^{-1}·K^{-1}
Temperature range 86 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=207.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 58.20 J·mol^{-1}·K^{-1}.
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ1Y1&1 -DL
Evaluation B(C_p),C(S)

$C_6H_{13}NO_2$ (c) 63HUT/COI
Leucine(L); 2-Amino-4-methylpentanoic acid(L)
Heat Capacity 298.15 K, C_p=200.96 J·mol^{-1}·K^{-1}
Temperature range 11 to 310 K.
Entropy 298.15 K, S=211.79 J·mol^{-1}·K^{-1}
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ1Y1&1 -L
Evaluation A

$C_6H_{13}NO_2$ (c) 75SPI/WAL
Leucine(L); 2-Amino-4-methylpentanoic acid(L)
Heat Capacity 298.15 K, C_p=201.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ1Y1&1 -L
Evaluation B

$C_6H_{13}NO_2$ (c) 84GRU/BOU
Leucine(L); 2-Amino-4-methylpentanoic acid(L)
Phase Changes
c,II/c,I 352 K, ΔH=200 J·mol^{-1}
ΔS=0.57 J·mol^{-1}·K^{-1}
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ1Y1&1 -L
Evaluation B

$C_6H_{13}NO_2$ (c) 89KUL/KOZ
Leucine(L); 2-Amino-4-methylpentanoic acid(L)
Heat Capacity 298 K, C_p=190.6 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ1Y1&1 -L
Evaluation C

$C_6H_{13}NO_2$ (c) 90BAD/KUI
Leucine(L); 2-Amino-4-methylpentanoic acid(L)
Heat Capacity 298 K, C_p=191 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ1Y1&1 -L
Evaluation D

$C_6H_{13}NO_2$ (c) 84GRU/BOI
Norleucine(L); α-Aminocaproic acid(L)
Phase Changes
c,II/c,I 389 K, ΔH=110 J·mol^{-1}
ΔS=0.28 J·mol^{-1}·K^{-1}
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ4 -L
Evaluation B

$C_6H_{13}NO_2$ (c) 84GRU/BO
Norleucine(DL); α-Aminocaproic acid(DL)
Phase Changes
c,II/c,I 390 K, ΔH=4410 J·mol^{-1}
ΔS=11.31 J·mol^{-1}·K^{-}
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ4
Evaluation B

$C_6H_{13}NO_2$ (c) 88PET/TSY
Norleucine(DL); α-Aminocaproic acid(DL)
Phase Changes
c,II/c,I 390.4 K, $\Delta H = 4200$ J·mol^{-1}
$\Delta S = 10.7$ J·mol^{-1}·K^{-1}
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ4
Evaluation A

$C_6H_{13}NO_2$ (c) 63HUT/COL
2-Amino-3-methylpentanoic acid(L); Isoleucine(L)
Heat Capacity 298.15 K, $C_p = 188.28$ J·mol^{-1}·K^{-1}
Temperature range 11 to 310 K.
Entropy 298.15 K, $S = 207.99$ J·mol^{-1}·K^{-1}
Molecular Weight 131.1742
Wiswesser Line Notation QVYZY2&1 -L
Evaluation A

$C_6H_{13}NO_2$ (c) 83SKO/SAB
6-Aminohexanoic acid
Heat Capacity 298 K, $C_p = 175.6$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 131.1742
Wiswesser Line Notation Z5VQ
Evaluation B

$C_6H_{13}N_3O_3$ (c) 40HUF/FOX
Citrulline(DL)
Heat Capacity 300.8 K, $C_p = 232.80$ J·mol^{-1}·K^{-1}
Temperature range 90 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S = 254.4$ J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 75.94 J·mol^{-1}·K^{-1}.
Molecular Weight 175.1870
Wiswesser Line Notation ZVM3YZVQ
Evaluation B(C_p),C(S)

C_6H_{14} (liq) 37STU
2,3-Dimethylbutane
Heat Capacity 298.1 K, $C_p = 184.35$ J·mol^{-1}·K^{-1}
Temperature range 140 to 320 K.
Molecular Weight 86.1766
Wiswesser Line Notation 1Y1&Y1&1
Evaluation B(C_p)

C_6H_{14} (liq) 46DOU/HUF
2,3-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 188.74$ J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, $S = 277.52$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 136.07 K, $\Delta H = 6494$ J·mol^{-1}
$\Delta S = 47.72$ J·mol^{-1}·K^{-1}
c,I/liq 145.19 K, $\Delta H = 800.8$ J·mol^{-1}
$\Delta S = 5.52$ J·mol^{-1}·K^{-1}
Molecular Weight 86.1766
Wiswesser Line Notation 1Y1&Y1&1
Evaluation A

C_6H_{14} (liq) 71ADA/SUG
2,3-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 189.70$ J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, $S = 278.85$ J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,I 107 K, $\Delta H = 2370$ J·mol^{-1}
$\Delta S = 22.15$ J·mol^{-1}·K^{-1}
c,III has residual entropy of 2.7 J·mol^{-1}·K^{-1}.
c,II/c,I 136.02 K, $\Delta H = 6425$ J·mol^{-1}
$\Delta S = 47.24$ J·mol^{-1}·K^{-1}
c,II stable form to 10 K; apparently has no zero point entropy.
c,I/liq 145.04 K, $\Delta H = 793.7$ J·mol^{-1}
$\Delta S = 5.47$ J·mol^{-1}·K^{-1}
Molecular Weight 86.1766
Wiswesser Line Notation 1Y1&Y1&1
Evaluation A

C_6H_{14} (liq) 82WIL/FAR
2,3-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 188.80$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 1Y1&Y1&1
Evaluation B

C_6H_{14} (liq) 83AIC/KUM
2,3-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 188.77$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 1Y1&Y1&1
Evaluation B

C_6H_{14} (liq) 83BEN/DAR
2,3-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 188.77$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 1Y1&Y1&1
Evaluation B

C_6H_{14} (liq) 84BEN/DAR
2,3-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 188.67$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 1Y1&Y1&1
Evaluation B

C_6H_{14} (liq) 86BEN/DAR3
2,3-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 189.04$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 1Y1&Y1&1
Evaluation B

C_6H_{14} (liq) 89OHN/FUJ
2,3-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 189.02\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 1Y1&Y1&1
Evaluation B

C_6H_{14} (liq) 37STU
2,2-Dimethylbutane
Heat Capacity 298.1 K, $C_p = 183.18\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 320 K.
Entropy 298.1 K, $S = 269.4\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, 17.76 $cal \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c,II/c,I 127.11 K, $\Delta H = 4581\ J \cdot mol^{-1}$
$\Delta S = 36.04\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 172.13 K, $\Delta H = 464\ J \cdot mol^{-1}$
$\Delta S = 2.70\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 86.1766
Wiswesser Line Notation 2X1&1&1
Evaluation B(C_p),C(S)

C_6H_{14} (liq) 46DOU/HUF
2,2-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 188.74\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 13 to 300 K.
Entropy 298.15 K, $S = 272.00\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,III/c,II 126.81 K, $\Delta H = 5410\ J \cdot mol^{-1}$
$\Delta S = 42.66\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I 140.79 K, $\Delta H = 285.3\ J \cdot mol^{-1}$
$\Delta S = 2.03\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 174.28 K, $\Delta H = 579.1\ J \cdot mol^{-1}$
$\Delta S = 3.32\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 86.1766
Wiswesser Line Notation 2X1&1&1
Evaluation A

C_6H_{14} (liq) 46KIL/PIT
2,2-Dimethylbutane
Heat Capacity 290 K, $C_p = 186.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 20 to 290 K.
Entropy 298.15 K, $S = 272.5\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,III/c,II 126.81 K, $\Delta H = 5394\ J \cdot mol^{-1}$
$\Delta S = 42.5\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I 140.88 K, $\Delta H = 283\ J \cdot mol^{-1}$
$\Delta S = 2.01\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 174.66 K, $\Delta H = 579\ J \cdot mol^{-1}$
$\Delta S = 3.33\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 86.1766
Wiswesser Line Notation 2X1&1&1
Evaluation A

C_6H_{14} (liq) 50AUE/SAG
2,2-Dimethylbutane
Heat Capacity 300 K, $C_p = 191.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 300 to 366 K. C_p given as 0.5312 $Btu(lb)^{-1}(°R)^{-1}$ at 80 °F.
Molecular Weight 86.1766
Wiswesser Line Notation 2X1&1&1
Evaluation B

C_6H_{14} (liq) 83AIC/KUM
2,2-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 189.14\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2X1&1&1
Evaluation B

C_6H_{14} (liq) 83BEN/DAR
2,2-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 189.14\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2X1&1&1
Evaluation B

C_6H_{14} (liq) 86BEN/DAR3
2,2-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 189.44\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2X1&1&1
Evaluation B

C_6H_{14} (liq) 88COS/HUU
2,2-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 191.88\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2X1&1&1
Evaluation B

C_6H_{14} (liq) 88PER/AIC
2,2-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 191.88\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2X1&1&1
Evaluation A

C_6H_{14} (liq) 89OHN/FU.
2,2-Dimethylbutane
Heat Capacity 298.15 K, $C_p = 189.67\ J \cdot mol^{-1} \cdot K^{-}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2X1&1&1
Evaluation B

C_6H_{14} (liq) 37STI
3-Methylpentane
Heat Capacity 298.1 K, $C_p = 187.36\ J \cdot mol^{-1} \cdot K^{-}$
Temperature range 90 to 320 K.
Molecular Weight 86.1766
Wiswesser Line Notation 2Y2&1
Evaluation B(C_p),C(S)

C_6H_{14} (c) 46DOU/HUI
3-Methylpentane
Heat Capacity 298.15 K, $C_p = 190.83\ J \cdot mol^{-1} \cdot K^{-}$
Temperature range 13 to 300 K.
Molecular Weight 86.1766
Wiswesser Line Notation 2Y2&1
Evaluation A

C_6H_{14} (liq) 73FIN/MES
3-Methylpentane
Heat Capacity 298.15 K, $C_p = 190.67\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 330 K.
Entropy 298.15 K, $S = 292.5\ J \cdot mol^{-1} \cdot K^{-1}$
Thermodynamic properties calculated from a Debye function at 10 K.
Phase Changes
c,I/liq 110.26 K, $\Delta H = 5303.2\ J \cdot mol^{-1}$
$\Delta S = 48.101\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 86.1766
Wiswesser Line Notation 2Y2&1
Evaluation A

C_6H_{14} (liq) 82CZA
3-Methylpentane
Heat Capacity 298.95 K, $C_p = 186.8\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2Y2&1
Evaluation B

C_6H_{14} (liq) 82OGU/WAT
3-Methylpentane
Heat Capacity 288.19 K, $C_p = 187.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 80 to 370 K. Unsmoothed experimental datum. Heat capacity measured as a check of the calorimeter's performance.
Molecular Weight 86.1766
Wiswesser Line Notation 2Y2&1
Evaluation B

C_6H_{14} (liq) 83AIC/KUM
3-Methylpentane
Heat Capacity 298.15 K, $C_p = 190.77\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2Y2&1
Evaluation B

C_6H_{14} (liq) 83BEN/DAR
3-Methylpentane
Heat Capacity 298.15 K, $C_p = 190.77\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2Y2&1
Evaluation B

C_6H_{14} (liq) 84BEN/DAR
3-Methylpentane
Heat Capacity 298.15 K, $C_p = 190.86\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2Y2&1
Evaluation B

C_6H_{14} (liq) 86BEN/DAR3
3-Methylpentane
Heat Capacity 298.15 K, $C_p = 190.99\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2Y2&1
Evaluation B

C_6H_{14} (liq) 89OHN/FUJ
3-Methylpentane
Heat Capacity 298.15 K, $C_p = 191.16\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 2Y2&1
Evaluation B

C_6H_{14} (liq) 37STU
2-Methylpentane
Heat Capacity 298.1 K, $C_p = 198.45\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 320 K.
Entropy 298.1 K, $S = 292.5\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, $103.72\ J \cdot mol^{-1} \cdot K^{-1}$.
Molecular Weight 86.1766
Wiswesser Line Notation 3Y1&1
Evaluation B(C_p),C(S)

C_6H_{14} (liq) 46DOU/HUF
2-Methylpentane
Heat Capacity 298.15 K, $C_p = 193.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 13 to 300 K.
Entropy 298.15 K, $S = 290.58\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 119.55 K, $\Delta H = 6268\ J \cdot mol^{-1}$
$\Delta S = 52.43\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 86.1766
Wiswesser Line Notation 3Y1&1
Evaluation A

C_6H_{14} (liq) 83AIC/KUM
2-Methylpentane
Heat Capacity 298.15 K, $C_p = 193.84\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 3Y1&1
Evaluation B

C_6H_{14} (liq) 83BEN/DAR
2-Methylpentane
Heat Capacity 298.15 K, $C_p = 193.84\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 3Y1&1
Evaluation B

C_6H_{14} (liq) 84BEN/DAR
2-Methylpentane
Heat Capacity 298.15 K, $C_p = 193.92\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 3Y1&1
Evaluation B

C_6H_{14} (liq) 86BEN/DAR3
2-Methylpentane
Heat Capacity 298.15 K, $C_p = 193.96\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 3Y1&1
Evaluation B

C_6H_{14} (liq) 89OHN/FUJ
2-Methylpentane
Heat Capacity 298.15 K, $C_p = 194.19\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 3Y1&1
Evaluation B

C_6H_{14} (liq) 1881REI
n-Hexane
Heat Capacity 298 K, $C_p = 194.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 290 to 363 K.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation D

C_6H_{14} (liq) 30PAR/HUF
n-Hexane
Heat Capacity 295.1 K, $C_p = 191.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 295 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S = 297.5\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, 65.44 $J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 178.6 K, $\Delta H = 12581\ J \cdot mol^{-1}$
$\Delta S = 70.44\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B(C_p),C(S)

C_6H_{14} (liq) 31HUF/PAR
n-Hexane
Heat Capacity 293.5 K, $C_p = 193.3\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 140 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, $S = 295.4\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, 64.02 $J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 177.9 K, $\Delta H = 13033\ J \cdot mol^{-1}$
$\Delta S = 73.3\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B(C_p),C(S)

C_6H_{14} (liq) 37STU
n-Hexane
Heat Capacity 298.1 K, $C_p = 189.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 320 K. Hump about 262 K with abnormal curve to 320 K.
Entropy 298.1 K, $S = 289.5\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 91 K, 54.68 $J \cdot mol^{-1} \cdot K^{-1}$.
Phase Changes
c/liq 177.90 K, $\Delta H = 12343\ J \cdot mol^{-1}$
$\Delta S = 69.38\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B(C_p),C(S)

C_6H_{14} (liq) 39PHI
n-Hexane
Heat Capacity 300.7 K, $C_p = 186.2\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation C

C_6H_{14} (liq) 46DOU/HUI
n-Hexane
Heat Capacity 298.15 K, $C_p = 194.97\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 13 to 300 K.
Entropy 298.15 K, $S = 296.06\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 177.84 K, $\Delta H = 13079\ J \cdot mol^{-1}$
$\Delta S = 73.54\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 51CON/SAC
n-Hexane
Heat Capacity 299.8 K, $C_p = 196.10\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 80 to 200 °F.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 74DIA/REI
n-Hexane
Heat Capacity 298.15 K, $C_p = 198.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 298 to 325 K.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation A

C_6H_{14} (liq) 75GRI/RAS
n-Hexane
Heat Capacity 298 K, $C_p = 196.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 300 to 463 K.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 79CZA
n-Hexane
Heat Capacity 300 K, $C_p = 184.2\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 80KAL/JEI
n-Hexane
Heat Capacity 297.316 K, $C_p = 195.64\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 185 to 300 K. Unsmoothed experimental datum.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 81GRO/IN
n-Hexane
Heat Capacity 298.15 K, $C_p = 195.76\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 82WIL/ING
n-Hexane
Heat Capacity 298.15 K, C_p=195.33 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation A

C_6H_{14} (liq) 82ZAR
n-Hexane
Heat Capacity 298 K, C_p=195.1 J·mol^{-1}·K^{-1}
Temperature range 298, 323 K.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 83AIC/KUM
n-Hexane
Heat Capacity 298.15 K, C_p=195.80 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 83BEN/DAR
n-Hexane
Heat Capacity 298.15 K, C_p=195.80 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 84BEN/DAR
n-Hexane
Heat Capacity 298.15 K, C_p=195.80 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 84BRA/PIN
n-Hexane
Heat Capacity 298.15 K, C_p=195.33 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 84GRI/AND
n-Hexane
Heat Capacity 297.32 K, C_p=196.1 J·mol^{-1}·K^{-1}
Temperature range 293 to 324 K. Unsmoothed experimental datum given as 2.276 kJ/kg·K.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 85COS/PAT
n-Hexane
Heat Capacity 298.15 K, C_p=194.96 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 86BEN/DAR3
n-Hexane
Heat Capacity 298.15 K, C_p=195.84 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 86NAZ/BAS2
n-Hexane
Heat Capacity 308.35 K, C_p=203.0 J·mol^{-1}·K^{-1}
Temperature range 308.35, 333.15. p=0.1 MPa. Unsmoothed experimental datum given as 2.356 kJ/kg·K.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 86TAR/AIC
n-Hexane
Heat Capacity 298.15 K, C_p=197.66 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 88AND/PAT
n-Hexane
Heat Capacity 298.15 K, C_p=197.66 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 88PER/AIC
n-Hexane
Heat Capacity 298.15 K, C_p=197.66 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation A

C_6H_{14} (liq) 88SAI/TAN
n-Hexane
Heat Capacity 298.15 K, C_p=195.64 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 89OHN/FUJ
n-Hexane
Heat Capacity 298.15 K, C_p=195.52 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation B

C_6H_{14} (liq) 91PRU
n-Hexane
Heat Capacity 298.15 K, C_p=265.2 J·mol^{-1}·K^{-1}
Molecular Weight 86.1766
Wiswesser Line Notation 6H
Evaluation A
C_p(liq)=1.1999+4.959×10^{-3}(T/K)−1.02177×10^{-5}(T/K)^2 +1.91869×10^{-8}(T/K)^3 (90 to 401 K).

$C_6H_{14}N_4O_2$ (c) 37HUF/ELL
Arginine(D)
Heat Capacity 296.8 K, C_p=232.8 J·mol^{-1}·K^{-1}
Temperature range 86 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=250.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 73.30 J·mol^{-1}·K^{-1}.
Molecular Weight 174.2022
Wiswesser Line Notation QVYZ3MYZUM -D
Evaluation B(C_p),C(S)

$C_6H_{14}N_4O_2 \cdot H_3PO_4 \cdot H_2O$ (c) 89YAN/YAN
Arginine phosphate monohydrate(L)
Heat Capacity 300 K, C_p=365.53 J·mol^{-1}·K^{-1}
Temperature range 290 to 350 K.
Molecular Weight 290.2125
Wiswesser Line Notation QVYZ3MYZUM &QPQQO &QH -L
Evaluation B

$C_6H_{14}O$ (liq) 33PAR/HUF
2,4-Dimethyl-3-oxapentane; Isopropyl ether
Heat Capacity 293.1 K, C_p=216.31 J·mol^{-1}·K^{-1}
Temperature range 92 to 213 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=294.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 61.30 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 186.3 K, ΔH=11025 J·mol^{-1}
ΔS=59.18 J·mol^{-1}·K^{-1}
Molecular Weight 102.1760
Wiswesser Line Notation 1Y1&OY1&1
Evaluation B(C_p),C(S)

$C_6H_{14}O$ (liq) 74AND/COU
2,4-Dimethyl-3-oxapentane; Isopropyl ether
Heat Capacity 298.15 K, C_p=216.1 J·mol^{-1}·K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S=304.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 187.77 K, ΔH=12035 J·mol^{-1}
ΔS=64.09 J·mol^{-1}·K^{-1}
Molecular Weight 102.1760
Wiswesser Line Notation 1Y1&OY1&1
Evaluation A

$C_6H_{14}O$ (liq) 93GRO/ROU
2,4-Dimethyl-3-oxapentane; Isopropyl ether
Heat Capacity 298.15 K, C_p=216.74 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation 1Y1&OY1&1
Evaluation B

$C_6H_{14}O$ (liq) 36EVA/EDL
4,4-Dimethyl 3 oxapentane; tert Butyl ethyl ether
Heat Capacity 298 K, C_p=218 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation 2OX1&1&1
Evaluation C

$C_6H_{14}O$ (liq) 36EVA/EDL
3,3-Dimethyl-2-oxapentane; tert-Amyl methyl ether
Heat Capacity 298 K, C_p=222 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation 2X1&1&O1
Evaluation C

$C_6H_{14}O$ (liq) 75AND/COU
4-Oxaheptane; Di-n-propyl ether
Heat Capacity 298.15 K, C_p=221.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 330 K.
Entropy 298.15 K, S=323.9 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 149.40 K, ΔH=9540 J·mol^{-1}
ΔS=63.86 J·mol^{-1}·K^{-1}
c,II/liq 158.36 K, ΔH=10770 J·mol^{-1}
ΔS=68.01 J·mol^{-1}·K^{-1}
liq/g 363.22 K, ΔH=31274 J·mol^{-1}
ΔS=86.10 J·mol^{-1}·K^{-1}
P=101.30 kPa
Molecular Weight 102.1760
Wiswesser Line Notation 3O3
Evaluation A

$C_6H_{14}O$ (liq) 83KIM/TRE
4-Oxaheptane; Di-n-propyl ether
Heat Capacity 298.15 K, C_p=221.45 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation 3O3
Evaluation B

$C_6H_{14}O$ (liq) 85BEN/DAF
2-Ethyl-1-butanol
Heat Capacity 298.15 K, C_p=252.82 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q1Y2&2
Evaluation A

$C_6H_{14}O$ (liq) 86ORT
2-Ethyl-1-butanol
Heat Capacity 298.15 K, C_p=246.65 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q1Y2&2
Evaluation B

$C_6H_{14}O$ (liq) 83AIC/KUM
2-Methyl-1-pentanol
Heat Capacity 298.15 K, C_p=248.40 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q1Y3&1
Evaluation B

$C_6H_{14}O$ (liq) 84BRA/PIN
2-Methyl-1-pentanol
Heat Capacity 298.15 K, C_p=247.63 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q1Y3&1
Evaluation B

$C_6H_{14}O$ (liq) 85BEN/DAR
2-Methyl-1-pentanol
Heat Capacity 298.15 K, C_p=249.21 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q1Y3&1
Evaluation B

$C_6H_{14}O$ (liq) 86BEN/KUM
3,3-Dimethyl-1-butanol
Heat Capacity 298.15 K, C_p=236.08 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q2X1&1&1
Evaluation B

$C_6H_{14}O$ (liq) 29KEL2
1-Hexanol; n-Hexyl alcohol
Heat Capacity 290.01 K, C_p=232.46 J·mol^{-1}·K^{-1}
Temperature range 16 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=287.4 J mol^{-1} K^{-1}
Phase Changes
c/liq 225.8 K, ΔH=15380 J·mol^{-1}
ΔS=68.11 J·mol^{-1}·K^{-1}
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 59HUT/BAI
1-Hexanol; n-Hexyl alcohol
Heat Capacity 298 K, C_p=244.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation C

$C_6H_{14}O$ (liq) 79GRI/YAN
1-Hexanol; n-Hexyl alcohol
Heat Capacity 303.74 K, C_p=247.7 J·mol^{-1}·K^{-1}
Temperature range 303 to 462 K. p=0.98 bar.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 81ARU
1-Hexanol; n-Hexyl alcohol
Heat Capacity 293.15 K, C_p=236.5 J·mol^{-1}·K^{-1}
Temperature range 273 to 533 K. p=0.1 MPa. Unsmoothed experimental datum at 293.15 K, C_p=2.315 kJ/kg·K.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 81ARU
1-Hexanol; n-Hexyl alcohol
Heat Capacity 293.15 K, C_p=236.5 J·mol^{-1}·K^{-1}
Temperature range 293 to 393 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.315 kJ/kg·K. C_p given from 293.15 to 533.15 K for pressure range 10 to 60 MPa.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 83BEN/DAR
1-Hexanol; n-Hexyl alcohol
Heat Capacity 298.15 K, C_p=240.65 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 84BRA/PIN
1-Hexanol; n-Hexyl alcohol
Heat Capacity 298.15 K, C_p=239.62 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 84KAL/WOY
1-Hexanol; n-Hexyl alcohol
Heat Capacity 300.607 K, C_p=249.15 J·mol^{-1}·K^{-1}
Temperature range 230 to 300 K. Value is unsmoothed experimental datum.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 84ZEG/SOM
1-Hexanol; n-Hexyl alcohol
Heat Capacity 298.15 K, C_p=241.32 J·mol^{-1}·K^{-1}
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation C

$C_6H_{14}O$ (liq) 85COS/PAT
1-Hexanol; n-Hexyl alcohol
Heat Capacity 298.15 K, C_p=239.68 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 86ORT
1-Hexanol; n-Hexyl alcohol
Heat Capacity 298.15 K, C_p=237.85 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 86TAN/TOY
1-Hexanol; n-Hexyl alcohol
Heat Capacity 298.15 K, C_p=240.57 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102:1760
Wiswesser Line Notation Q6
Evaluation A

$C_6H_{14}O$ (liq) 88AND/PAT
1-Hexanol; n-Hexyl alcohol
Heat Capacity 298.15 K, C_p=241.32 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 89VES/BAR
1-Hexanol; n-Hexyl alcohol
Heat Capacity 298.15 K, C_p=242.5 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation A

$C_6H_{14}O$ (liq) 91ATR/NES
1-Hexanol; n-Hexyl alcohol
Heat Capacity 298.15 K, C_p=243.2 J·mol^{-1}·K^{-1}
Temperature range 227 to 363 K. C_p(liq)=2.37095 −0.0851173(T/100)−0.195794(T/100)^2−0.00639224(T/100)^3 +0.0530459(T/100)^4 −0.00859433(T/100)^5 kJ/kg·K.
Molecular Weight 102.1760
Wiswesser Line Notation Q6
Evaluation B

$C_6H_{14}O$ (liq) 86ORT
2-Methyl-2-pentanol
Heat Capacity 298.15 K, C_p=289.03 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QX1&1&3
Evaluation B

$C_6H_{14}O$ (liq) 86ORT
3-Methyl-3-pentanol
Heat Capacity 298.15 K, C_p=293.83 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QX2&2&1
Evaluation B

$C_6H_{14}O$ (liq) 84BRA/PIN
3-Methyl-3-pentanol
Heat Capacity 298.15 K, C_p=293.38 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QX2&2&1
Evaluation B

$C_6H_{14}O$ (liq) 88CAC/COS
3-Methyl-3-pentanol
Heat Capacity 298.15 K, C_p=302.25 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QX2&2&1
Evaluation B

$C_6H_{14}O$ (liq) 84BRA/PIN
4-Methyl-2-pentanol
Heat Capacity 298.15 K, C_p=273.01 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QY1&1Y1&1
Evaluation B

$C_6H_{14}O$ (liq) 86ORT
4-Methyl-2-pentanol
Heat Capacity 298.15 K, C_p=272.34 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QY1&1Y1&1
Evaluation B

$C_6H_{14}O$ (liq) 86ORT
2-Hexanol
Heat Capacity 298.15 K, C_p=260.34 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QY1&4
Evaluation B

$C_6H_{14}O$ (liq) 88TAN/LUO
2-Hexanol
Heat Capacity 298.15 K, C_p=256.31 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QY1&4
Evaluation B

$C_6H_{14}O$ (liq) 84BRA/PIN
3-Methyl-2-pentanol
Heat Capacity 298.15 K, C_p=275.89 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QY1&Y2&1
Evaluation B

$C_6H_{14}O$ (liq) 76CON/GIN
3-Hexanol
Heat Capacity 298 K, C_p=286.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QY3&2
Evaluation B

$C_6H_{14}O$ (liq) 88TAN/LUO
3-Hexanol
Heat Capacity 298.15 K, C_p=269.27 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1760
Wiswesser Line Notation QY3&2
Evaluation B

$C_6H_{14}O_2$ (liq) 73KUS/SUU
3,6-Dioxaoctane; 1,2-Diethoxyethane
Heat Capacity 298.15 K, C_p=259.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 118.1754
Wiswesser Line Notation 2O2O2
Evaluation B

$C_6H_{14}O_2$ (liq) 82VIL/CAS
3,6-Dioxaoctane; 1,2-Diethoxyethane
Heat Capacity 298.15 K, C_p=261.08 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 118.1754
Wiswesser Line Notation 20202
Evaluation B

$C_6H_{14}O_2$ (liq) 1881REI
4-Methyl-3,5-dioxaheptane; Acetal; 1,1-Diethoxyethane
Heat Capacity 298 K, C_p=237.7 J·mol^{-1}·K^{-1}
Temperature range 289 to 382 K.
Molecular Weight 118.1754
Wiswesser Line Notation 2OY1&O2
Evaluation D

$C_6H_{14}O_2$ (liq) 73KUS/SUU
2,5-Dioxaoctane; 1-n-Propoxy-2-methoxyethane
Heat Capacity 298.15 K, C_p=248.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 118.1754
Wiswesser Line Notation 3O2O1
Evaluation B

$C_6H_{14}O_2$ (liq) 59ONK
2-n-Butoxy-1-ethanol; Butylglycol; 2-n-Butoxyethanol; 3-Oxa-1-heptanol
Heat Capacity 298.15 K, C_p=273.3 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K. C_p given as 65.33 cal·mol^{-1}·C^{-1}.
Molecular Weight 118.1754
Wiswesser Line Notation Q2O4
Evaluation C

$C_6H_{14}O_2$ (liq) 73KUS/SUU
2-n-Butoxy-1-ethanol; Butylglycol; 2-n-Butoxyethanol; 3-Oxa-1-heptanol
Heat Capacity 298.15 K, C_p=273.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 118.1754
Wiswesser Line Notation Q2O4
Evaluation B

$C_6H_{14}O_2$ (liq) 78ROU/PER
2-n-Butoxy-1-ethanol; Butylglycol; 2-n-Butoxyethanol; 3-Oxa-1-heptanol
Heat Capacity 298.15 K, C_p=270.6 J·mol^{-1}·K^{-1}
Temperatures 278.15, 283.15, 298.15, 313.15, 328.15 K.
Molecular Weight 118.1754
Wiswesser Line Notation Q2O4
Evaluation C

$C_6H_{14}O_2$ (liq) 72GAR/HUS
1,6-Hexanediol
Phase Changes
c/liq 320.6 K, ΔH=25522 J·mol^{-1}
ΔS=79.61 J·mol^{-1}·K^{-1}
Molecular Weight 118.1754
Wiswesser Line Notation Q6Q
Evaluation A

$C_6H_{14}O_2$ (c) 92STE/CHI
1,6 Hexanediol
Heat Capacity 298.15 K, C_p=202.9 J·mol^{-1}·K^{-1}
Temperature range 268 to 413 K. C/R(c)=0.128T−13.72 (268 to 315 K); C/R(liq)=0.1123T−1.91 (315 to 413 K), R=8.31451 J/K·mol.
Phase Changes
c/liq 315 K, ΔH=22600 J·mol^{-1}
Molecular Weight 118.1754
Wiswesser Line Notation Q6Q
Evaluation A

$C_6H_{14}O_3$ (liq) 66BEA/CLE
2,5,8-Trioxanonane; Diglyme
Heat Capacity 298.15 K, C_p=274.1 J·mol^{-1}·K^{-1}
Temperature range 90 to 350 K.
Entropy 298.15 K, S=352.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 79.91 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 209.1 K, ΔH=17795 J·mol^{-1}
ΔS=85.1 J·mol^{-1}·K^{-1}
Molecular Weight 134.1748
Wiswesser Line Notation 1O2O2O1
Evaluation A(C_p),C(S)

$C_6H_{14}O_3$ (liq) 82VIL/CAS
2,5,8-Trioxanonane; Diglyme
Heat Capacity 298.15 K, C_p=279.84 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 134.1748
Wiswesser Line Notation 1O2O2O1
Evaluation B

$C_6H_{14}O_3$ (liq) 82ZAR
Dipropylene glycol
Heat Capacity 298 K, C_p=322.1 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 134.1748
Wiswesser Line Notation QY1&1O1YQ&1
Evaluation B

$C_6H_{14}O_3$ (c) 89ZHA/YAN
1,1,1-Trihydroxymethylpropane; 2-Ethyl-2-(hydroxymethyl) -1,3-propanediol
Heat Capacity 301.29 K C_p=213.79 J·mol^{-1}·K^{-1}
Temperature range 270 to 354 K; value is unsmoothed experimental datum.
Phase Changes
c/liq 333.40 K ΔH=21450 J·mol^{-1}
ΔS=64.3 J·mol^{-1}·K^{-1}
Molecular Weight 134.1748
Wiswesser Line Notation Q1X1Q1Q2
Evaluation A

$C_6H_{14}O_3$ (liq) 91TRE/COS
2,5,8-Trioxanonane; Diglyme
Heat Capacity 298.15 K, C_p=277.76 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 134.1748
Wiswesser Line Notation 1O2O2O1
Evaluation B

$C_6H_{14}O_4$ (liq) 79STE/TAM
1,8-Dihydroxy-3,6-dioxaoctane; Triethylene glycol
Heat Capacity 298 K, C_p=327.6 J·mol^{-1}·K^{-1}
Temperature range 273 to 533 K. Temperature range 298, 323, 363 K.
Molecular Weight 150.1742
Wiswesser Line Notation Q2O2O2Q
Evaluation B

$C_6H_{14}O_4$ (liq) 82ZAR
1,8-Dihydroxy-3,6-dioxaoctane; Triethylene glycol
Heat Capacity 298 K, C_p=333.7 J·mol^{-1}·K^{-1}
Molecular Weight 150.1742
Wiswesser Line Notation Q2O2O2Q
Evaluation B

$C_6H_{14}O_6$ (c) 82LIA/CHE
Sorbitol(D)
Heat Capacity 298.15 K, C_p=241.43 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQ 2 -BBAA
Evaluation B

$C_6H_{14}O_6$ (c) 90BAR/DEL
Sorbitol(D)
Phase Changes
c/liq 366.5 K, ΔH=30200 J·mol^{-1}
ΔS=82.5 J·mol^{-1}·K^{-1}
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQ 2 -BBAA
Evaluation A

$C_6H_{14}O_6$ (c) 03MAG
Mannitol
Heat Capacity 298 K, C_p=240.1 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.315 cal·g^{-1}·K^{-1}.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q -DDLL -D
Evaluation D

$C_6H_{14}O_6$ (c) 82LIA/CHE
Mannitol(D)
Heat Capacity 298.15 K, C_p=239.00 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q -DDLL -D
Evaluation B

$C_6H_{14}O_6$ (c) 03MAG
Dulcite; Dulcitol; Galactitol
Heat Capacity 298 K, C_p=215.7 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.283 cal·g^{-1}·K^{-1}.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q -DLLD
Evaluation D

$C_6H_{14}O_6$ (c) 26PAR/HUI
Dulcite; Dulcitol; Galactitol
Heat Capacity 292.8 K, C_p=238.5 J·mol^{-1}·K^{-1}
Temperature range 88 to 293 K. Value is unsmoothed experimenta datum.
Entropy 298.1 K, S=247.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 73.35 J·mol^{-1}·K^{-1}.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q -DLLD
Evaluation B(C_p),C(S)
Meso form.

$C_6H_{14}O_6$ (c) 29PAR/KEI
Dulcite; Dulcitol; Galactitol
Entropy 298.1 K, S=234.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 60.25 J·mol^{-1}·K^{-1}. Revision o previous data.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q -DLLD
Evaluation C
Meso form.

$C_6H_{14}O_6$ (c) 90BAR/DEI
Dulcite; Dulcitol; Galactitol
Phase Changes
c/liq 460.3 K, ΔH=65100 J·mol^{-1}
ΔS=141.4 J·mol^{-1}·K^{-1}
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q -DLLD
Evaluation A

$C_6H_{14}O_6$ (c) 32SPA/THC
Mannitol
Heat Capacity 303 K, C_p=244.8 J·mol^{-1}·K^{-1}
Temperature range 30 to 200 °C.
Phase Changes
c/liq 433.2 K, ΔH=53580 J·mol^{-1}
ΔS=123.7 J·mol^{-1}·K^{-1}
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q -DDLL
Evaluation B

$C_6H_{14}O_6$ (c) 26PAR/AND
Mannitol(D)
Heat Capacity 294.1 K, C_p=236.0 J·mol^{-1}·K^{-1}
Temperature range 88 to 294 K. Value is unsmoothed experimental datum.
Entropy 298 K, S=253.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 78.66 J·mol^{-1}·K^{-1}.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q -DDLL -D
Evaluation B(C_p),C(S)

$C_6H_{14}O_6$ (c) 29PAR/KEL
Mannitol(D)
Entropy 298.1 K, S=238.5 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 64.02 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q -DDLL -D
Evaluation C

$C_6H_{14}O_6$ (c) 90BAR/DEL
Mannitol(D)
Phase Changes
c/liq 439.1 K, ΔH=56100 J·mol^{-1}
ΔS=127.8 J·mol^{-1}·K^{-1}
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q -BBAA -D
Evaluation A

$C_6H_{14}S$ (liq) 67MES/TOD
2,4-Dimethyl-3-thiapentane; Diisopropyl sulfide
Heat Capacity 298.15 K, C_p=232.00 J·mol^{-1}·K^{-1}
Temperature range 10 to 390 K.
Entropy 298.15 K, S=313.05 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 195.07 K, ΔH=10414 J·mol^{-1}
ΔS=53.39 J·mol^{-1}·K^{-1}
Molecular Weight 118.2366
Wiswesser Line Notation 1Y1&SY1&1
Evaluation A

$C_6H_{14}S$ (liq) 61MCC/FIN
4-Thiaheptane; Dipropyl sulfide
Heat Capacity 298.15 K, C_p=225.48 J·mol^{-1}·K^{-1}
Temperature range 11 to 370 K.
Entropy 298.15 K, S=338.28 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 170.44 K, ΔH=12142 J·mol^{-1}
ΔS=71.24 J·mol^{-1}·K^{-1}
Molecular Weight 118.2366
Wiswesser Line Notation 3S3
Evaluation A

$C_6H_{14}S$ (liq) 66GOO/DEP
1-Hexanethiol; n-Hexyl mercaptan
Heat Capacity 298.15 K, C_p=230.68 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 118.2366
Wiswesser Line Notation SH6
Evaluation A

$C_6H_{14}S$ (liq) 70FIN/MCC
1-Hexanethiol; n-Hexyl mercaptan
Heat Capacity 298.15 K, C_p=230.71 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=343.21 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 192.62 K, ΔH=18012 J·mol^{-1}
ΔS=93.51 J·mol^{-1}·K^{-1}
Molecular Weight 118.2366
Wiswesser Line Notation SH6
Evaluation A

$C_6H_{14}S$ (liq) 82TUT/GAB
1-Hexanethiol; n-Hexyl mercaptan
Heat Capacity 300 K, C_p=237.90 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K. C_p=221.21+3.060×10^{-2}T +8.343×10^{-5}T2.
Molecular Weight 118.2366
Wiswesser Line Notation SH6
Evaluation B

$C_6H_{14}S_2$ (liq) 58HUB/DOU
4,5-Dithiaoctane; Dipropyl disulfide
Heat Capacity 298.15 K, C_p=262.46 J·mol^{-1}·K^{-1}
Temperature range 10 to 360 K.
Entropy 298.15 K, S=373.55 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 187.66 K, ΔH=13807 J·mol^{-1}
ΔS=73.57 J·mol^{-1}·K^{-1}
Molecular Weight 150.2966
Wiswesser Line Notation 3SS3
Evaluation A

$C_6H_{15}Al$ (liq) 84SHE/NIS
Triethylaluminum
Heat Capacity 298.15 K, C_p=239.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=307.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 225.00 K, ΔH=10600 J·mol^{-1}
ΔS=47.11 J·mol^{-1}·K^{-1}
Molecular Weight 114.1660
Wiswesser Line Notation 2-AL-2&2
Evaluation A

$C_6H_{15}Al$ (liq) 89RAB/NIS
Triethylaluminum
Heat Capacity 298.15 K, C_p=239.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 313 K.
Entropy 298.15 K, S=308.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 225.00 K, ΔH=10600 J·mol^{-1}
ΔS=47.11 J·mol^{-1}·K^{-1}
Molecular Weight 114.1660
Wiswesser Line Notation 2-AL-2&2
Evaluation A

$C_6H_{15}As$ (liq) 72MAS/FAM
Triethylarsine
Heat Capacity 298.15 K, C_p=234.30 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Phase Changes
c/liq 181.8 K, ΔH=11058 J·mol^{-1}
ΔS=60.83 J·mol^{-1}·K^{-1}
Molecular Weight 162.1061
Wiswesser Line Notation 2-AS-2&2
Evaluation B

$C_6H_{15}B$ (c) 55FUR
Triethylboron
Heat Capacity 300 K, C_p=241.4 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 300 K, S=338.1 J·mol^{-1}·K^{-1}
Below 15°. Debye extrapolation.
Phase Changes
c,l/liq 180.3 K, ΔH=11853 J·mol^{-1}
ΔS=65.7 J·mol^{-1}·K^{-1}
liq/g 300 K, ΔH=3669 J·mol^{-1}
ΔS=122 J·mol^{-1}·K^{-1}
P=56.27 mmHg
Molecular Weight 97.9945
Wiswesser Line Notation 2B2&2
Evaluation B

$C_6H_{15}B$ (c) 77KOS/SAM
Triethylboron
Heat Capacity 298.15 K, C_p=240 J·mol^{-1}·K^{-1}
Temperature range 12 to 322 K. Data calculated from equation. C_p=6.2328+0.17161 T cal·mol^{-1}·K^{-1}.
Entropy 298.15 K, S=330.05 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 180.21 K, ΔH=11522 J·mol^{-1}
ΔS=63.94 J·mol^{-1}·K^{-1}
liq/g 321.81 K
Molecular Weight 97.9945
Wiswesser Line Notation 2B2&2
Evaluation B

$C_6H_{15}Bi$ (liq) 89NIS/RAB
Triethylbismuth
Heat Capacity 298.15 K, C_p=242.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K. C_p data also given for the glassy state (0–94.8 K) and the supercooled liquid (94.8–145.8 K). T(glass)=94.8 K.
Entropy 298.15 K, S=379.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 145.80 K, ΔH=8695 J·mol^{-1}
ΔS=59.64 J·mol^{-1}·K^{-1}
Molecular Weight 296.1649
Wiswesser Line Notation 2-BI-2&2
Evaluation A

$C_6H_{15}ClN_4O_2$ (c) 63COL/HUT2
Arginine hydrochloride(L)
Heat Capacity 298.15 K, C_p=260.96 J·mol^{-1}·K^{-1}
Temperature range 11 to 305 K.
Entropy 298.15 K, S=286.31 J·mol^{-1}·K^{-1}
Molecular Weight 210.6631
Wiswesser Line Notation QVYZ3MYZUM &GH -L
Evaluation A

$C_6H_{15}ErO_{12}S_3\cdot 9H_2O$ (c) 62GER/PEN
Erbium ethylsulfate nonahydrate
Heat Capacity 298.15 K, C_p=801.21 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=881.24 J·mol^{-1}·K^{-1}
Molecular Weight 704.7541
Wiswesser Line Notation WSO2&O 3 .ER &QH 9
Evaluation A

$C_6H_{15}Ga$ (liq) 72MAS/FAM
Triethylgallium; Gallium triethyl
Heat Capacity 298.15 K, C_p=278.03 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Phase Changes
c/liq 193.5 K, ΔH=11644 J·mol^{-1}
ΔS=60.18 J·mol^{-1}·K^{-1}
Molecular Weight 156.9045
Wiswesser Line Notation 2-GA-2&2
Evaluation B

$C_6H_{15}In$ (liq) 73MAS/NOV
Triethylindium
Heat Capacity 298.15 K, C_p=297.27 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Phase Changes
Anomaly in specific heat at 194.8 K.
c/liq 237.6 K, ΔH=13012 J·mol^{-1}
ΔS=54.77 J·mol^{-1}·K^{-1}
Molecular Weight 202.0045
Wiswesser Line Notation 2-IN-2&2
Evaluation B

$C_6H_{15}LuO_{12}S_3\cdot 9H_2O$ (c) 60GER/SPE
Lutetium ethylsulfate nonahydrate
Heat Capacity 295 K, C_p=802.7 J·mol^{-1}·K^{-1}
Temperature range 5 to 295 K.
Molecular Weight 712.4611
Wiswesser Line Notation WSO2&O 3 .LU &QH 9
Evaluation A

$C_6H_{15}N$ (liq) 1881RE
Triethylamine
Heat Capacity 298 K, C_p=177.0 J·mol^{-1}·K^{-1}
Temperature range 293 to 378 K.
Molecular Weight 101.1912
Wiswesser Line Notation 2N2&2
Evaluation D

$C_6H_{15}N$ (liq) 85HEP/KOC
Triethylamine
Heat Capacity 298.15 K, C_p=218.10 J·mol^{-1}·K^{-}
One temperature.
Molecular Weight 101.1912
Wiswesser Line Notation 2N2&2
Evaluation B

$C_6H_{15}N$ (liq) 93GRO/ROL
Triethylamine
Heat Capacity 298.15 K, C_p=216.43 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 101.1912
Wiswesser Line Notation 2N2&2
Evaluation B

$C_6H_{15}N$ (liq) 01KAH
Dipropylamine
Heat Capacity C_p=252.6 J·mol^{-1}·K^{-1}
Temperature range 294.15 to 403.15 K. Heat capacity is an average value over the temperature range.
Molecular Weight 101.1912
Wiswesser Line Notation 3M3
Evaluation D

$C_6H_{15}N$ (liq) 71KON/WAD
1-Aminohexane; n-Hexylamine
Heat Capacity 298.15 K, C_p=252 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 101.1912
Wiswesser Line Notation Z6
Evaluation B

$C_6H_{15}N_3$ (liq) 88BOB/KAM
N-(2-Aminoethyl)piperazine
Heat Capacity 333 K, C_p=284 J·mol^{-1}·K^{-1}
Temperature range 333 to 473 K.
Molecular Weight 129.2046
Wiswesser Line Notation T6M DNTJ D2Z
Evaluation D

$C_6H_{15}NO_3$ (liq) 82MIN/SAB
Triethanolamine
Heat Capacity 298.15 K, C_p=389 J·mol^{-1}·K^{-1}
One temperature. C_p given as 2.6 J·K^{-1}·g^{-1}.
Molecular Weight 149.1894
Wiswesser Line Notation Q2N2Q2Q
Evaluation C

$C_6H_{15}O_{12}S_3Y·9H_2O$ (c) 62GER/PEN
Yttrium ethylsulfate nonahydrate
Heat Capacity 298.15 K, C_p=799.40 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=853.84 J·mol^{-1}·K^{-1}
Molecular Weight 626.4000
Wiswesser Line Notation WSO2&O 3 .Y &QH 9
Evaluation A

$C_6H_{15}Sb$ (liq) 73MAS/NOV
Triethylstibine; Triethylantimony
Heat Capacity 298.15 K, C_p=242.25 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Phase Changes
c/liq 153.9 K, ΔH=9452 J·mol^{-1}
ΔS=61.42 J·mol^{-1}·K^{-1}
Molecular Weight 208.9345
Wiswesser Line Notation 2-SB-2&2
Evaluation B

$C_6H_{16}CdCl_4N_2$ (c) 82WHI/STA
Tetrachlorobis-(2-propeneammonium) cadmium II
Heat Capacity 298.15 K, C_p=362.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=497.0 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 206.9 K, ΔH=2140 J·mol^{-1}
ΔS=7.87 J·mol^{-1}·K^{-1}
c,II/c,I 266.7 K, ΔH=2000 J·mol^{-1}
ΔS=7.87 J·mol^{-1}·K^{-1}
Molecular Weight 370.4278
Wiswesser Line Notation Z2U1 2 -CD- G4
Evaluation A

$C_6H_{16}N_4O_6$ (c) 85NUR/BER
Triacetamide nitrate
Heat Capacity 298.15 K, C_p=383.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 330 K.
Entropy 298.15 K, S=443.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 337 K
Molecular Weight 240.2156
Wiswesser Line Notation ZV1 3 &WNQ
Evaluation A

$C_6H_{16}Si_2$ (liq) 73DZH/GUS
Tetramethyldisiletan; Tetramethyldisilacyclobutane;
1,1,3,3-Tetramethyl-1,3-disilacyclobutane
Heat Capacity
Temperature range 12 to 300 K. C_p data only in complete paper deposited at VINITI, No. 5024-72, 3 Nov 1972.
Entropy 298.15 K, S=296.27 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 266.02 K, ΔH=10259 J·mol^{-1}
ΔS=38.56 J·mol^{-1}·K^{-1}
Molecular Weight 144.3634
Wiswesser Line Notation T4-SI-C-SI-TJ A1 A1 C1 C1
Evaluation B

$C_6H_{16}Si_2$ (c) 75GUS/KAR
Tetramethyldisiletan; Tetramethyldisilacyclobutane;
1,1,3,3-Tetramethyl-1,3-disilacyclobutane
Heat Capacity 298.15 K, C_p=216.94 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K. Data given graphically.
Entropy 298.15 K, S=296.27 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 266.02 K, ΔH=10259 J·mol^{-1}
ΔS=38.58 J·mol^{-1}·K^{-1}
liq/g 390.93 K, ΔH=39480 J·mol^{-1}
ΔS=91.34 J·mol^{-1}·K^{-1}
Molecular Weight 144.3634
Wiswesser Line Notation T4-SI-TJ A1 A1 C1 C1
Evaluation B

$C_6H_{17}BeF_4N_3O_6$ (c) 79LOI/OSB
Triglycine fluoroberyllate
Heat Capacity 300 K, C_p=412.8 J·mol^{-1}·K^{-1}
Temperature range 294 to 340 K. C_p given as 0.316 cal·g^{-1}·K^{-1}.
Molecular Weight 312.2226
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4
Evaluation B

$C_6H_{17}BeF_4N_3O_6$ (c) 81LOI/KOS
Triglycine fluoroberyllate
Heat Capacity 308 K, C_p=444 J·mol^{-1}·K^{-1}
One temperature. C_p(35 °C)=0.34 cal·g^{-1}·°C^{-1}.
Molecular Weight 312.2226
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4
Evaluation B

$C_6H_{17}BeF_4N_3O_6$ (c) 81LOI/KOS2
Triglycine fluoroberyllate
Phase Changes
c,II/c,I 345 K, ΔH=1254 J·mol^{-1}
ΔS=3.63 J·mol^{-1}·K^{-1}
Ferroelectric transition.
Molecular Weight 312.2226
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4
Evaluation C

$C_6H_{17}N_3O_{10}S$ (c,II) 68AGU/TEL
Triglycine sulfate
Heat Capacity
C_p data only graphically. Temperature range 12 to 60 °C.
Phase Changes
c,II/c,I 322 K, $\Delta H = 1079$ J·mol^{-1}
$\Delta S = 3.26$ J·mol^{-1}·K^{-1}
Molecular Weight 323.2804
Wiswesser Line Notation Z1VQ 3 &WSQQ
Evaluation C

$C_6H_{17}N_3O_{10}S$ (c) 75CAM/GON
Triglycine sulfate
Heat Capacity 300 K, $C_p = 420$ J·mol^{-1}·K^{-1}
Temperature range 100 to 400 K. Data given graphically; C_p estimated from graph.
Phase Changes
c,II/c,I 322.55 K, $\Delta H = 614$ J·mol^{-1}
$\Delta S = 1.9$ J·mol^{-1}·K^{-1}
Molecular Weight 323.2804
Wiswesser Line Notation Z1VQ 3 &WSQQ
Evaluation C_p(D); Phase change(B)

$C_6H_{17}N_3O_{10}S$ (c) 79LOI/OSB
Triglycine sulfate
Heat Capacity 300 K, $C_p = 407$ J·mol^{-1}·K^{-1}
Temperature range 294 to 340 K. $C_p = 0.301$ cal·g^{-1}·K^{-1}.
Phase Changes
c,II/c,I $\Delta H = 622$ J·mol^{-1}
No temperature given.
Molecular Weight 323.2804
Wiswesser Line Notation Z1VQ 3 &WSQQ
Evaluation B

$C_6H_{17}N_3O_{10}S$ (c) 80RAM/CER
Triglycine sulfate
Heat Capacity 322 K, $C_p = 426.7$ J·mol^{-1}·K^{-1}
Temperature 322 K. One temperature near the critical temperature.
Phase Changes
c,II/c,I 322 K
Specific heat anomaly at 322 K equal to 0.28 J·g^{-1}·K^{-1}.
Molecular Weight 323.2804
Wiswesser Line Notation Z1VQ 3 &WSQQ
Evaluation A

$C_6H_{17}N_3O_{10}S$ (c) 81LOI/KOS
Triglycine sulfate
Heat Capacity 308 K, $C_p = 419$ J·mol^{-1}·K^{-1}
One temperature. C_p(35 °C) = 0.31 cal·g^{-1}·°C^{-1}.
Molecular Weight 323.2804
Wiswesser Line Notation Z1VQ 3 &WSQQ
Evaluation B

$C_6H_{17}N_3O_{10}S \cdot C_6H_{17}N_3O_{10}Se$ (c) 83GUL/POL
Triglycine sulfate-triglycine selenate
Heat Capacity 303 K, $C_p = 461$ J·mol^{-1}·K^{-1}
One temperature. $C_p = 1.26$ J·g^{-1}·C^{-1}.
Molecular Weight 365.4850
Wiswesser Line Notation Z1VQ 3 &WSQQ−&Z1VQ 3 &W-SE-QQ
Evaluation C
TGS0.10−TGSe0.90

$C_6H_{18}BN$ (liq) 67SMI/GOO
Triethylamineborane
Heat Capacity 298.15 K, $C_p = 256.9$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 115.0249
Wiswesser Line Notation 2N2&2 &BHHH
Evaluation B

$C_6H_{18}BN$ (liq) 70FIN/TOD
Triethylamineborane
Heat Capacity 298.15 K, $C_p = 257.11$ J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, $S = 301.71$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.48 K, $\Delta H = 14906.3$ J·mol^{-1}
$\Delta S = 55.32$ J·mol^{-1}·K^{-1}
Molecular Weight 115.0249
Wiswesser Line Notation 2N2&2 &BHHH
Evaluation A

$C_6H_{18}N_3OP$ (liq) 82VOR/YAK
Hexamethylphosphoramide; Hexamethylphosphoric triamide
Heat Capacity 298.15 K, $C_p = 321.3$ J·mol^{-1}·K^{-1}
Temperature range 297.15 to 299.15 K. C_p given as 1.793 J·K^{-1}·g^{-1}.
Molecular Weight 179.2015
Wiswesser Line Notation OPN1&1&N1&1&N1&1
Evaluation B

$C_6H_{18}N_4$ (liq) 88BOB/KAM
Triethylenetetramine
Heat Capacity 333 K, $C_p = 376$ J·mol^{-1}·K^{-1}
Temperature range 333 to 473 K.
Molecular Weight 146.2350
Wiswesser Line Notation Z2M2M2Z
Evaluation D

$C_6H_{18}OSi_2$ (liq) 61SCO/MES
Hexamethyldisiloxane
Heat Capacity 298.15 K, $C_p = 311.37$ J·mol^{-1}·K^{-1}
Temperature range 12 to 371 K.
Entropy 298.15 K, $S = 433.84$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 204.93 K, $\Delta H = 11921.9$ J·mol^{-1}
$\Delta S = 58.18$ J·mol^{-1}·K^{-1}
Molecular Weight 162.3786
Wiswesser Line Notation 1-SI-1&1&O-SI-1&1&1
Evaluation A

$C_6H_{18}OSi_2$ (liq) 86DZH/KUL
Hexamethyldisiloxane
Heat Capacity 298.15 K, $C_p = 311.4$ J·mol^{-1}·K^{-1}
Temperature range 4 to 300 K. C_p(liq) = 275.5−34.48×10^{-2}T+21.7×10^{-1}T^2 (204 to 375 K).
Entropy 298.15 K, $S = 433.8$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 204.93 K, $\Delta H = 11920$ J·mol^{-1}
Molecular Weight 162.3786
Wiswesser Line Notation 1-SI-1&1&O-SI-1&1&1
Evaluation A

$C_6H_{18}O_3Si_3$ (liq) 77KUL/DZH2
Hexamethylcyclotrisiloxane
Heat Capacity
Temperature range 12 to 350 K. Data deposited in VINITI, No. 987-77, 14 March 1977. Includes C_p, S, ΔH phase transitions.
Molecular Weight 222.4629
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A1 A1 C1 C1 E1 E1
Evaluation C

$C_6H_{18}O_3Si_3$ (c) 82KUL/DZH
Hexamethylcyclotrisiloxane
Heat Capacity 298.15 K, C_p=360.0 J·mol^{-1}·K^{-1}
Temperature range 4.2 to 370 K. Data given graphically except for data at 298.15 K.
Entropy 298.15 K, S=412.1 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 335.22 K, ΔH=16611 J·mol^{-1}
ΔS=49.5 J·mol^{-1}·K^{-1}
Molecular Weight 222.4629
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A1 A1 C1 C1 E1 E1
Evaluation B

$C_6H_{18}Si_2$ (liq) 59SUG/SEK
Hexamethyldisilane
Heat Capacity 295.67 K, C_p=255.89 J·mol^{-1}·K^{-1}
Temperature range 200 to 300 K. Value is unsmoothed experimental datum.
Phase Changes
c,II/c,I 221.8 K, ΔH=9750 J·mol^{-1}
ΔS=43.96 J·mol^{-1}·K^{-1}
c,I/liq 287.7 K, ΔH=3017 J·mol^{-1}
ΔS=10.49 J·mol^{-1}·K^{-1}
Molecular Weight 146.3792
Wiswesser Line Notation 1-SI-1&1-SI-1&1&1
Evaluation B

$C_6H_{20}CdCl_4N_2$ (c) 81WHI/GRA
Tetrachlorobis-(n-propylammonium) cadmium II
Heat Capacity 298.15 K, C_p=380.3 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=519.7 J·mol^{-1}·K^{-1}
Phase Changes
c,IV/c.III 105.5 K, ΔH=1472 J·mol^{-1}
ΔS=13.96 J·mol^{-1}·K^{-1}
c.III/c.II 156.8 K, ΔH=598 J·mol^{-1}
ΔS=3.85 J·mol^{-1}·K^{-1}
c.II/c,I 178.7 K, ΔH=1021 J·mol^{-1}
ΔS=6.15 J·mol^{-1}·K^{-1}
Molecular Weight 374.4594
Wiswesser Line Notation Z3H 2 -CD- G4
Evaluation A

$C_6H_{20}Cl_4MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(n-propylammonium) manganese II
Phase Changes
c.IV/c.III 323 K, ΔH=67.2 J·mol^{-1}
ΔS=0.22 J·mol^{-1}·K^{-1}
c.III/c.II 383 K, ΔH=14.4 J·mol^{-1}
ΔS=0.036 J·mol^{-1}·K^{-1}
c.II/c.I 445 K, ΔH=5.3 J·mol^{-1}
ΔS=0.12 J·mol^{-1}·K^{-1}
Molecular Weight 316.9874
Wiswesser Line Notation Z3H 2 -MN- G4
Evaluation A

$C_6H_{20}Cl_4MnN_2$ (c) 81WHI/GRA
Tetrachlorobis-(n-propylammonium) manganese II
Heat Capacity 298.15 K, C_p=391.2 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=516.3 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 112.8 K, ΔH=586 J·mol^{-1}
ΔS=5.48 J·mol^{-1}·K^{-1}
c,II/c,I 164.3 K, ΔH=498 J·mol^{-1}
ΔS=3.31 J·mol^{-1}·K^{-1}
Molecular Weight 316.9874
Wiswesser Line Notation Z3H 2 -MN- G4
Evaluation A

$C_6H_{20}Cl_4N_2Pb$ (c) 91CHA/COU
Bis(propylammonium) tetrachloroplumbate(II)
Phase Changes
c,II/c,I 339.5 K, ΔH=3250 J·mol^{-1}
Molecular Weight 469.2494
Wiswesser Line Notation ZH&3 2 -PB- G4
Evaluation B

$C_6H_{20}Cl_4N_2Pb$ (c) 91ROM/LAU
Bis(propylammonium) tetrachloroplumbate(II)
Phase Changes
c,IV/c,III 340 K, ΔH=3730 J·mol^{-1}
ΔS=11 J·mol^{-1}·K^{-1}
c,III/c,II 371 K, ΔH=220 J·mol^{-1}
ΔS=0.59 J·mol^{-1}·K^{-1}
c,II/c,I 406 K, ΔH=250 J·mol^{-1}
ΔS=0.61 J·mol^{-1}·K^{-1}
Molecular Weight 469.2494
Wiswesser Line Notation ZH&3 2 -PB- G4
Evaluation B

$C_6H_{20}Cl_4N_2Pb$ (c) 92ROM/LAU
Bis(propylammonium) tetrachloroplumbate(II)
Phase Changes
c,IV/c,III 340 K, ΔH=3730 J·mol^{-1}
ΔS=11 J·mol^{-1}·K^{-1}
c,III/c,II 371 K, ΔH=220 J·mol^{-1}
ΔS=0.59 J·mol^{-1}·K^{-1}
c,II/c,I 406 K, ΔH=250 J·mol^{-1}
ΔS=0.61 J·mol^{-1}·K^{-1}
Molecular Weight 469.2494
Wiswesser Line Notation 3ZH 2 -PB- G4
Evaluation A

$C_6H_{21}N_3Si_3$ (liq) 81MEK/KAR
Hexamethylcyclotrisilazane
Heat Capacity 298.15 K, C_p=428.0 J·mol^{-1}·K^{-1}
Temperature range 13 to 390 K. Data given graphically.
Entropy 298.15 K, S=460 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 254.4 K, ΔH=15171 J·mol^{-1}
ΔS=61.38 J·mol^{-1}·K^{-1}
Molecular Weight 219.5085
Wiswesser Line Notation T6-SI-M-SI-M-SI-MTJ A1 A1 C1 C1 E1 E1
Evaluation A

$C_6O_{12}Ce_2$ (c) 85GAL/DWO
Cerium(III) oxalate
Heat Capacity 418 K, C_p=499.2 J·mol^{-1}·K^{-1}
Temperature range 298 to 773 K. C_p=3.2177×10^1−(1.9668×10^{-1})T+(4.0732×10^{-1})T^2−(2.7686×10^{-1})T^3 J·K^{-1}·g^{-1} over the temperature range 418 to 538 K.
Molecular Weight 544.2888
Wiswesser Line Notation OV1 3 .CE 2
Evaluation B

C_7F_8 (liq) 74AND/MAR
Octafluorotoluene; Perfluorotoluene
Heat Capacity 298.15 K, C_p=262.3 J·mol^{-1}·K^{-1}
Temperature range 10 to 315 K.
Entropy 298.15 K, S=355.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 207.69 K, ΔH=11490 J·mol^{-1}
ΔS=55.32 J·mol^{-1}·K^{-1}
Molecular Weight 236.0642
Wiswesser Line Notation FXFFR BF CF DF EF FF
Evaluation A

C_7F_8 (liq) 75PAU
Octafluorotoluene; Perfluorotoluene
Heat Capacity 298.15 K, C_p=266.4 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=360.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 207.62 K, ΔH=11581 J·mol^{-1}
Molecular Weight 236.0642
Wiswesser Line Notation FXFFR BF CF DF EF FF
Evaluation A

C_7F_{14} (liq) 57YAR/KAY
Perfluoromethylcyclohexane
Heat Capacity 298 K, C_p=353.1 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K. Equation only.
Molecular Weight 350.0546
Wiswesser Line Notation L6TJ AXFFF AF BF BF CF CF DF DF EF EF FF FF
Evaluation B

C_7F_{16} (liq) 51OLI/GRI
Perfluoroheptane; Hexadecafluoroheptane
Heat Capacity 300 K, C_p=419.47 J·mol^{-1}·K^{-1}
Temperature range 18 to 310 K.
Entropy 298.15 K, S=561.80 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 180.45 K, ΔH=6670.6 J·mol^{-1}
ΔS=36.97 J·mol^{-1}·K^{-1}
c,I/liq 221.86 K, ΔH=6947.2 J·mol^{-1}
ΔS=31.31 J·mol^{-1}·K^{-1}
Molecular Weight 388.0514
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFXFFF
Evaluation A

C_7F_{16} (liq) 57YAR/KAY
Perfluoroheptane; Hexadecafluoroheptane
Heat Capacity 298 K, C_p=411.3 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K. Equation only.
Molecular Weight 388.0514
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFXFFF
Evaluation B

C_7F_{16} (liq) 83CAM/DIA
Perfluoroheptane; Hexadecafluoroheptane
Heat Capacity 293 K, C_p=322.2 J·mol^{-1}·K^{-1}
Interpolated data.
Molecular Weight 388.0514
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFXFFF
Evaluation C

$C_7H_3F_5$ (liq) 68COU/HAL
2,3,4,5,6-Pentafluorotoluene
Heat Capacity 298.15 K, C_p=225.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 376 K.
Entropy 298.15 K, S=306.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 70.3 K, ΔH=210.3 J·mol^{-1}
ΔS=2.94 J·mol^{-1}·K^{-1}
c,II/c,I 243.35 K, ΔH=12990 J·mol^{-1}
ΔS=53.38 J·mol^{-1}·K^{-1}
Molecular Weight 182.0927
Wiswesser Line Notation FR BF CF DF EF F1
Evaluation A

$C_7H_3F_5$ (liq) 71PAL
2,3,4,5,6-Pentafluorotoluene
Heat Capacity 298.15 K, C_p=231.12 J·mol^{-1}·K^{-1}
Temperature range 12 to 305 K. Data deposited VINITI, No 2538-71, 20 Jan 1971.
Entropy 298.15 K, S=310.87 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 243.7 K, ΔH=13280 J·mol^{-1}
ΔS=54.49 J·mol^{-1}·K^{-1}
Transition 0.3 K below mp, ΔH is sum of transition and fusion.
Molecular Weight 182.0927
Wiswesser Line Notation FR BF CF DF EF F1
Evaluation A

C_7H_4ClNO (liq) 65ZAL/KOC
m-Chlorophenylisocyanate
Heat Capacity 294.2 K, C_p=187.0 J·mol^{-1}·K^{-1}
Temperature range 294, 323 K.
Molecular Weight 153.5677
Wiswesser Line Notation OCNR CG
Evaluation C

C_7H_4ClNO (c) 65ZAL/KOC
p-Chlorophenylisocyanate
Heat Capacity 282 K, C_p=210.9 J·mol^{-1}·K^{-1}
Temperature range 273 to 290 K. Mean value.
Molecular Weight 153.5677
Wiswesser Line Notation OCNR DG
Evaluation C

$C_7H_4CrO_3S$ (c) 78POM/CHI
Thiophene chromium tricarbonyl
Heat Capacity 298.15 K, C_p=193.0 J·mol^{-1}·K^{-1}
Temperature range 120 to 300 K. Data given graphically C_p = 71.02 − 4.41 × 10^{-1}T+4.61×10^{-3}T^2−5.96×10^{-6}T J·mol^{-1}·K^{-1} (105 to 130 K; 245 to 300 K). C_p value calculated from equation.
Phase Changes
c,II/c,I 185 K, ΔH=1650 J·mol^{-1}
ΔS=8.95 J·mol^{-1}·K^{-1}
Molecular Weight 220.1628
Wiswesser Line Notation T5SϕJ ϕ-CR- CO 3
Evaluation C (C_p), A (Phase changes)

$C_7H_4CrO_3Se$ (c) 78POM/CHH
Selenophene chromium tricarbonyl
Heat Capacity 298.15 K, C_p=272.9 J·mol^{-1}·K^{-1}
Temperature range 125 to 337 K. Data given graphically. Sp=116.8+2.69×10^{-1}T+1.48×10^{-3}T^2−2.08×10^{-6}T^3 J·mol^{-1}·K^{-1} (125 to 337 K). C_p value calculated from equation.
Molecular Weight 267.0628
Wiswesser Line Notation T5-SE-ϕJ ϕ-CR− CO 3
Evaluation C (C_p), A (Phase changes)

$C_7H_4CrO_3Se$ (c) 81CHH/POM
Selenophene chromium tricarbonyl
Heat Capacity 298.15 K, C_p=272.9 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K. Data given graphically. C_p=116.8+2.69×10^{-1}T+1.48×10^{-3}T^2−2.08×$^{-6}$T^3 J·mol^{-1}·K^{-1}. C_p value calculated from equation.
Molecular Weight 267.0628
Wiswesser Line Notation T5-SE-ϕJ ϕ-CR− CO 3
Evaluation B

$C_7H_4CrO_3Te$ (c) 78POM/CHH
Tellurophene chromium tricarbonyl
Heat Capacity 298.15 K, C_p=278.7 J·mol^{-1}·K^{-1}
Temperature range 124 to 326 K. Data given graphically. C_p=96.85+1.67×10^{-1}T+2.44×10^{-3}T^2−3.19×10^{-6}T^3 J·mol^{-1}·K^{-1} (124 to 326 K). C_p value calculated from equation.
Molecular Weight 315.7028
Wiswesser Line Notation T5-TE-ϕJ ϕ-CR− CO 3
Evaluation C (C_p), A (Phase changes)

$C_7H_4CrO_3Te$ (c) 81CHH/POM
Tellurophene chromium tricarbonyl
Heat Capacity 298.15 K, C_p=278.7 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K. Data given graphically. C_p=96.85+1.67×10^{-1}T+2.44×10^{-3}T^2−3.19×10^{-6}T^3 J·mol^{-1}·K^{-1}. C_p value calculated from equation.
Molecular Weight 315.7028
Wiswesser Line Notation T5-TE-ϕJ ϕ-CR− CO 3
Evaluation B

$C_7H_4F_3NO_2$ (liq) 81LEB/RYA
3-Trifluoromethyl nitrobenzene
Heat Capacity C_p=224.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K. Data given over temperature range.
Molecular Weight 191.1093
Wiswesser Line Notation WNR CXFFF
Evaluation B

$C_7H_4MnNO_3$ (c) 78POM/CHH
Azacymantrene; Pyrroyl manganese tricarbonyl
Heat Capacity 298.15 K, C_p=236.3 J·mol^{-1}·K^{-1}
Temperature range 124 to 293 K. Data given graphically. C_p=172.3−1.16T+7.86×10^{-3}T^2−1.09×10^{-5}T^3 J·mol^{-1}·K^{-1} (124 to 150 K; 240 to 293 K). C_p value calculated from equation.
Phase Changes
c,II/c,I 150–240 K, ΔH=702 J·mol^{-1}
ΔS=3.55 J·mol^{-1}·K^{-1}
Molecular Weight 205.0515
Wiswesser Line Notation T5NϕJ ϕ-MN− CO 3
Evaluation C (C_p), A (Phase changes)

$C_7H_4MnNO_3$ (c) 83CHH/POM
Azacymantrene; Pyrroyl manganese tricarbonyl
Heat Capacity 298.15 K, C_p=216.2 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=250.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 305 K, ΔH=1910 J·mol^{-1}
ΔS=6.3 J·mol^{-1}·K^{-1}
c,I/liq 315.5 K, ΔH=13010 J·mol^{-1}
ΔS=41 J·mol^{-1}·K^{-1}
Molecular Weight 205.0515
Wiswesser Line Notation T5NϕJ ϕ-MN− CO 3
Evaluation A

$C_7H_5BrO_2$ (c) 87FER/PIL
2-Bromobenzoic acid
Heat Capacity 298.15 K, C_p=153.8 J·mol^{-1}·K^{-1}
One temperature. Value given as C_p=0.765 J·K^{-1}·g^{-1}.
Molecular Weight 201.0193
Wiswesser Line Notation QVR BE
Evaluation C

$C_7H_5BrO_2$ (c) 87FER/PIL
3-Bromobenzoic acid
Heat Capacity 298.15 K, C_p=151.4 J·mol^{-1}·K^{-1}
One temperature. Value given as C_p=0.753 J·K^{-1}·g^{-1}.
Molecular Weight 201.0193
Wiswesser Line Notation QVR CE
Evaluation C

$C_7H_5BrO_2$ (c) 87FER/PIL
4-Bromobenzoic acid
Heat Capacity 298.15 K, C_p=151.4 J·mol^{-1}·K^{-1}
One temperature. Value given as C_p=0.753 J·K^{-1}·g^{-1}.
Molecular Weight 201.0193
Wiswesser Line Notation QVR DE
Evaluation B

C_7H_5ClO (liq) 1881REI
Benzoyl chloride
Heat Capacity 298 K, C_p=187.0 J·mol^{-1}·K^{-1}
Temperature range 290 to 477 K.
Molecular Weight 140.5689
Wiswesser Line Notation GVR
Evaluation D

$C_7H_5ClO_2$ (c) 26AND/LYN
2-Chlorobenzoic acid
Heat Capacity 298 K, C_p=163.2 J·mol^{-1}·K^{-1}
Temperature range 22 to 200 °C.
Phase Changes
c/liq 413.4 K, ΔH=25730 J·mol^{-1}
ΔS=62.2 J·mol^{-1}·K^{-1}
Molecular Weight 156.5683
Wiswesser Line Notation QVR BG
Evaluation C

$C_7H_5ClO_2$ (c) 91SAB/HIR
2-Chlorobenzoic acid
Phase Changes
c/liq 414.10 K, ΔH=26290 J·mol^{-1}
Molecular Weight 156.5683
Wiswesser Line Notation QVR BG
Evaluation A

$C_7H_5ClO_2$ (c) 26AND/LYN
3-Chlorobenzoic acid
Heat Capacity 298 K, $C_p = 163.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 22 to 205 °C.
Phase Changes
c/liq 427.4 K, $\Delta H = 23850\ J \cdot mol^{-1}$
$\Delta S = 55.8\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 156.5683
Wiswesser Line Notation QVR CG
Evaluation C

$C_7H_5ClO_2$ (c) 91SAB/HIR
3-Chlorobenzoic acid
Phase Changes
c/liq 427.83 K, $\Delta H = 22000\ J \cdot mol^{-1}$
Molecular Weight 156.5683
Wiswesser Line Notation QVR CG
Evaluation A

$C_7H_5ClO_2$ (c) 26AND/LYN
4-Chlorobenzoic acid
Heat Capacity 298 K, $C_p = 167.8\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 22 to 265 °C.
Phase Changes
c/liq 512.9 K, $\Delta H = 32260\ J \cdot mol^{-1}$
$\Delta S = 62.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 156.5683
Wiswesser Line Notation QVR DG
Evaluation C

$C_7H_5ClO_2$ (c) 91SAB/HIR
4-Chlorobenzoic acid
Phase Changes
c/liq 513.53 K, $\Delta H = 34260\ J \cdot mol^{-1}$
Molecular Weight 156.5683
Wiswesser Line Notation QVR DG
Evaluation A

$C_7H_5Cl_3$ (liq) 87GOA/BOE
Benzotrichloride; α,α,α-Trichlorotoluene
Phase Changes
c,l/liq 235.99 K, $\Delta H = 13950\ J \cdot mol^{-1}$
$\Delta S = 59.11\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 108.1396
Wiswesser Line Notation GXGGR
Evaluation A

$C_7H_5F_3$ (liq) 59SCO/DOU
Benzotrifluoride; α,α,α-Trifluorotoluene
Heat Capacity 298.15 K, $C_p = 188.45\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 12 to 365 K.
Entropy 298.15 K, $S = 271.50\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 244.14 K, $\Delta H = 13782\ J \cdot mol^{-1}$
$\Delta S = 56.45\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 146.1117
Wiswesser Line Notation FXFFR
Evaluation A

$C_7H_5IO_2$ (c) 92SAB/ELW
4-Iodobenzoic acid
Phase Changes
c/liq 544.74 K, $\Delta H = 33940\ J \cdot mol^{-1}$
Molecular Weight 248.0198
Wiswesser Line Notation QVR DI
Evaluation A

C_7H_5N (liq) 83BYK/LEI
Benzonitrile
Heat Capacity 298.15 K, $C_p = 165.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 330 K.
Entropy 298.15 K, $S = 209.1\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 260.33 K, $\Delta H = 10980\ J \cdot mol^{-1}$
$\Delta S = 42.16\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation A

C_7H_5N (liq) 84BYK/KI
Benzonitrile
Heat Capacity 298.15 K, $C_p = 165.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 14 to 330 K.
Phase Changes
c,l/liq 260.33 K, $\Delta H = 10980\ J \cdot mol^{-1}$
$\Delta S = 42.16\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation A

C_7H_5N (liq) 84LEB/BYK
Benzonitrile
Heat Capacity 298.15 K, $C_p = 165.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 25 to 330 K.
Entropy 298.15 K, $S = 209.1\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 260.332 K, $\Delta H = 10980\ J \cdot mol^{-1}$
$\Delta S = 42.16\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation A

C_7H_5N (liq) 85LAI/ROI
Benzonitrile
Heat Capacity 298.15 K. $C_p = 166.24\ J \cdot mol^{-1} \cdot K^{-}$
One temperature.
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation B

C_7H_5N (liq) 85LEB/BYI
Benzonitrile
Heat Capacity 298.15 K, $C_p = 165.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 330 K.
Entropy 298.15 K, $S = 209.1\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 260.33 K, $\Delta H = 10980\ J \cdot mol^{-1}$
$\Delta S = 42.16\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation A

C_7H_5N (liq) 85TAN/NAK
Benzonitrile
Heat Capacity 298.15 K, C_p=166.52 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation B

C_7H_5N (liq) 87MIR/SHA
Benzonitrile
Heat Capacity 298.15 K, C_p=161.1 J·mol^{-1}·K^{-1}
Temperature range 273 to 453 K. Unsmoothed experimental datum given as 1.496 kJ/kg·K at 293 K. C_p(liq)=1.2396 +8.7×10^{-5} T/K+3.3333×10^{-6} T^2/K^2 kJ/kg·K (273 to 453 K).
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation C

C_7H_5NO (c,I) 92STE/CHI4
Benzoxazole
Heat Capacity 298.15 K, C_p=141.59 J·mol^{-1}·K^{-1}
Temperature range 5 to 650 K. C_p(liq, 298.15 K)=178.50 J/K·mol. C_p value for the liquid at 298.15 K was calculated with graphically extrapolated data.
Entropy 298.15 K, S=148.95 J·mol^{-1}·K^{-1}
S(liq, 298.15 K)=203.91 J/K·mol. S value for the liquid at 298.15 K was calculated with graphically extrapolated data.
Phase Changes
c,II/c,I 247.0 K, ΔH=18.29 J·mol^{-1}
c,I/liq 302.505 K, ΔH=16784 J·mol^{-1}
Molecular Weight 119.1226
Wiswesser Line Notation T56 BN DOJ
Evaluation A

C_7H_5NO (liq) 93STE/CHI2
Phenyl isocyanate
Heat Capacity 298.15 K, C_p=186.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 119.1226
Wiswesser Line Notation OCNR
Evaluation A

$C_7H_5NO_4$ (c) 26AND
2-Nitrobenzoic acid
Heat Capacity 297.9 K, C_p=190.0 J·mol^{-1}·K^{-1}
Temperature range 110 to 344 K. Value is unsmoothed experimental datum.
Molecular Weight 167.1208
Wiswesser Line Notation WNR BVQ
Evaluation C

$C_7H_5NO_4$ (c) 26AND/LYN
2-Nitrobenzoic acid
Heat Capacity 298 K, C_p=191.6 J·mol^{-1}·K^{-1}
Temperature range 22 to 240 °C.
Phase Changes
c/liq 419.0 K, ΔH=27990 J·mol^{-1}
ΔS=66.8 J·mol^{-1}·K^{-1}
Molecular Weight 167.1208
Wiswesser Line Notation WNR BVQ
Evaluation C

$C_7H_5NO_4$ (c) 41SAT/SOG
2-Nitrobenzoic acid
Heat Capacity 323 K, C_p=202.1 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 167.1208
Wiswesser Line Notation WNR BVQ
Evaluation C
Same data in 40SAT/SOG2.

$C_7H_5NO_4$ (c) 26AND
3-Nitrobenzoic acid
Heat Capacity 297.9 K, C_p=179.9 J·mol^{-1}·K^{-1}
Temperature range 110 to 344 K. Value is unsmoothed experimental datum.
Molecular Weight 167.1208
Wiswesser Line Notation WNR CVQ
Evaluation C

$C_7H_5NO_4$ (c) 26AND/LYN
3-Nitrobenzoic acid
Heat Capacity 298 K, C_p=173.2 J·mol^{-1}·K^{-1}
Temperature range 22 to 225 °C.
Phase Changes
c/liq 414.3 K, ΔH=19330 J·mol^{-1}
ΔS=46.7 J·mol^{-1}·K^{-1}
Molecular Weight 167.1208
Wiswesser Line Notation WNR CVQ
Evaluation C

$C_7H_5NO_4$ (c) 41SAT/SOG
3-Nitrobenzoic acid
Heat Capacity 323 K, C_p=201.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 167.1208
Wiswesser Line Notation WNR CVQ
Evaluation C
Same data in 40SAT/SOG2.

$C_7H_5NO_4$ (c) 90RAI/MAN
3-Nitrobenzoic acid
Phase Changes
c/liq 413 K, ΔH=21400 J·mol^{-1}
ΔS=51.6 J·mol^{-1}·K^{-1}
Temperature from graph.
Molecular Weight 167.1208
Wiswesser Line Notation WNR CVQ
Evaluation A

$C_7H_5NO_4$ (c) 26AND
4-Nitrobenzoic acid
Heat Capacity 297.9 K, C_p=182.8 J·mol^{-1}·K^{-1}
Temperature range 110 to 344 K. Value is unsmoothed experimental datum.
Molecular Weight 167.1208
Wiswesser Line Notation WNR DVQ
Evaluation C

$C_7H_5NO_4$ (c) 26AND/LYN
4-Nitrobenzoic acid
Heat Capacity 298 K, C_p=180.3 J·mol^{-1}·K^{-1}
Temperature range 22 to 245 °C.
Phase Changes
c/liq 512.4 K, ΔH=36900 J·mol^{-1}
ΔS=72.0 J·mol^{-1}·K^{-1}
Molecular Weight 167.1208
Wiswesser Line Notation WNR DVQ
Evaluation C

$C_7H_5NO_4$ (c) 41SAT/SOG
4-Nitrobenzoic acid
Heat Capacity 323 K, C_p=197.9 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 167.1208
Wiswesser Line Notation WNR DVQ
Evaluation C
Same data in 40SAT/SOG2.

$C_7H_5NO_4$ (c) 72BOO/HAU
4-Nitrobenzoic acid
Phase Changes
c/liq 512.35 K, ΔH=36900 J·mol^{-1}
ΔS=72.0 J·mol^{-1}·K^{-1}
Molecular Weight 167.1208
Wiswesser Line Notation WNR DVQ
Evaluation C

C_7H_5NS (liq) 36KUR/VOS
Phenyl isothiocyanate
Heat Capacity 290 K, C_p=186.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 135.1832
Wiswesser Line Notation SCNR
Evaluation D

C_7H_5NS (liq) 68GOU/WES4
Benzothiazole
Heat Capacity 298.15 K, C_p=189.54 J·mol^{-1}·K^{-1}
Temperature range 25 to 325 K.
Entropy 298.15 K, S=209.83 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 275.596 K, ΔH=12782 J·mol^{-1}
ΔS=46.40 J·mol^{-1}·K^{-1}
Molecular Weight 135.1832
Wiswesser Line Notation T56 BN DSJ
Evaluation A

C_7H_5NS (liq) 69GOU/WES
Benzothiazole
Heat Capacity 298.15 K, C_p=189.54 J·mol^{-1}·K^{-1}
Temperature range 5 to 325 K.
Entropy 298.15 K, S=209.83 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 275.60 K, ΔH=12782 J·mol^{-1}
ΔS=46.38 J·mol^{-1}·K^{-1}
Molecular Weight 135.1832
Wiswesser Line Notation T56 BN DSJ
Evaluation A

C_7H_5NS (liq) 92STE/CHI
Benzothiazole
Heat Capacity 298.15 K, C_p=189.25 J·mol^{-1}·K^{-1}
Temperature range 5 to 445 K.
Entropy 298.15 K, S=209.88 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 245.0 K, ΔH=37.4 J·mol^{-1}
c,I/liq 275.651 K, ΔH=12591 J·mol^{-1}
Molecular Weight 135.1832
Wiswesser Line Notation T56 BN DSJ
Evaluation A

$C_7H_5N_3O_6$ (c) 24TAY/RI
2,4,6-Trinitrotoluene
Heat Capacity 293 K, C_p=311.7 J·mol^{-1}·K^{-1}
Temperature range 90 to 352 K.
Molecular Weight 227.1330
Wiswesser Line Notation WNR B1 CNW ENW
Evaluation C

$C_7H_5N_3O_6$ (c,II) 71CHI/TH
2,4,5-Trinitrotoluene; γ-TNT
Heat Capacity 313.2 K, C_p=312 J·mol^{-1}·K^{-1}
Temperature range 313 to 333 K. At 313.2 K, C_p of c,I is 248 ·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 319.2 K, ΔH=5700 J·mol^{-1}
ΔS=18 J·mol^{-1}·K^{-1}
c,I/liq 376.2 K, ΔH=24700 J·mol^{-1}
ΔS=66 J·mol^{-1}·K^{-1}
c,II/liq 347.2 K, ΔH=13300 J·mol^{-1}
ΔS=38 J·mol^{-1}·K^{-1}
Molecular Weight 227.1330
Wiswesser Line Notation WNR B1 DNW ENW
Evaluation C

$C_7H_5N_3O_6$ (c) 91YIN/LI
2,4,6-Trinitrotoluene
Heat Capacity 298 K, C_p=243.3 J·mol^{-1}·K^{-1}
Temperature range 290 to 345 K. C_p value reported at 298 K i 1.07-1 J/g·K.
Molecular Weight 227.1330
Wiswesser Line Notation WNR B1 CNW ENW
Evaluation B

$C_7H_5N_5O_8$ (c) 24TAY/RI
2,4,6-Trinitrophenylmethyl nitramine; Tetryl; N-Methyl-2,4,6, N-tetranitroaniline
Heat Capacity 293 K, C_p=260.7 J·mol^{-1}·K^{-1}
Temperature range 90 to 370 K.
Molecular Weight 287.1452
Wiswesser Line Notation WNN1&R BNW DNW FNW
Evaluation C

$C_7H_5N_5O_8$ (c) 71HA
2,4,6-Trinitrophenylmethyl nitramine; Tetryl; N-Methyl-2,4,6, N-tetranitroaniline
Phase Changes
c/liq 400.5 K, ΔH=25857 J·mol^{-1}
Molecular Weight 287.1452
Wiswesser Line Notation WNN1&R BNW DNW FNW
Evaluation C

$C_7H_5N_5O_8$ (c) 73KRI/LIC
2,4,6-Trinitrophenylmethyl nitramine; Tetryl; N-Methyl-2,4,6, N-tetranitroaniline
Heat Capacity 298 K, C_p=302.1 J·mol^{-1}·K^{-1}
Temperature range 200 to 403 K. Equation only.
Phase Changes
c/liq 402.6 K, ΔH=22930 J·mol^{-1}
ΔS=57.0 J·mol^{-1}·K^{-1}
Molecular Weight 287.1452
Wiswesser Line Notation WNN1&R BNW DNW FNW
Evaluation C

$C_7H_5N_5O_8$ (c) 91YIN/LIU
2,4,6-Trinitrophenylmethyl nitramine; Tetryl; N-Methyl-2,4,6-N-tetranitroaniline
Heat Capacity 298 K, C_p=290.9 J·mol^{-1}·K^{-1}
Temperature range 290 to 345 K. C_p value reported at 298 K is 1.013 J/g·K.
Molecular Weight 287.1452
Wiswesser Line Notation WNN1&R BNW DNW FNW
Evaluation B

$C_7H_6F_8O_3$ (liq) 80LEB/DOB
Bis-(tetrafluoropropyl)carbonate
Heat Capacity 298.15 K, C_p=389.87 J·mol^{-1}·K^{-1}
Temperature range 12 to 360 K. Data given in tables and by equations.
Entropy 298.15 K, S=539.02 J·mol^{-1}·K^{-1}
Phase Changes
c,l/liq 253.35 K, ΔH=41049 J·mol^{-1}
ΔS=162.0 J·mol^{-1}·K^{-1}
Molecular Weight 290.1098
Wiswesser Line Notation 1XFFXFF&O 2V
Evaluation A

$C_7H_6N_2$ (c) 87JIM/ROU
Benzimidazole
Heat Capacity 298.15 K, C_p=128.8 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.09 J·K^{-1}·g^{-1}.
Molecular Weight 118.1378
Wiswesser Line Notation T56 BM DNJ
Evaluation B

$C_7H_6N_2$ (c) 87JIM/ROU
Indazole
Heat Capacity 298.15 K, C_p=128.8 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.09 J·K^{-1}·g^{-1}.
Molecular Weight 118.1378
Wiswesser Line Notation T56 BMNJ
Evaluation B

$C_7H_6N_2O_4$ (c) 64DAV
2,4-Dinitrotoluene
Heat Capacity 325 K. C_p=255 J·mol^{-1}·K^{-1}
Temperature range 298 to 340 K. Mean value. Temperature range uncertain.
Phase Changes
c/liq 345 K. ΔH=20900 J·mol^{-1}
ΔS=61 J·mol^{-1}·K^{-1}
Temperature not measured.
Molecular Weight 182.1354
Wiswesser Line Notation WNR B1 ENW
Evaluation D

$C_7H_6N_2O_4$ (c) 90FIN/PAY
2,6-Dinitrotoluene
Heat Capacity 305 K, C_p=217 J·mol^{-1}·K^{-1}
Temperature range 305 to 365 K. Unsmoothed mexperimental datum.
Phase Changes
c/liq 340 K, ΔH=19280 J·mol^{-1}
c,form A/liq.
Molecular Weight 182.1354
Wiswesser Line Notation WNR B1 CNW
Evaluation A
Data given in the solid and liquid state for form A.

$C_7H_6N_2O_4$ (c) 90FIN/PAY
2,6-Dinitrotoluene
Heat Capacity 305 K, C_p=224 J·mol^{-1}·K^{-1}
Temperature range 305 to 365 K. Unsmoothed experimental datum.
Phase Changes
c/liq 340 K, ΔH=16070 J·mol^{-1}
c,form B/liq.
Molecular Weight 182.1354
Wiswesser Line Notation WNR B1 CNW
Evaluation A
Data given in the solid and liquid state for form B.

C_7H_6O (liq) 34KOL/UDO
Benzaldehyde
Heat Capacity 302.4 K, C_p=171.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1238
Wiswesser Line Notation VHR
Evaluation C

C_7H_6O (liq) 34KOL/UDO2
Benzaldehyde
Heat Capacity 302.3 K, C_p=171.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1238
Wiswesser Line Notation VHR
Evaluation C

C_7H_6O (liq) 75AMB/CON
Benzaldehyde
Heat Capacity 298.15 K, C_p=172.0 J·mol^{-1}·K^{-1}
Temperature range 13 to 425 K.
Entropy 298.15 K, S=221.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 216.02 K, ΔH=9320 J·mol^{-1}
ΔS=43.14 J·mol^{-1}·K^{-1}
Molecular Weight 106.1238
Wiswesser Line Notation VHR
Evaluation A

$C_7H_6O_2$ (c) 26AND/LYN
Benzoic acid
Heat Capacity 298 K, C_p=155.2 J·mol^{-1}·K^{-1}
Temperature range 22 to 200 °C.
Phase Changes
c/liq 395.0 K, ΔH=17320 J·mol^{-1}
ΔS=43.8 J·mol^{-1}·K^{-1}
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation C

$C_7H_6O_2$ (c) 33PAR/HUF
Benzoic acid
Heat Capacity 295.1 K, C_p=145.10 J·mol^{-1}·K^{-1}
Temperature range 93 to 295 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=170.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 59.25 J·mol^{-1}·K^{-1}.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation B(C_p),C(S)

$C_7H_6O_2$ (c) 39SAT/SOG2
Benzoic acid
Heat Capacity 323 K, C_p=160.2 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation C
Same data in 40SAT/SOG.

$C_7H_6O_2$ (c) 51FUR/MCC
Benzoic acid
Heat Capacity 298.15 K, C_p=146.81 J·mol^{-1}·K^{-1}
Temperature range 13 to 410 K.
Entropy 298.15 K, S=167.59 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 395.52 K, ΔH=18000 J·mol^{-1}
ΔS=45.51 J·mol^{-1}·K^{-1}
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 53GIN/FUR
Benzoic acid
Heat Capacity 298.15 K, C_p=146.81 J·mol^{-1}·K^{-1}
Temperature range 14 to 410 K.
Phase Changes
c/liq 395.52 K, ΔH=18006 J·mol^{-1}
ΔS=45.52 J·mol^{-1}·K^{-1}
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 56POP/KOL
Benzoic acid
Heat Capacity 298.15 K, C_p=149.79 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 57DAV/STA
Benzoic acid
Heat Capacity 298.15 K, C_p=147.02 J·mol^{-1}·K^{-1}
Temperature range 20 to 298 K.
Entropy 298.15 K, S=167.82 J·mol^{-1}·K^{-1}
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation B

$C_7H_6O_2$ (c) 62KOL/SEF
Benzoic acid
Heat Capacity 298.15 K, C_p=146.31 J·mol^{-1}·K^{-1}
Temperature range 22 to 310 K.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 64DA
Benzoic acid
Heat Capacity 340 K, C_p=130 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K. Mean value. Temperature rang uncertain.
Phase Changes
c/liq 395 K, ΔH=17400 J·mol^{-1}
ΔS=44 J·mol^{-1}·K^{-1}
Temperature not measured.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation D

$C_7H_6O_2$ (c) 65SUG/SEI
Benzoic acid
Heat Capacity 299.99 K, C_p=147.14 J·mol^{-1}·K
Temperature range 13 to 300 K. Value is unsmoothed experiment datum.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (liq) 67PA
Benzoic acid
Heat Capacity 413 K, C_p=259 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 395 K, ΔH=16230 J·mol^{-1}
ΔS=41.1 J·mol^{-1}·K^{-1}
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation C

$C_7H_6O_2$ (c) 69JU
Benzoic acid
Heat Capacity 298.15 K, C_p=167.40 J·mol^{-1}·K
As check on system. Only value at 298 K given.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation B

$C_7H_6O_2$ (c) 71KON/SU
Benzoic acid
Heat Capacity 298.15 K, C_p=146.80 J·mol^{-1}·K
One temperature.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation B

$C_7H_6O_2$ (c) 74MOS/MO
Benzoic acid
Heat Capacity 301 K, C_p=149 J·mol^{-1}·K^{-1}
One temperature, ΔT=5 K. Value ±5 J·mol^{-1}·K^{-1}.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation B

$C_7H_6O_2$ (c) 75TAT/MAT
Benzoic acid
Heat Capacity 299.62 K, $C_p = 147.07\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 12 to 304 K.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 76ARV/FAI
Benzoic acid
Heat Capacity 298.15 K, $C_p = 146.79\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 6 to 341 K.
Entropy 298.15 K, $S = 167.73\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 80AND/CON
Benzoic acid
Phase Changes
c,I/liq 395.527 K, $\Delta H = 18062\ J \cdot mol^{-1}$
$\Delta S = 45.67\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 82MOR/MAT
Benzoic acid
Heat Capacity 296.29 K, $C_p = 146.23\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 13 to 355 K. NBS SRM 29.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 80SHA/LYU
Benzoic acid
Heat Capacity 298.15 K, $C_p = 146.65\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 20 to 300 K.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 88TOR/BAR
Benzoic acid
Phase Changes
liq/g 335 K, $\Delta H = 87450\ J \cdot mol^{-1}$
$\Delta S = 261.0\ J \cdot mol^{-1} \cdot K^{-1}$
c/g 298.15 K, $\Delta H = 89230\ J \cdot mol^{-1}$
$\Delta S = 299.3\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 92SOR/KAJ
Benzoic acid
Heat Capacity 298.902 K, $C_p = 147.03\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 15 to 305 K. Unsmoothed experimental datum.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 93KAJ/TOC
Benzoic acid
Heat Capacity 300 K, $C_p = 147.78\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 19 to 312 K. Unsmoothed experimental datum.
Entropy 298.15 K, $S = 165.71\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (liq) 07WAL
2-Hydroxybenzaldehyde; Salicylaldehyde
Heat Capacity 291 K, $C_p = 222\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 122.1232
Wiswesser Line Notation VHR BQ
Evaluation D

$C_7H_6O_3$ (c) 34PAR/LIG
Salicylic acid; o-Hydroxybenzoic acid
Heat Capacity 288.6 K, $C_p = 159.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 96 to 289 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S = 178.2\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K. $57.32\ J \cdot mol^{-1} \cdot K^{-1}$.
Molecular Weight 138.1226
Wiswesser Line Notation QVR BQ
Evaluation B(C_p),C(S)

$C_7H_6O_3$ (c) 40CAM/CAM
Salicylic acid; o-Hydroxybenzoic acid
Heat Capacity 293 K, $C_p = 104.2\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 138.1226
Wiswesser Line Notation QVR BQ
Evaluation C

$C_7H_6O_3$ (c) 86RAB/SHE
Salicylic acid; o-Hydroxybenzoic acid
Heat Capacity 298.15 K, $C_p = 160.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 460 K.
Entropy 298.15 K, $S = 172.4\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 431.8 K, $\Delta H = 24600\ J \cdot mol^{-1}$
$\Delta S = 56.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 138.1226
Wiswesser Line Notation QVR BQ
Evaluation A

$C_7H_6O_3$ (c) 93SAB/LE
Salicylic acid; o-Hydroxybenzoic acid
Phase Changes
c/liq/g 433 K
c/liq $\Delta H = 18200\ J \cdot mol^{-1}$
c/g 298.15 K $\Delta H = 96270\ J \cdot mol^{-1}$
Molecular Weight 138.1226
Wiswesser Line Notation QVR BQ
Evaluation B

$C_7H_6O_3$ (c) 34PAR/LIG
m-Hydroxybenzoic acid
Heat Capacity 288.4 K, C_p=157.3 J·mol^{-1}·K^{-1}
Temperature range 94 to 288 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=177.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 56.48 J·mol^{-1}·K^{-1}.
Molecular Weight 138.1226
Wiswesser Line Notation QVR CQ
Evaluation B(C_p),C(S)

$C_7H_6O_3$ (c) 93SAB/LE
m-Hydroxybenzoic acid
Phase Changes
c/liq/g 475 K
c/liq ΔH=26200 J·mol^{-1}
c/g 298.15 K ΔH=124990 J·mol^{-1}
Molecular Weight 138.1226
Wiswesser Line Notation QVR CQ
Evaluation B

$C_7H_6O_3$ (c) 34PAR/LIG
p-Hydroxybenzoic acid
Heat Capacity 283.8 K, C_p=155.2 J·mol^{-1}·K^{-1}
Temperature range 95 to 284 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=175.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 55.35 J·mol^{-1}·K^{-1}.
Molecular Weight 138.1226
Wiswesser Line Notation QVR DQ
Evaluation B(C_p),C(S)

$C_7H_6O_3$ (c) 93SAB/LE
p-Hydroxybenzoic acid
Phase Changes
c/g 298.15 K ΔH=114050 J·mol^{-1}
Molecular Weight 138.1226
Wiswesser Line Notation QVR DQ
Evaluation B

$C_7H_6O_3$ (c) 81LEB/RYA
3,4-Dihydroxybenzaldehyde
Heat Capacity C_p=205.7 J·mol^{-1}·K^{-1}
Temperature range 298 to 413 K. Data given over temperature range.
Molecular Weight 138.1226
Wiswesser Line Notation VHR CQ DQ
Evaluation B

C_7H_7Cl (liq) 31SMI/AND
Benzyl chloride; α-Chlorotoluene; Phenylchloromethane
Heat Capacity 298.5 K, C_p=182.4 J·mol^{-1}·K^{-1}
Temperature range 102 to 299 K. Value is unsmoothed experimental datum.
Molecular Weight 126.5853
Wiswesser Line Notation G1R
Evaluation C

C_7H_7F (liq) 90MEV/LIC
2-Fluorotoluene
Phase Changes
c/liq 210.65 K, ΔH=9800 J·mol^{-1}
ΔS=46.0 J·mol^{-1}·K^{-1}
Molecular Weight 110.1307
Wiswesser Line Notation FR B1
Evaluation A

C_7H_7F (liq) 90MEV/LI
3-Fluorotoluene
Phase Changes
c/liq 183.95 K, ΔH=8300 J·mol^{-1}
ΔS=45 J·mol^{-1}·K^{-1}
Molecular Weight 110.1307
Wiswesser Line Notation FR C1
Evaluation A

C_7H_7F (liq) 62GOO/LA
4-Fluorotoluene
Heat Capacity 298.15 K, C_p=172.3 J·mol^{-1}·K^{-}
One temperature.
Molecular Weight 110.1307
Wiswesser Line Notation FR D1
Evaluation B

C_7H_7F (liq) 62SCO/MI
4-Fluorotoluene
Heat Capacity 298.15 K, C_p=171.17 J·mol^{-1}·K
Temperature range 13 to 361 K.
Entropy 298.15 K, S=237.11 J·mol^{-1}·K^{-}
Phase Changes
c/liq 216.49 K, ΔH=9351 J·mol^{-1}
ΔS=43.19 J·mol^{-1}·K^{-}
Molecular Weight 110.1307
Wiswesser Line Notation FR D1
Evaluation A

C_7H_7F (liq) 90MEV/L
4-Fluorotoluene
Heat Capacity 298.15 K, C_p=173.7 J·mol^{-1}·K^{-}
Temperature range 216 to 298 K. C_p(liq)=164.969+0.35
J·mol^{-1}·K^{-1} (−57 to 25 °C).
Phase Changes
c/liq 215.55 K, ΔH=8800 J·mol^{-1}
ΔS=41 J·mol^{-1}·K^{-1}
Molecular Weight 110.1307
Wiswesser Line Notation FR D1
Evaluation A

C_7H_7NO (c) 90STE/C
Benzamide
Heat Capacity 298.15 K, C_p=153.8 J·mol^{-1}·K^{-}
Temperature range 315 to 475 K. C/R(c)=0.067T−1.51 (315
375 K): C/R(liq)=0.0288T+21.03 (415 to 475 K). R=8.31441
·mol.
Phase Changes
c/liq 403 K, ΔH=23760 J·mol^{-1}
Molecular Weight 121.1384
Wiswesser Line Notation ZVR
Evaluation B

$C_7H_7NO_2$ (liq) 34KOL/UD
2-Nitrotoluene
Heat Capacity 302.3 K, C_p=202.5 J·mol^{-1}·K
One temperature.
Molecular Weight 137.1378
Wiswesser Line Notation WNR B1
Evaluation C

$C_7H_7NO_2$ (liq) 34KOL/UDO
3-Nitrotoluene
Heat Capacity 302.4 K, C_p=202.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 137.1378
Wiswesser Line Notation WNR C1
Evaluation C

$C_7H_7NO_2$ (c,I) 79RIC/SAV
4-Nitrotoluene
Heat Capacity 298.15 K, C_p=172.3 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Equations only. Data for stable and metastable crystal form.
Phase Changes
c,II/liq 318.5 K, ΔH=70781 J·mol^{-1}
ΔS=222.2 J·mol^{-1}·K^{-1}
Metastable form.
c,I/liq 324.7 K, ΔH=69802 J·mol^{-1}
ΔS=215.0 J·mol^{-1}·K^{-1}
Molecular Weight 137.1378
Wiswesser Line Notation WNR D1
Evaluation B

$C_7H_7NO_2$ (c) 80AND/CON
4-Nitrotoluene
Phase Changes
c,I/liq 324.788 K, ΔH=16811 J·mol^{-1}
ΔS=51.76 J·mol^{-1}·K^{-1}
Molecular Weight 137.1378
Wiswesser Line Notation WNR D1
Evaluation A

$C_7H_7NO_2$ (c) 26AND/LYN
2-Aminobenzoic acid
Heat Capacity 298 K, C_p=165.3 J·mol^{-1}·K^{-1}
Temperature range 22 to 160 °C.
Phase Changes
c/liq 417.8 K, ΔH=20380 J·mol^{-1}
ΔS=48.8 J·mol^{-1}·K^{-1}
Molecular Weight 137.1378
Wiswesser Line Notation ZR BVQ
Evaluation C

$C_7H_7NO_2$ (c) 41SAT/SOG2
2-Aminobenzoic acid
Heat Capacity 323 K, C_p=187.0 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 137.1378
Wiswesser Line Notation ZR BVQ
Evaluation C
Same data as 40SAT/SOG3.

$C_7H_7NO_2$ (c) 26AND/LYN
3-Aminobenzoic acid
Heat Capacity 298 K, C_p=162.8 J·mol^{-1}·K^{-1}
Temperature range 22 to 180 °C.
Phase Changes
c/liq 452.9 K, ΔH=21840 J·mol^{-1}
ΔS=48.2 J·mol^{-1}·K^{-1}
Molecular Weight 137.1378
Wiswesser Line Notation ZR CVQ
Evaluation C

$C_7H_7NO_2$ (c) 41SAT/SOG2
3-Aminobenzoic acid
Heat Capacity 323 K, C_p=179.9 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 137.1378
Wiswesser Line Notation ZR CVQ
Evaluation C
Same data as 40SAT/SOG3.

$C_7H_7NO_2$ (c) 26AND/LYN
4-Aminobenzoic acid
Heat Capacity 298 K, C_p=177.8 J·mol^{-1}·K^{-1}
Temperature range 22 to 190 °C.
Phase Changes
c/liq 461.4 K, ΔH=20920 J·mol^{-1}
ΔS=45.3 J·mol^{-1}·K^{-1}
Molecular Weight 137.1378
Wiswesser Line Notation ZR DVQ
Evaluation C

$C_7H_7NO_2$ (c) 41SAT/SOG2
4-Aminobenzoic acid
Heat Capacity 323 K, C_p=187.4 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 137.1378
Wiswesser Line Notation ZR DVQ
Evaluation C
Same data as 40SAT/SOG3.

$C_7H_7NO_3$ (c) 81LEB/RYA
p-Nitroanisole; 4-Nitromethoxybenzene
Heat Capacity C_p=279.9 J·mol^{-1}·K^{-1}
Temperature range 298 to 320 K. Data given over temperature range.
Molecular Weight 153.1372
Wiswesser Line Notation WNR DO1
Evaluation B

C_7H_7NS (c) 82SAB/TOR
Thiobenzamide
Heat Capacity 298 K, C_p=152.8 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.114 J·K^{-1}·g^{-1}.
Phase Changes
c/g 298.15 K, ΔH=97200 J·mol^{-1}
ΔS=326.0 J·mol^{-1}·K^{-1}
Molecular Weight 137.1990
Wiswesser Line Notation ZYR&US
Evaluation B

C_7H_8 (liq) 1881REI
Toluene
Heat Capacity 298 K, C_p=158.2 J·mol^{-1}·K^{-1}
Temperature range 292 to 390 K.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation D

C_7H_8 (liq) 24WIL/DAN
Toluene
Heat Capacity 303 K, C_p=153.6 J·mol^{-1}·K^{-1}
Temperature range 303 to 343 K. Equation only.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation C

C_7H_8 (liq) 25WIL/DAN
Toluene
Heat Capacity 293.2 K, $C_p = 151.0\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 20 to 60 °C.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 29KEL4
Toluene
Heat Capacity 28.444 K, $C_p = 153.09\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 14 to 284 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S = 219.2\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 177.95 K, $\Delta H = 6619\ J \cdot mol^{-1}$
$\Delta S = 37.20\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation A

C_7H_8 (liq) 31SMI/AND
Toluene
Heat Capacity 298.15 K, $C_p = 161.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 102 to 299 K. Value is unsmoothed experimental datum.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation C

C_7H_8 (liq) 32RIC/WAL
Toluene
Heat Capacity 298.1 K, $C_p = 156.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 333 K.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation C

C_7H_8 (liq) 35AOY/KAN
Toluene
Heat Capacity 227.8 K, $C_p = 142.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 78 to 228 K. Value is unsmoothed experimental datum.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 37VOL
Toluene
Heat Capacity 298 K, $C_p = 156.5\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 40BUR
Toluene
Heat Capacity 298.2 K, $C_p = 157.07\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 281 to 383 K.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 41ZHD
Toluene
Heat Capacity 298.1 K, $C_p = 156.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 47 °C.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation C

C_7H_8 (liq) 42ZIE/ANI
Toluene
Phase Changes
c/liq 178.0 K, $\Delta H = 6548\ J \cdot mol^{-1}$
$\Delta S = 36.79\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 47KUI
Toluene
Heat Capacity 298 K, $C_p = 158.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range −76 to 60 °C, mean C_p, four temperatures.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation D

C_7H_8 (liq) 48TS(
Toluene
Heat Capacity 295 K, $C_p = 140\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation C

C_7H_8 (liq) 58SWI/ZIE
Toluene
Heat Capacity 324 K, $C_p = 166.9\ J \cdot mol^{-1} \cdot K^{-1}$
Mean value 21 to 81 °C.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation C

C_7H_8 (liq) 62SCO/GU
Toluene
Heat Capacity 298.15 K, $C_p = 157.23\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 360 K.
Entropy 298.15 K, $S = 220.96\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 178.15 K, $\Delta H = 6636\ J \cdot mol^{-1}$
$\Delta S = 37.25\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation A

C_7H_8 (liq) 66HWA/Z
Toluene
Heat Capacity 298.711 K, $C_p = 157.33\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 181 to 304 K. Unsmoothed experiment datum.
Phase Changes
c/liq 178.159 K
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 67RAS/GAN
Toluene
Heat Capacity 293 K, C_p=158.6 J·mol^{-1}·K^{-1}
Temperature range 293 to 373 K.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation C

C_7H_8 (liq) 71DES/BHA
Toluene
Heat Capacity 298 K, C_p=156.5 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 74RAJ/SUB
Toluene
Heat Capacity 298.15 K, C_p=156.8 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 323.15 K.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 75HOL/ZIE
Toluene
Heat Capacity 298.15 K, C_p=156.99 J·mol^{-1}·K^{-1}
Temperature range 165 to 312 K. C_p=187.43814−0.73026493T +0.0029613602T^2−2.8661704×10^{-6}T^3 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 178.166 K
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation A

C_7H_8 (liq) 75PED/KAY
Toluene
Heat Capacity 298.15 K, C_p=158.4 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K. C_p(liq)=154.73+0.0981(T/K −273.15) +0.001949(T/K−273.15)^2 J/K·mol (298 to 348 K).
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 76FOR/BEN2
Toluene
Heat Capacity 298.15 K, C_p=157.026 J·mol^{-1}·K^{-1}
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation A
Data from 76FOR/BEN.

C_7H_8 (liq) 77FOR/BEN
Toluene
Heat Capacity 298.15 K, C_p=157.081 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 77WIL/GRO
Toluene
Heat Capacity 298.15 K, C_p=156.94 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 79AND/GRI
Toluene
Heat Capacity 294.71 K, C_p=157.0 J·mol^{-1}·K^{-1}
Temperature range 293 to 373 K. Unsmoothed experimental datum given as 1.704 KJ/kg·K.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 79FOR/BEN
Toluene
Heat Capacity 298.15 K, C_p=157.057 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 81ATA/ELS
Toluene
Heat Capacity 293.15 K, C_p=156.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 82GRO/ING
Toluene
Heat Capacity 298.15 K, C_p=157.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation A

C_7H_8 (liq) 82WIL/FAR
Toluene
Heat Capacity 298.15 K, C_p=157.15 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 84STE/OLS
Toluene
Heat Capacity 298.15 K, C_p=158.7 J·mol^{-1}·K^{-1}
Temperature range 266 to 318 K. C_p given as 0.4117 cal·g^{-1}·C^{-1}.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 86RED
Toluene
Heat Capacity 303.15 K, C_p=159.9 J·mol^{-1}·K^{-1}
Temperature range 303.15, 313.15 K.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 86ROU/GRO
Toluene
Heat Capacity 298.15 K, C_p=157.08 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 86TAR/AIC
Toluene
Heat Capacity 298.15 K, C_p=158.70 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 88SHI/OGA
Toluene
Heat Capacity 298.15 K, C_p=155.96 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation A

C_7H_8 (liq) 93GRO/ROU
Toluene
Heat Capacity 298.15 K, C_p=157.09 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 73HAL/SMI
Quadricyclane; Tetracyclo[3.2.0.0.^{2,7}0^{4,6}]heptane
Heat Capacity 297 K, C_p=139.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation L435 B3 2AB GTJ
Evaluation C

C_7H_8 (liq) 78STE
Quadricyclane; Tetracyclo[3.2.0.0.^{2,7}0^{4,6}]heptane
Heat Capacity 298.15 K, C_p=157.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation L435 B3 2AB GTJ
Evaluation B

C_7H_8 (liq) 92KAW/GII
Quadricyclane; Tetracyclo[3.2.0.0^{2,7}.0^{4,6}]heptane
Phase Changes
c,II/c,I 180 K, ΔS=40.0 J·mol^{-1}·K^{-1}
c,I/liq 228 K, ΔS=4.8 J·mol^{-1}·K^{-1}
Molecular Weight 92.1402
Wiswesser Line Notation L435 B3 2AB GTJ
Evaluation B

C_7H_8 (liq) 73HAL/SM
Norbornadiene; Bicyclo[2.2.1]hept-2,5-diene
Heat Capacity 297 K, C_p=116.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation L55 A CU FUTJ
Evaluation C

C_7H_8 (liq) 78ST
Norbornadiene; Bicyclo[2.2.1]hept-2,5-diene
Heat Capacity 298.15 K, C_p=161.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation L55 A CU FUTJ
Evaluation B

C_7H_8 (liq) 56FIN/SC
Cycloheptatriene
Heat Capacity 298.15 K, C_p=162.76 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=214.64 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 153.98 K, ΔH=2346.8 J·mol^{-1}
ΔS=15.24 J·mol^{-1}·K^{-1}
c,I/liq 197.92 K, ΔH=1160.6 J·mol^{-1}
ΔS=5.86 J·mol^{-1}·K^{-1}
Molecular Weight 92.1402
Wiswesser Line Notation L7HJ
Evaluation A

$C_7H_8N_2O$ (c) 87FER/DI
Phenylurea; Monophenylurea
Phase Changes
c/liq 420.6 K, ΔH=23680 J·mol^{-1}
ΔS=56.3 J·mol^{-1}·K^{-1}
Molecular Weight 136.1530
Wiswesser Line Notation ZVMR
Evaluation A

$C_7H_8N_2O_2$ (c) 41SAT/SO
5-Nitro-2-aminotoluene
Heat Capacity 323 K, C_p=217.1 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 152.1524
Wiswesser Line Notation ZR B1 DNW
Evaluation C
Same data as 40SAT/SOG4.

$C_7H_8N_2O_2$ (c) 41SAT/SOG3
3-Nitro-4-aminotoluene
Heat Capacity 323 K, C_p=205.4 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 152.1524
Wiswesser Line Notation ZR D1 BNW
Evaluation C
Same data as 40SAT/SOG4.

C_7H_8O (liq) 1889EYK
Anisole; Methyl phenyl ether; Methoxybenzene
Phase Changes
c/liq 293.2 K, ΔH=17029 J·mol^{-1}
ΔS=58.1 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation 1OR
Evaluation C

C_7H_8O (liq) 02LOU
Anisole; Methyl phenyl ether; Methoxybenzene
Heat Capacity 360 K, C_p=218 J·mol^{-1}·K^{-1}
Mean value 20 to 152 °C.
Molecular Weight 108.1396
Wiswesser Line Notation 1OR
Evaluation D

C_7H_8O (liq) 33KOL/UDO
Anisole; Methyl phenyl ether; Methoxybenzene
Heat Capacity 297.2 K, C_p=191.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 108.1396
Wiswesser Line Notation 1OR
Evaluation C

C_7H_8O (liq) 39PHI
Anisole; Methyl phenyl ether; Methoxybenzene
Heat Capacity 304.8 K, C_p=208.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 108.1396
Wiswesser Line Notation 1OR
Evaluation C

C_7H_8O (liq) 75FEN/HAR
Anisole; Methyl phenyl ether; Methoxybenzene
Heat Capacity 298.15 K, C_p=199.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 108.1396
Wiswesser Line Notation 1OR
Evaluation B

C_7H_8O (liq) 87GOA/BOE
Anisole; Methyl phenyl ether; Methoxybenzene
Phase Changes
c,l/liq 268.73 K, ΔH=12890 J·mol^{-1}
ΔS=48.0 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation 1OR
Evaluation A

C_7H_8O (liq) 1881REI
Benzyl alcohol
Heat Capacity 298 K, C_p=220.5 J·mol^{-1}·K^{-1}
Temperature range 290 to 485 K.
Molecular Weight 108.1396
Wiswesser Line Notation Q1R
Evaluation D

C_7H_8O (liq) 31SMI/AND
Benzyl alcohol
Heat Capacity 298.5 K, C_p=215.9 J·mol^{-1}·K^{-1}
Temperature range 102 to 299 K. Value is unsmoothed experimental datum.
Molecular Weight 108.1396
Wiswesser Line Notation Q1R
Evaluation C

C_7H_8O (liq) 36PAR/TOD
Benzyl alcohol
Heat Capacity 298.1 K, C_p=217.86 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 298.1 K, S=216.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 54.06 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 257.6 K, ΔH=8970 J·mol^{-1}
ΔS=34.82 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation Q1R
Evaluation B(C_p),C(S)

C_7H_8O (liq) 75NIC/WAD
Benzyl alcohol
Heat Capacity 298.15 K, C_p=215.94 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 108.1396
Wiswesser Line Notation Q1R
Evaluation B

C_7H_8O (liq) 79GRI/YAN
Benzyl alcohol
Heat Capacity 307.5 K, C_p=223.6 J·mol^{-1}·K^{-1}
Temperature range 307 to 461 K. p=0.98 bar.
Molecular Weight 108.1396
Wiswesser Line Notation Q1R
Evaluation B

C_7H_8O (liq) 16BRA
2-Methylphenol; o-Hydroxytoluene; o-Cresol
Heat Capacity 283 K, C_p=225.9 J·mol^{-1}·K^{-1}
Mean value, 0 to 20 °C.
Molecular Weight 108.1396
Wiswesser Line Notation QR B1
Evaluation C

C_7H_8O (c) 67AND/COU
2-Methylphenol; o-Hydroxytoluene; o-Cresol
Heat Capacity 298.15 K, C_p=154.56 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=165.44 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 304.20 K, ΔH=15820 J·mol^{-1}
ΔS=52.00 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR B1
Evaluation A

C_7H_8O (liq) 67RAS/GAN
2-Methylphenol; o-Hydroxytoluene; o-Cresol
Heat Capacity 313 K, C_p=233.6 J·mol^{-1}·K^{-1}
Temperature range 313 to 373 K.
Molecular Weight 108.1396
Wiswesser Line Notation QR B1
Evaluation C

C_7H_8O (c) 82POE/FAN
2-Methylphenol; o-Hydroxytoluene; o-Cresol
Phase Changes
c/liq 303.0 K, ΔH=13938 J·mol^{-1}
ΔS=46.00 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR B1
Evaluation A

C_7H_8O (c) 90MEV/LIC
2-Methylphenol; o-Hydroxytoluene; o-Cresol
Phase Changes
c/liq 304.05 K, ΔH=14800 J·mol^{-1}
ΔS=49 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR B1
Evaluation A

C_7H_8O (liq) 16BRA
3-Methylphenol; m-Hydroxytoluene; m-Cresol
Heat Capacity 283 K, C_p=216.7 J·mol^{-1}·K^{-1}
Mean value, 0 to 20 °C.
Molecular Weight 108.1396
Wiswesser Line Notation QR C1
Evaluation C

C_7H_8O (liq) 51TSC/KRI
3-Methylphenol; m-Hydroxytoluene; m-Cresol
Heat Capacity 298 K, C_p=218.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 108.1396
Wiswesser Line Notation QR C1
Evaluation C

C_7H_8O (liq) 67RAS/GAN
3-Methylphenol; m-Hydroxytoluene; m-Cresol
Heat Capacity 93 K, C_p=220.9 J·mol^{-1}·K^{-1}
Temperature range 293 to 373 K.
Molecular Weight 108.1396
Wiswesser Line Notation QR C1
Evaluation C

C_7H_8O (liq) 67AND/COU
3-Methylphenol; m-Hydroxytoluene; m-Cresol
Heat Capacity 298.15 K, C_p=224.93 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=212.59 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 285.40 K, ΔH=10707 J·mol^{-1}
ΔS=27.53 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR C1
Evaluation A

C_7H_8O (liq) 82POE/FAI
3-Methylphenol; m-Hydroxytoluene; m-Cresol
Phase Changes
c/liq 285.0 K, ΔH=9413 J·mol^{-1}
ΔS=33.03 J·mol^{-1}·K^{-}
Molecular Weight 108.1396
Wiswesser Line Notation QR C1
Evaluation A

C_7H_8O (liq) 90MEV/LI
3-Methylphenol; m-Hydroxytoluene; m-Cresol
Phase Changes
c/liq 280.75 K, ΔH=9100 J·mol^{-1}
ΔS=32 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR C1
Evaluation A

C_7H_8O (c) 1889EY
4-Methylphenol; p-Hydroxytoluene; p-Cresol
Phase Changes
c/liq 309 K, ΔH=12247 J·mol^{-1}
ΔS=39.6 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR D1
Evaluation C

C_7H_8O (c) 67AND/CC
4-Methylphenol; p-Hydroxytoluene; p-Cresol
Heat Capacity 298.15 K, C_p=150.25 J·mol^{-1}·K
Temperature range 10 to 400 K.
Entropy 298.15 K, S=167.32 J·mol^{-1}·K^{-}
Phase Changes
c/liq 307.94 K, ΔH=12707 J·mol^{-1}
ΔS=41.26 J·mol^{-1}·K^{-}
Molecular Weight 108.1396
Wiswesser Line Notation QR D1
Evaluation A

C_7H_8O (c) 67RAS/G
4-Methylphenol; p-Hydroxytoluene; p-Cresol
Heat Capacity 313 K, C_p=226.2 J·mol^{-1}·K^{-}
Temperature range 313 to 373 K.
Molecular Weight 108.1396
Wiswesser Line Notation QR D1
Evaluation C

C_7H_8O (c) 75NIC/W
4-Methylphenol; p-Hydroxytoluene; p-Cresol
Heat Capacity 298.15 K, C_p=221.03 J·mol^{-1}·K
One temperature.
Molecular Weight 108.1396
Wiswesser Line Notation QR D1
Evaluation B

C_7H_8O (c) 82POE/F
4-Methylphenol; p-Hydroxytoluene; p-Cresol
Phase Changes
c/liq 309.0 K, ΔH=11887 J·mol^{-1}
ΔS=38.47 J·mol^{-1}·K
Molecular Weight 108.1396
Wiswesser Line Notation QR D1
Evaluation A

C_7H_8O (c) 90MEV/LIC
4-Methylphenol; p-Hydroxytoluene; p-Cresol
Heat Capacity 298.15 K, C_p=163.5 J·mol^{-1}·K^{-1}
Temperature range 173 to 353 K. C_p(c)=145.401 +0.616T+3.728×10^{-3}T^2+2.145×10^{-5}T^3 J·mol^{-1}·K^{-1} (−100 to 22 °C). C_p(liq)=232.122+0.178T J·mol^{-1}·K^{-1} (40 to 80 °C).
Phase Changes
c/liq 307.35 K, ΔH=11800 J·mol^{-1}
ΔS=38 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR D1
Evaluation A

$C_7H_8O_2$ (c) 41SAT/SOG3
2,5-Dihydroxytoluene
Heat Capacity 323 K, C_p=174.9 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 124.1390
Wiswesser Line Notation QR DQ B1
Evaluation C
Same data as 40SAT/SOG4.

$C_7H_8O_2·H_2O$ (c) 82VII/GAM
Orcinol monohydrate; 3,5-Dihydroxytoluene monohydrate
Phase Changes
c/liq 328.0 K, ΔH=26360 J·mol^{-1}
ΔS=80.4 J·mol^{-1}·K^{-1}
Molecular Weight 142.1542
Wiswesser Line Notation QR CQ E1 &QH
Evaluation B

C_7H_8S (liq) 74MES/FIN
Methyl phenyl sulfide
Heat Capacity 298.15 K, C_p=206.02 J·mol^{-1}·K^{-1}
Temperature range 10 to 330 K.
Entropy 298.15 K, S=252.50 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 256.44 K, ΔH=14835.8 J·mol^{-1}
ΔS=57.85 J·mol^{-1}·K^{-1}
Molecular Weight 124.2002
Wiswesser Line Notation 1SR
Evaluation A

C_7H_9N (liq) 02LOU
N-Methylaniline
Heat Capacity 380 K, C_p=230 J·mol^{-1}·K^{-1}
Mean value 20 to 196 °C.
Molecular Weight 107.1548
Wiswesser Line Notation 1MR
Evaluation D

C_7H_9N (liq) 36KUR/VOS
N-Methylaniline
Heat Capacity 290 K, C_p=230.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 107.1548
Wiswesser Line Notation 1MR
Evaluation D

C_7H_9N (liq) 87LES/LIC
N-Methylaniline
Heat Capacity 298 K, C_p=207.1 J·mol^{-1}·K^{-1}
Temperature range 220 to 325 K.
Phase Changes
c/liq 216 K
Molecular Weight 107.1548
Wiswesser Line Notation 1MR
Evaluation B

C_7H_9N (liq) 71HAL/BAL
1-Bicyclo[3.1.0]hexyl cyanide; 1-Cyanobicyclo[3.1.0]hexane
Heat Capacity 297 K, C_p=170.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 107.1548
Wiswesser Line Notation L35TJ ACN
Evaluation C

C_7H_9N (liq) 86STE/CHI
2,3-Dimethylpyridine; 2,3-Lutidine
Heat Capacity 298.15 K, C_p=189.55 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S=243.70 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 47.350 K
c,I/liq 258.565 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ B1 C1
Evaluation A

C_7H_9N (liq) 86STE/CHI
2,4-Dimethylpyridine
Heat Capacity 298.15 K, C_p=184.76 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S=248.50 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 209.415 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ B1 D1
Evaluation A

C_7H_9N (liq) 86STE/CHI
2,5-Dimethylpyridine
Heat Capacity 298.15 K, C_p=184.70 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S=248.81 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 182.200 K
c/liq 259.070 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ B1 E1
Evaluation A

C_7H_9N (liq) 86STE/CHI
2,6-Dimethylpyridine
Heat Capacity 298.15 K, C_p=185.17 J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, S=244.24 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 35.816 K
c,I/liq 267.033 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ B1 F1
Evaluation A

C_7H_9N (liq) 84POD/RAC
3,4-Dimethylpyridine
Heat Capacity 298 K, C_p=196 J·mol^{-1}·K^{-1}
Temperature range 265 to 380 K. Data graphically only. Value given is estimated from graph.
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ C1 D1
Evaluation B
Specific heat anomaly with peak at 293.5 K, $\Delta\Delta H$=65.6 J·mol^{-1}, $\Delta\Delta S$=0.16 J·mol^{-1}·K^{-1}. Temperature range of anomaly is 280 to 310 K.

C_7H_9N (liq) 86STE/CHI
3,4-Dimethylpyridine
Heat Capacity 298.15 K, C_p=191.84 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S=240.72 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 241.100 K
c,I/liq 262.704 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ C1 D1
Evaluation A

C_7H_9N (liq) 86STE/CHI
3,5-Dimethylpyridine
Heat Capacity 298.15 K, C_p=184.55 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S=241.72 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 266.823 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ C1 E1
Evaluation A

C_7H_9N (liq) 75NIC/WAD
Benzylamine; Phenylmethylamine
Heat Capacity 298.15 K, C_p=207.18 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 107.1548
Wiswesser Line Notation Z1R
Evaluation B

C_7H_9N (liq) 1881REI
2-Methylaniline; o-Toluidine
Heat Capacity 298 K, C_p=211.3 J·mol^{-1}·K^{-1}
Temperature range 294 to 485 K.
Molecular Weight 107.1548
Wiswesser Line Notation ZR B1
Evaluation D

C_7H_9N (liq) 02LOU
2-Methylaniline; o-Toluidine
Heat Capacity 380 K, C_p=234 J·mol^{-1}·K^{-1}
Mean value 20 to 196 °C.
Molecular Weight 107.1548
Wiswesser Line Notation ZR B1
Evaluation D

C_7H_9N (liq) 34KOL/UDC
2-Methylaniline; o-Toluidine
Heat Capacity 302.5 K, C_p=209.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 107.1548
Wiswesser Line Notation ZR B1
Evaluation C

C_7H_9N (liq) 34KOL/UDO
2-Methylaniline; o-Toluidine
Heat Capacity 302.5 K, C_p=209.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 107.1548
Wiswesser Line Notation ZR B1
Evaluation C

C_7H_9N (liq) 34RAD/JUI
2-Methylaniline; o-Toluidine
Heat Capacity 288 K, C_p=201.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 107.1548
Wiswesser Line Notation ZR B1
Evaluation C

C_7H_9N (liq) 88GUS/MII
2-Methylaniline; o-Toluidine
Heat Capacity 303.15 K, C_p=164.4 J·mol^{-1}·K^{-1}
Temperature range 303 to 463 K. p=0.1 MPa. Unsmoothed experimental datum. C_p(liq)=0.8056+0.0023634T+(0.001736−8.1591×10^{-6}T)P kJ/kg·K (303.15 to 523.15 K, 0.1 to 25 MPa
Molecular Weight 107.1548
Wiswesser Line Notation ZR B1
Evaluation B

C_7H_9N (liq) 90MEV/LI
2-Methylaniline; o-Toluidine
Phase Changes
c/liq 249.55 K, ΔH=8100 J·mol^{-1}
ΔS=32 J·mol^{-1}·K^{-1}
Molecular Weight 107.1548
Wiswesser Line Notation ZR B1
Evaluation A

C_7H_9N (liq) 34KOL/UD
3-Methylaniline; m-Toluidine
Heat Capacity 302.7 K, C_p=216.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 107.1548
Wiswesser Line Notation ZR C1
Evaluation C

C_7H_9N (liq) 34KOL/UDO
3-Methylaniline; m-Toluidine
Heat Capacity 302.7 K, C_p=216.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 107.1548
Wiswesser Line Notation ZR C1
Evaluation C

C_7H_9N (liq) 88GUS/MIR
3-Methylaniline; m-Toluidine
Heat Capacity 303.15 K, C_p=167.2 J·mol^{-1}·K^{-1}
Temperature range 303 to 463 K. p=0.1 MPa. Unsmoothed experimental datum. C_p(liq)=0.8666+0.0022600+(0.0007010 −6.0538×10^{-6}T)P kJ/kg·K (303.15 to 523.25 K, 0.1 to 25 MPa).
Molecular Weight 107.1548
Wiswesser Line Notation ZR C1
Evaluation B

C_7H_9N (liq) 90MEV/LIC
3-Methylaniline; m-Toluidine
Phase Changes
c/liq 241.65 K, ΔH=8800 J·mol^{-1}
ΔS=36 J·mol^{-1}·K^{-1}
Molecular Weight 107.1548
Wiswesser Line Notation ZR C1
Evaluation A

C_7H_9N (c) 1889FYK
4-Methylaniline; p-Toluidine
Phase Changes
c/liq 315.6 K, ΔH=17280 J·mol^{-1}
Molecular Weight 107.1548
Wiswesser Line Notation ZR D1
Evaluation C

C_7H_9N (c) 40CAM/CAM
4-Methylaniline; p-Toluidine
Heat Capacity 293 K, C_p=124.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 107.1548
Wiswesser Line Notation ZR D1
Evaluation C

C_7H_9N (c) 90MEV/LIC
4-Methylaniline; p-Toluidine
Heat Capacity 298.15 K, C_p=165.2 J·mol^{-1}·K^{-1}
Temperature range 273 to 368 K. C_p(c)=147.505+0.604T +3.525×10^{-3}T^2+2.351×10^{-5}T^3 J·mol^{-1}·K^{-1} (−100 to 30 °C). C_p(liq) =212.982+0.182T J·mol^{-1}·K^{-1} (50 to 95 °C).
Phase Changes
c/liq 316.55 K, ΔH=17300 J·mol^{-1}
ΔS=55 J·mol^{-1}·K^{-1}
Molecular Weight 107.1548
Wiswesser Line Notation ZR D1
Evaluation A

C_7H_9NO (c) 81LEB/RYA
p-Anisidine
Heat Capacity C_p=236.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 320 K. Data given over temperature range.
Molecular Weight 123.1542
Wiswesser Line Notation ZR DO1
Evaluation B

C_7H_9NO (c) 82KIS/SAN
Aniline· formaldehyde
Heat Capacity C_p=132.2 J·mol^{-1}·K^{-1}
Temperature range 298 to 303 K. C_p data given as 1.0736 J·K^{-1}·g^{-1} over a 25 to 30 °C temperature range.
Molecular Weight 123.1542
Wiswesser Line Notation ZR &VH
Evaluation C
C_p data given for 1:1 molar proportion of aniline formaldehyde. C_p data also given for the solid compounds of molar proportion: 1:2, 1:3, 1:4, 1:4.5, 1:4.75, 1:5, 1:7, 2:1 and 4:1.

$C_7H_9NO_2$ (c) 39SAT/SOG2
Ammonium benzoate
Heat Capacity 323 K, C_p=212.5 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 129.1536
Wiswesser Line Notation QVR &ZH
Evaluation C
Same data in 40SAT/SOG.

C_7H_{10} (c) 73HAL/SMI
Nortricyclene; Tricyclo[2.2.1.0^{2,6}]heptane
Heat Capacity 297 K, C_p=110.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 94.1560
Wiswesser Line Notation L535 B 1A GTJ
Evaluation C

C_7H_{10} (c) 78STE
Nortricyclene; Tricyclo[2.2.1.0^{2,6}]heptane
Heat Capacity 298.15 K, C_p=129.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 94.1560
Wiswesser Line Notation L535 B 1A GTJ
Evaluation B

C_7H_{10} (c) 73HAL/SMI
Norbornene; Bicyclo[2.2.1]heptene
Heat Capacity 297 K, C_p=129.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 94.1560
Wiswesser Line Notation L55 A CUTJ
Evaluation C

C_7H_{10} (liq) 78STE
Norbornene; Bicyclo[2.2.1]heptene
Heat Capacity 298.15 K, C_p=129.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 94.1560
Wiswesser Line Notation L55 A CUTJ
Evaluation B

$C_7H_{10}ClN$ (c) 89VAN/WHI
Phenylmethylammonium chloride
Phase Changes
c.II/c.I 416 K, ΔH=4240 J·mol^{-1}
ΔS=1.23 J·mol^{-1}·K^{-1}
Molecular Weight 143.6157
Wiswesser Line Notation Z1R &GH
Evaluation A

$C_7H_{10}N_2O$ (c) 80BYS
6,7-Diazatricyclo[3.2.2.0^{2,4}]non-6-ene N-oxide
Phase Changes
c,II/c,I 372.6 K, ΔH=15800 J·mol^{-1}
ΔS=42.4 J·mol^{-1}·K^{-1}
c,I/liq 411.4 K, ΔH=2600 J·mol^{-1}
ΔS=6.32 J·mol^{-1}·K^{-1}
Molecular Weight 138.1692
Wiswesser Line Notation T366/DI 2AC I ENUNTJ EUO
Evaluation A

$C_7H_{10}N_2O_2$ (c) 84ZIE/ZIE
1,3,6-Trimethyluracil
Phase Changes
c/liq 384.5 K, ΔH=21200 J·mol^{-1}
ΔS=55.1 J·mol^{-1}·K^{-1}
Molecular Weight 154.1682
Wiswesser Line Notation T6NVNVJ A1 C1 F1
Evaluation B

$C_7H_{10}N_2O_3$ (c) 89VAN/WHI
Phenylmethylammonium nitrate
Phase Changes
c,II/c,I 227 K, ΔH=900 J·mol^{-1}
ΔS=0.48 J·mol^{-1}·K^{-1}
Molecular Weight 170.1676
Wiswesser Line Notation Z1R &WNQ
Evaluation A

$C_7H_{10}O$ (liq) 88AND/PAT
1-Heptanol; n-Heptyl alcohol
Heat Capacity 298.15 K, C_p=272.29 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.2028
Wiswesser Line Notation Q7
Evaluation B

$C_7H_{11}N$ (liq) 71HAL/BAL
Cyclohexyl cyanide; Cyanocyclohexane
Heat Capacity 297 K, C_p=177.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 109.1706
Wiswesser Line Notation L6TJ ACN
Evaluation C

$C_7H_{11}N$ (liq) 91KIS/PIN
Cyclohexyl cyanide; Cyanocyclohexane
Phase Changes
c,II/c,I 215.0 K, ΔH=7425 J·mol^{-1}
ΔS=34.5 J·mol^{-1}·K^{-1}
c,I/liq 285.1 K, ΔH=3635 J·mol^{-1}
ΔS=12.75 J·mol^{-1}·K^{-1}
Molecular Weight 109.1706
Wiswesser Line Notation L6TJ ACN
Evaluation A
Data cited in 91KIS/PIN is from: Pinvidic, J.-J.: Ph.D. Thesis. Universite de Paris Sud (1988).

$C_7H_{11}N$ (liq) 91KIS/PIN
Cyclohexyl isocyanide; Isocyanocyclohexane
Heat Capacity
Temperature range 5 to 300 K. Data given graphically. C_p(liq)=195 J·mol^{-1}·K^{-1} is a graphical estimate.
Phase Changes
c,II/c,I 192.6 K, ΔH=6177 J·mol^{-1}
ΔS=32.07 J·mol^{-1}·K^{-1}
c,I/liq 279.6 K, ΔH=4227 J·mol^{-1}
ΔS=15.12 J·mol^{-1}·K^{-1}
Molecular Weight 109.1706
Wiswesser Line Notation L6TJ ANC
Evaluation A
T(glass-1)=160 K; T(glass-2)=130 K; T(glass-3)=55 K.

C_7H_{12} (liq) 70CHA/MCC
cis-Bicyclo[4.1.0]heptane
Heat Capacity 315 K, C_p=187.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 96.1718
Wiswesser Line Notation L36TJ -C
Evaluation B

C_7H_{12} (c) 78STE
Norbornane: Bicyclo[2.2.1]heptane
Heat Capacity 298.15 K, C_p=151.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 96.1718
Wiswesser Line Notation L55 ATJ
Evaluation B

C_7H_{12} (liq) 79FUC/PEA
1-Ethylcyclopentene
Heat Capacity 298.15 K, C_p=188.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 96.1718
Wiswesser Line Notation L5UTJ A2
Evaluation B

C_7H_{12} (liq) 79FUC/PEA
Ethylidenecyclopentane
Heat Capacity 298.15 K, C_p=181.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 96.1718
Wiswesser Line Notation L5YTJ AU2
Evaluation B

C_7H_{12} (liq) 88LEB/KUI
4-Methylcyclohexene
Heat Capacity 298.15 K, C_p=180.42 J mol^{-1}·K^{-1}
Temperature range 13.4 to 350 K.
Entropy 298.15 K, S=253.01 J·mol^{-1}·K^{-1}
Molecular Weight 96.1718
Wiswesser Line Notation L6UTJ D1
Evaluation A

C_7H_{12} (liq) 79FUC/PEA
Methylenecyclohexane
Heat Capacity 298.15 K, C_p=177.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 96.1718
Wiswesser Line Notation L6YTJ AU1
Evaluation B

C_7H_{12} (liq) 90HAI/GIL2
Cycloheptene
Phase Changes
c,III/c,II 154 K, ΔH=5280 J·mol^{-1}
ΔS=34.3 J·mol^{-1}·K^{-1}
c,II/c,I 210 K, ΔH=710 J·mol^{-1}
ΔS=3.4 J·mol^{-1}·K^{-1}
c,I/liq 217 K, ΔH=970 J·mol^{-1}
ΔS=4.5 J·mol^{-1}·K^{-1}
Molecular Weight 96.1718
Wiswesser Line Notation L7UTJ
Evaluation B

C_7H_{12} (liq) 89LEB/SMI
cis-Cycloheptene
Heat Capacity 298.15 K, C_p=171.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 310 K.
Entropy 298.15 K, S=241.0 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 154.22 K, ΔH=7070 J·mol^{-1}
ΔS=45.8 J·mol^{-1}·K^{-1}
c,II/c,I 208.26 K, ΔH=730 J·mol^{-1}
ΔS=3.5 J·mol^{-1}·K^{-1}
c,I/liq 217.75 K, ΔH=820 J·mol^{-1}
ΔS=4.1 J·mol^{-1}·K^{-1}
Molecular Weight 96.1718
Wiswesser Line Notation L7UTJ -C
Evaluation A
T_1(glass)=97 K; T_2(glass)=135 K.

$(C_7H_{12})_n$ (liq) 80LEB/MUK
Butadiene-propylene copolymer
Heat Capacity 298.15 K, C_p=192.4 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=209.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 262 K, ΔH=7800 J·mol^{-1}
ΔS=29.8 J·mol^{-1}·K^{-1}
100% crystallinity.
Molecular Weight 96.1718
Wiswesser Line Notation /*1Y1&2U2*/
Evaluation A
T(glass)=198 K.

$C_7H_{12}O$ (liq) 24HER/BLO
2-Methylcyclohexanone
Heat Capacity 290 K, C_p=204.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 122.1712
Wiswesser Line Notation L6VTJ B1
Evaluation C

$C_7H_{12}O$ (liq) 24HER/BLO
3-Methylcyclohexanone
Heat Capacity 290 K, C_p=207.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 122.1712
Wiswesser Line Notation L6VTJ C1
Evaluation C

$C_7H_{12}O$ (liq) 24HER/BLO
4-Methylcyclohexanone
Heat Capacity 290 K, C_p=207.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 122.1712
Wiswesser Line Notation L6VTJ D1
Evaluation C

$C_7H_{12}O_2$ (liq) 85KAR/ABD2
Butyl acrylate
Phase Changes
c/liq 209.5 K, ΔH=17307 J·mol^{-1}
ΔS=82.61 J·mol^{-1}·K^{-1}
Molecular Weight 128.1706
Wiswesser Line Notation 4OV1U1
Evaluation A

$C_7H_{12}O_2$ (liq) 85KAR/SAI
Butyl acrylate
Heat Capacity 298.15 K, C_p=251.0 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K. C_p(c)=155.53+5.53T J/kg·K (100 to 175 K); C_p(liq)=1290.27+2.24T J/kg·K (209.5 to 300 K). C_p data calculated from equation.
Phase Changes
c/liq 209.5 K
Molecular Weight 128.1706
Wiswesser Line Notation 4OV1U1
Evaluation B

$C_7H_{12}O_4$ (liq) 92VER/BEC
Dimethylmalonic acid dimethyl ester
Heat Capacity 298.15 K, C_p=259.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 160.1694
Wiswesser Line Notation 1OVX1&1&VO1
Evaluation B

$C_7H_{12}O_4$ (c) 74CIN/BER
Pimelic acid
Phase Changes
c,II/c,I 369.0 K, ΔH=1322 J·mol^{-1}
ΔS=3.60 J·mol^{-1}·K^{-1}
c,I/liq 377.5 K, ΔH=27623 J·mol^{-1}
ΔS=73.18 J·mol^{-1}·K^{-1}
Molecular Weight 160.1694
Wiswesser Line Notation QV5VQ
Evaluation B

$C_7H_{12}O_4$ (c) 88PET/TSY
Pimelic acid
Phase Changes
c,II/c,I 369.7 K, ΔH=1000 J·mol^{-1}
ΔS=2.7 J·mol^{-1}·K^{-1}
Molecular Weight 160.1694
Wiswesser Line Notation QV5VQ
Evaluation A

$C_7H_{12}O_4$ (liq) 33KOL/UDO
Diethyl malonate
Heat Capacity 294.6 K, C_p=284.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 160.1694
Wiswesser Line Notation 2OV1VO2
Evaluation C

$C_7H_{12}O_4$ (liq) 34KOL/UDO2
Diethyl malonate
Heat Capacity 294.6 K, C_p=284.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 160.1694
Wiswesser Line Notation 2OV1VO2
Evaluation C

$C_7H_{12}O_4$ (liq) 92VER/BEC
Diethyl malonate
Heat Capacity 298.15 K, C_p=300.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 160.1694
Wiswesser Line Notation 2OV1VO2
Evaluation B

$C_7H_{13}LiO_2$ (c) 85FRA/WES
Lithium heptanoate
Heat Capacity 298.15 K, C_p=231.72 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=231.06 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 317.08 K. ΔH=5832 J·mol^{-1}
ΔS=18.39 J·mol^{-1}·K^{-1}
Molecular Weight 136.1195
Wiswesser Line Notation OV6 .LI
Evaluation A

$C_7H_{13}LiO_2$ (c) 86FRA/NGE
Lithium heptanoate
Heat Capacity 300 K, C_p=231.72 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 300 K, S=231.06 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 317.08 K, ΔH=5840 J·mol^{-1}
ΔS=18.52 J·mol^{-1}·K^{-1}
Molecular Weight 136.1195
Wiswesser Line Notation OV6 .LI
Evaluation A

$C_7H_{13}N$ (c,I) 70WES/WON
1-Azabicyclo[2.2.2]octane; Quinuclidine
Heat Capacity 298.15 K, C_p=169.37 J·mol^{-1}·K^{-1}
Temperature range 5 to 433 K.
Entropy 298.15 K, S=206.98 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 196 K, ΔH=5226 J·mol^{-1}
ΔS=26.52 J·mol^{-1}·K^{-1}
Transition region 190 to 200 K; maximum at 196 K. Entropy change obtained by difference of integrated heat input and lattice (extrapolated C_p) contribution.
c,I/liq 430 K, ΔH=5860 J·mol^{-1}
ΔS=13.6 J·mol^{-1}·K^{-1}
Molecular Weight 111.1864
Wiswesser Line Notation T66 A B CNTJ
Evaluation A

$C_7H_{13}NO$ (c) 59KOL/PAU
ζ-Enantholactam
Heat Capacity 290 K, C_p=196.1 J·mol^{-1}·K^{-1}
Temperature range 60 to 350 K.
Entropy 298.15 K, S=190.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 310.295 K, ΔH=13376 J·mol^{-1}
ΔS=43.1 J·mol^{-1}·K^{-1}
Molecular Weight 127.1835
Wiswesser Line Notation T8MVTJ
Evaluation B

$C_7H_{13}NO$ (c) 62KOL/PAU
ζ-Enantholactam
Heat Capacity 295.00 K, C_p=205.1 J·mol^{-1}·K^{-1}
Temperature range 60 to 350 K.
Entropy 298.15 K, S=190.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 310.295 K, ΔH=13376 J·mol^{-1}
ΔS=43.1 J·mol^{-1}·K^{-1}
Molecular Weight 127.1835
Wiswesser Line Notation T8MVTJ
Evaluation B

$C_7H_{13}N_3O_4$ (c) 89KUL/KO
α-Alanylasparagine (DL)
Heat Capacity 298 K, C_p=256.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 203.1974
Wiswesser Line Notation ZY1&VMYVQ1VZ
Evaluation C

$C_7H_{13}N_3O_4$ (c) 89KUL/KO
α-Alanylglycylglycine
Heat Capacity 298 K, C_p=236.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 203.1974
Wiswesser Line Notation ZY1VNV1Z1VQ
Evaluation C

$C_7H_{13}N_3O_4$ (c) 90BAD/KU
Alanylglycylglycine (DL)
Heat Capacity 298 K, C_p=236 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 203.1974
Wiswesser Line Notation ZY1&VM1VM1VQ -DL
Evaluation D

$C_7H_{13}N_3O_4 \cdot H_2O$ (c) 90BAD/KU
Alanylasparagine hydrate (DL)
Heat Capacity 298 K, C_p=256 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 221.2126
Wiswesser Line Notation ZY1&VMY1VZVQ &QH -DL
Evaluation D

$C_7H_{13}O_2Tl$ (c) 76MEI/SE
Thallium heptanoate
Phase Changes
c,II/c,I 299 K, ΔH=2761 J·mol^{-1}
ΔS=9.20 J·mol^{-1}·K^{-1}
c,I/liq 419 K, ΔH=6276 J·mol^{-1}
ΔS=15.1 J·mol^{-1}·K^{-1}
Solid-mesophase.
liq/liq 501 K, ΔH=3138 J·mol^{-1}
ΔS=6.28 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
Molecular Weight 333.5485
Wiswesser Line Notation OV6 .TL
Evaluation B

$C_7H_{13}O_2Tl$ (c) 84FER/LC
Thallium heptanoate
Heat Capacity 320 K, C_p=318 J·mol^{-1}·K^{-1}
Temperature range 320 to 480 K.
Phase Changes
c,II/c,I 301.9 K, ΔH=2652 J·mol^{-1}
ΔS=8.81 J·mol^{-1}·K^{-1}
c,I/liq 420.7 K, ΔH=6302 J·mol^{-1}
ΔS=15.0 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 333.5485
Wiswesser Line Notation OV6 .TL
Evaluation A
Mesophase to isotropic liquid phase change data also given: T=502.0 K; $\Delta\Delta H$=3301 J·mol; $\Delta\Delta S$=6.57 J·mol^{-1}·K^{-1}.

$C_7H_{13}O_2Tl$ (c) 85NGE/LOP

Thallium heptanoate

Heat Capacity	298.15 K,	C_p=367.50 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K. Estimated value.		
Entropy	298.15 K,	S=320.77 J·mol^{-1}·K^{-1}
Phase Changes		
c,VI/c,V	262.8 K,	ΔH=1966 J·mol^{-1}
		ΔS=7.44 J·mol^{-1}·K^{-1}
c,V/c,IV	267.8 K,	ΔH=1167 J·mol^{-1}
		ΔS=4.36 J·mol^{-1}·K^{-1}
c,IV/c,III	271.7 K,	ΔH=1176 J·mol^{-1}
		ΔS=4.32 J·mol^{-1}·K^{-1}
c,III/c,II	296.2 K,	ΔH=2956 J·mol^{-1}
		ΔS=10.02 J·mol^{-1}·K^{-1}
c,II/c,I	300.9 K,	ΔH=2546 J·mol^{-1}
		ΔS=8.40 J·mol^{-1}·K^{-1}
c,I/liq	420.7 K	Solid-mesomorphic liquid.

Molecular Weight 333.5485
Wiswesser Line Notation OV6 .TL
Evaluation A
Mesomorphic liquid-isotropic liquid transition at 502.7 K.

$C_7H_{13}O_2Tl$ (c) 89LAB/LOP

Thallium heptanoate

Heat Capacity	298.15 K,	C_p=354.19 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.		
Entropy	298.15 K,	S=330.83 J·mol^{-1}·K^{-1}
Phase Changes		
c,IV′/c,III′	269.3 K,	ΔH=1413 J·mol^{-1}
		ΔS=5.24 J·mol^{-1}·K^{-1}
c,III′/c,II	271.8 K,	ΔH=1413 J·mol^{-1}
		ΔS=5.15 J·mol^{-1}·K^{-1}
c,V/c,IV	262.3 K,	ΔH=2087 J·mol^{-1}
		ΔS=7.98 J·mol^{-1}·K^{-1}
c,IV/c,III	267.9 K	ΔH=2087 J·mol^{-1}
		ΔS=7.98 J·mol^{-1}·K^{-1}.
c,III/c,II	272.4 K,	ΔH=1588 J·mol^{-1}
		ΔS=5.82 J·mol^{-1}·K^{-1}
c,II/c,I	300.96 K	ΔH=3009 J·mol^{-1}
		ΔS=9.18 J·mol^{-1}·K^{-1}.
c,I/liq	420.7 K,	ΔH=6302 J·mol^{-1}
		ΔS=15.0 J·mol^{-1}·K^{-1}
c/liq	502.0 K	ΔH=3301 J·mol^{-1}
		ΔS=6.57 J·mol^{-1}·K^{-1}.

Molecular Weight 333.5485
Wiswesser Line Notation OV6 .TL
Evaluation A

C_7H_{14} (liq) 36PAR/TOD2

1-Heptene

Heat Capacity	295.1 K,	C_p=212.84 J·mol^{-1}·K^{-1}
Temperature range 80 to 295 K. Value is unsmoothed experimental datum.		
Entropy	298.15 K,	S=328.9 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 58.58 J·mol^{-1}·K^{-1}.		
Phase Changes		
c/liq	153.4 K,	ΔH=12661 J·mol^{-1}
		ΔS=82.54 J·mol^{-1}·K^{-1}

Molecular Weight 98.1876
Wiswesser Line Notation 6U1
Evaluation (C_p).C(S)

C_7H_{14} (liq) 57MCC/FIN2

1-Heptene

Heat Capacity	298.15 K,	C_p=211.79 J·mol^{-1}·K^{-1}
Temperature range 11 to 360 K.		
Entropy	298.15 K,	S=327.65 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/liq	153.89 K,	ΔH=12640 J·mol^{-1}
		ΔS=82.14 J·mol^{-1}·K^{-1}
c,I/liq	154.30 K,	ΔH=12401 J·mol^{-1}
		ΔS=80.37 J·mol^{-1}·K^{-1}

Molecular Weight 98.1876
Wiswesser Line Notation 6U1
Evaluation A

C_7H_{14} (liq) 53GRO/OLI

1,1-Dimethylcyclopentane

Heat Capacity	299.81 K,	C_p=187.36 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Unsmoothed experimental datum.		
Entropy	298.15 K,	S=265.01 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/c,I	146.80 K,	ΔH=6489.4 J·mol^{-1}
		ΔS=44.21 J·mol^{-1}·K^{-1}
c,I/liq	203.68 K,	ΔH=1078.6 J·mol^{-1}
		ΔS=5.30 J·mol^{-1}·K^{-1}

Molecular Weight 98.1876
Wiswesser Line Notation L5TJ A1 A1
Evaluation A

C_7H_{14} (liq) 31HUF/PAR

1,2-Dimethylcyclopentane

Heat Capacity	294.2 K,	C_p=187.4 J·mol^{-1}·K^{-1}
Temperature range 93 to 294 K. Value is unsmoothed experimental datum.		
Entropy	298.1 K,	S=269.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 69.75 J·mol^{-1}·K^{-1}.		
Phase Changes		
c/liq	154.1 K,	ΔH=6410 J·mol^{-1}
		ΔS=41.6 J·mol^{-1}·K^{-1}

Molecular Weight 98.1876
Wiswesser Line Notation L5TJ A1 B1
Evaluation B(C_p),C(S)

C_7H_{14} (liq) 53GRO/OLI

1-cis-2-Dimethylcyclopentane

Heat Capacity	302.84 K,	C_p=190.66 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Unsmoothed experimental datum.		
Entropy	298.15 K,	S=269.16 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/c,I	141.50 K,	ΔH=6668.9 J·mol^{-1}
		ΔS=47.13 J·mol^{-1}·K^{-1}
c,I/liq	219.45 K,	ΔH=1657.3 J·mol^{-1}
		ΔS=7.55 J·mol^{-1}·K^{-1}

Molecular Weight 98.1876
Wiswesser Line Notation L5TJ A1 B1 -C
Evaluation A

C_7H_{14} (liq) 53GRO/OLI

1-trans-3-Dimethylcyclopentane

Heat Capacity	304.03 K,	C_p=190.87 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Unsmoothed experimental datum.		
Entropy	298.15 K,	S=271.54 J·mol^{-1}·K^{-1}
Phase Changes		
c/liq	139.48 K,	ΔH=7398.1 J·mol^{-1}
		ΔS=53.04 J·mol^{-1}·K^{-1}

Molecular Weight 98.1876
Wiswesser Line Notation L5TJ A1 C1 -T
Evaluation A

C_7H_{14} (liq) 53GRO/OLI
Ethylcyclopentane
Heat Capacity 301.83 K, C_p=187.61 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Unsmoothed experimental datum.
Entropy 298.15 K, S=279.91 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 134.73 K, ΔH=6869.3 J·mol^{-1}
ΔS=50.99 J·mol^{-1}·K^{-1}
Form stable above 129.5 K.
c,II/liq 134.03 K, ΔH=2904.4 J·mol^{-1}
ΔS=58.97 J·mol^{-1}·K^{-1}
Form stable below 129.5 K.
Molecular Weight 98.1876
Wiswesser Line Notation L5TJ A2
Evaluation A

C_7H_{14} (liq) 30PAR/HUF2
Methylcyclohexane
Heat Capacity 294.2 K, C_p=182.0 J·mol^{-1}·K^{-1}
Temperature range 93 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=248.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 54.73 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 146.2 K, ΔH=6673 J·mol^{-1}
ΔS=45.14 J·mol^{-1}·K^{-1}
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation B(C_p),C(S)

C_7H_{14} (liq) 46DOU/HUF2
Methylcyclohexane
Heat Capacity 298.15 K, C_p=184.51 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=247.90 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 146.58 K, ΔH=6750.5 J·mol^{-1}
ΔS=46.05 J·mol^{-1}·K^{-1}
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation A

C_7H_{14} (liq) 66HWA/ZIE
Methylcyclohexane
Heat Capacity 298.055 K, C_p=185.27 J·mol^{-1}·K^{-1}
Temperature range 175 to 308 K. Unsmoothed experimental datum.
Phase Changes
c/liq 146.65 K
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation B

C_7H_{14} (liq) 75HOL/ZIE
Methylcyclohexane
Heat Capacity 298.15 K, C_p=184.84 J·mol^{-1}·K^{-1}
Temperature range 144 to 312 K. C_p=129.88277 −0.0054107773T+7.9975642×10^{-4}T^2 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 146.550 K
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation A

C_7H_{14} (liq) 79WIL/GRO
Methylcyclohexane
Heat Capacity 298.15 K, C_p=184.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation B

C_7H_{14} (liq) 82GRO/ING
Methylcyclohexane
Heat Capacity 298.15 K, C_p=185.29 J·mol^{-1}·K^{-1}
Temperature range 298.15 K. One temperature.
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation A

C_7H_{14} (liq) 83SID/SVE
Methylcyclohexane
Heat Capacity 293.15 K, C_p=183.88 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation B

C_7H_{14} (liq) 85TAN
Methylcyclohexane
Heat Capacity 298.15 K, C_p=184.96 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation A

C_7H_{14} (liq) 88SHI/OGA2
Methylcyclohexane
Heat Capacity 298.15 K, C_p=184.38 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation A

C_7H_{14} (liq) 56FIN/SCC
Cycloheptane
Heat Capacity 298.15 K, C_p=180.75 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=242.55 J·mol^{-1}·K^{-1}
Phase Changes
c,IV/c,III 134.8 K, ΔH=4966.4 J·mol^{-1}
ΔS=36.84 J·mol^{-1}·K^{-1}
c,III/c,II 198.2 K, ΔH=289.5 J·mol^{-1}
ΔS=1.46 J·mol^{-1}·K^{-1}
c,II/c,I 212.4 K, ΔH=449.8 J·mol^{-1}
ΔS=2.12 J·mol^{-1}·K^{-1}
c,I/liq 265.12 K, ΔH=1882.0 J·mol^{-1}
ΔS=7.10 J·mol^{-1}·K^{-1}
Molecular Weight 98.1876
Wiswesser Line Notation L7TJ
Evaluation A

C_7H_{14} (liq) 75JOL/BOI
Cycloheptane
Heat Capacity 298.15 K, C_p=180.47 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.1876
Wiswesser Line Notation L7TJ
Evaluation B

C_7H_{14} (liq) 79FOR/DAR
Cycloheptane
Heat Capacity 298.15 K, C_p=180.614 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.1876
Wiswesser Line Notation L7TJ
Evaluation B

C_7H_{14} (liq) 90HAI/GIL
Cycloheptane
Phase Changes
c,IV/c,III 135.7 K
c,III/c,I 206.3 K
Overlap of the III to II and the II to I transitions.
Molecular Weight 98.1876
Wiswesser Line Notation L7TJ
Evaluation A

$C_7H_{14}N_2O_2$ (c) 91ABA/DEL
α-Acetylaminoisobutyro-N′-methylamide(DL);
2-(Acetylamino)-N,2-dimethylpropanamide(DL)
Heat Capacity 298 K, C_p=229.10 J·mol^{-1}·K^{-1}
Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 158.1998
Wiswesser Line Notation 1X1&VM1&MV1 -DL
Evaluation C

$C_7H_{14}O$ (liq) 70AND/COU
2,4-Dimethyl-3-pentanone; Diisopropyl ketone
Heat Capacity 298.15 K, C_p=233.7 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=318.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 204.81 K, ΔH=11180 J·mol^{-1}
ΔS=54.58 J·mol^{-1}·K^{-1}
Molecular Weight 114.1870
Wiswesser Line Notation 1Y1&VY1&1
Evaluation A

$C_7H_{14}O$ (liq) 88CAC/COS
1-Methylcyclohexanol
Heat Capacity 298.15 K, C_p=279.05 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.1870
Wiswesser Line Notation L6TJ AQ A1
Evaluation B

$C_7H_{14}O$ (liq) 88CAC/COS
2-Methylcyclohexanol
Heat Capacity 298.15 K, C_p=267.44 J·mol^{-1}·K^{-1}
One temperature. Mixed isomers. C_p(trans isomer)=262.98; (cis isomer)=268.95 J/K·mol.
Molecular Weight 114.1870
Wiswesser Line Notation L6TJ AQ B1
Evaluation B

$C_7H_{14}O$ (liq) 24HER/BLO
2-Methylcyclohexanol
Heat Capacity 290 K, C_p=199.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.1870
Wiswesser Line Notation L6TJ AQ B1
Evaluation C

$C_7H_{14}O$ (liq) 24HER/BLO
3-Methylcyclohexanol
Heat Capacity 290 K, C_p=201.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.1870
Wiswesser Line Notation L6TJ AQ C1
Evaluation C

$C_7H_{14}O$ (liq) 24HER/BLO
4-Methylcyclohexanol
Heat Capacity 290 K, C_p=202.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.1870
Wiswesser Line Notation L6TJ AQ D1
Evaluation C

$C_7H_{14}O$ (liq) 72ADA/SUG
Cycloheptanol
Heat Capacity 298.15 K, C_p=250.22 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=241.638 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 258.45 K, ΔH=875 J·mol^{-1}
ΔS=3.39 J·mol^{-1}·K^{-1}
c,II′/c,II 172.23 K
ΔH=2925 J·mol^{-1} between 162.50 and 176.50
c,III/c,II 227.26 K, ΔH=554 J·mol^{-1}
ΔS=2.44 J·mol^{-1}·K^{-1}
c,III′/c,III 152.30 K, ΔH=58.07 J·mol^{-1}
ΔS=0.38 J·mol^{-1}·K^{-1}
c,III″/c,III 128.2 K
c,I/liq 280.30 K, ΔH=1604 J·mol^{-1}
ΔS=5.72 J·mol^{-1}·K^{-1}
Molecular Weight 114.1870
Wiswesser Line Notation L7TJ AQ
Evaluation A

$C_7H_{14}O$ (liq) 76CON/GIN
Cycloheptanol
Heat Capacity 298 K, C_p=244.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.1870
Wiswesser Line Notation L7TJ AQ
Evaluation B

$C_7H_{14}O$ (liq) 87MIL/FEN2
3-Methylhexanal
Heat Capacity 323.15 K, C_p=245.94 J·mol^{-1}·K^{-1}
Temperature range 323.15 to 428.15 K.
Molecular Weight 114.1870
Wiswesser Line Notation VH1Y3
Evaluation A

$C_7H_{14}O$ (liq) 87MIL/FEN2
3,4-Dimethylpentanal
Heat Capacity 323.15 K, C_p=235.60 J·mol^{-1}·K^{-1}
Temperature range 323.15 to 428.15 K.
Molecular Weight 114.1870
Wiswesser Line Notation VH1Y1&Y1&1
Evaluation A

$C_7H_{14}O$ (liq) 1881REI
Heptanal; Oenanthal; Enanthal; n-Heptaldehyde
Heat Capacity 298 K, C_p=204.6 J·mol^{-1}·K^{-1}
Temperature range 298 to 450 K.
Molecular Weight 114.1870
Wiswesser Line Notation VH6
Evaluation D

$C_7H_{14}O$ (liq) 56PAR/KEN
Heptanal; Oenanthal; Enanthal; n-Heptaldehyde
Heat Capacity 298.15 K, C_p=250.33 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.1 K, S=348.5 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 56.69 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 229.8 K, ΔH=23585 J·mol^{-1}
ΔS=102.63 J·mol^{-1}·K^{-1}
Molecular Weight 114.1870
Wiswesser Line Notation VH6
Evaluation B(C_p),C(S)

$C_7H_{14}O$ (liq) 82DYA/VAS
Heptanal; Oenanthal; Enanthal; n-Heptaldehyde
Heat Capacity 298.15 K, C_p=230.78 J·mol^{-1}·K^{-1}
Calculated from general equation: C_p(J·mol^{-1}·K^{-1})=(112.4±4.2) −(59.94±3.46)×10^{-2}T(K)+(10.93±0.74)×10^{-4}T^2+(20.66±0.57) × n_c (number of carbon atoms)+(2.65±0.19)×10^{-2}Tn$_c$.
Entropy 298.15 K, S=335.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq ΔH=22890 J·mol^{-1}
Molecular Weight 114.1870
Wiswesser Line Notation VH6
Evaluation B

$C_7H_{14}O$ (liq) 84VAS/PET
Heptanal; Oenanthal; Enanthal; n-Heptaldehyde
Heat Capacity 298.15 K, C_p=230.15 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S=335.43 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 229.20 K
Molecular Weight 114.1870
Wiswesser Line Notation VH6
Evaluation A

$C_7H_{14}O_2$ (liq) 86NIL/WAD
Ethyl-2,2-dimethylpropanoate
Heat Capacity 298.15 K, C_p=251.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.1864
Wiswesser Line Notation 2OVX1&1&1
Evaluation A

$C_7H_{14}O_2$ (liq) 92VER/BEC
Ethyl-2,2-dimethylpropanoate
Heat Capacity 298.15 K, C_p=277.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.1864
Wiswesser Line Notation 2OVX1&1&1
Evaluation B

$C_7H_{14}O_2$ (liq) 92VER/BEC
2-Methylbutanoic acid ethyl ester
Heat Capacity 298.15 K, C_p=327.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.1864
Wiswesser Line Notation 2Y1&VO2
Evaluation B

$C_7H_{14}O_2$ (liq) 82SCH/MIL
Heptanoic acid
Heat Capacity 298.15 K, C_p=265.43 J·mol^{-1}·K^{-1}
Temperature range 80 to 305 K.
Phase Changes
c,II/c,I 224.8 K, ΔH=2038 J·mol^{-1}
ΔS=9.07 J·mol^{-1}·K^{-1}
c,I/liq 265.83 K, ΔH=15437 J·mol^{-1}
ΔS=58.07 J·mol^{-1}·K^{-1}
Molecular Weight 130.1864
Wiswesser Line Notation QV6
Evaluation B

$C_7H_{14}O_2$ (liq) 91LAB/WES
Heptanoic acid
Heat Capacity 298.15 K, C_p=267.31 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=323.35 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 219.99 K, ΔH=2163.4 J·mol^{-1}
ΔS=9.412 J·mol^{-1}·K^{-1}
c,I/liq 265.98 K, ΔH=15129.9 J·mol^{-1}
ΔS=57.295 J·mol^{-1}·K^{-1}
Molecular Weight 130.1864
Wiswesser Line Notation QV6
Evaluation A

$C_7H_{14}O_2$ (liq) 39PHI
Pentyl ethanoate; n-Amyl acetate
Heat Capacity 304.0 K, C_p=276.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.1864
Wiswesser Line Notation 5OV1
Evaluation C

$C_7H_{14}O_3$ (liq) 82BIR/SIK
2-Hydroxyethyl-2′,2′-dimethylpropionate; 2-Hydroxyethyl pivalate
Heat Capacity 298.15 K, C_p=308.0 J·mol^{-1}·K^{-1}
Temperature range 270 to 370 K. Equation only. C_p=15.79 +1.337T−0.001197T^2 J·mol^{-1}·K^{-1}.
Molecular Weight 146.1858
Wiswesser Line Notation Q2OVX1&1&1
Evaluation C

$C_7H_{15}Br$ (liq) 93SHE
1-Bromoheptane; n-Heptyl bromide
Heat Capacity 298.15 K, C_p=247.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 179.0995
Wiswesser Line Notation E7
Evaluation B

$C_7H_{15}Cl$ (liq) 93SHE
1-Chloroheptane; n-Heptyl chloride
Heat Capacity 298.15 K, C_p=245.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 134.6485
Wiswesser Line Notation G7
Evaluation B

$C_7H_{15}I$ (liq) 93SHE
1-Iodoheptane; n-Heptyl iodide
Heat Capacity 298.15 K, C_p=251.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.1000
Wiswesser Line Notation I7
Evaluation B

$C_7H_{15}N$ (liq) 76CON/GIN
Octahydroazocine
Heat Capacity 298 K, C_p=230 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 113.2022
Wiswesser Line Notation T8MTJ
Evaluation C

$C_7H_{15}NO_2$ (liq) 92VER/BEC
N,N,2-Trimethylalanine methyl ester
Heat Capacity 298.15 K, C_p=315.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 145.2010
Wiswesser Line Notation 1OVX1&1&N1&1
Evaluation B

C_7H_{16} (liq) 30HUF/PAR2
2,4-Dimethylpentane
Heat Capacity 294.4 K, C_p=220.9 J·mol^{-1}·K^{-1}
Temperature range 92 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=291.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 65.90 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 152.5 K, ΔH=6694 J·mol^{-1}
ΔS=43.90 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 1Y1&1Y&1
Evaluation B(C_p),C(S)

C_7H_{16} (liq) 61HUF/GRO
2,4-Dimethylpentane
Heat Capacity 298.15 K, C_p=224.22 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=303.17 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 153.97 K, ΔH=6845 J·mol^{-1}
ΔS=44.46 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 1Y1&1Y&1
Evaluation A

C_7H_{16} (liq) 30HUF/PAR2
2,2,3-Trimethylbutane
Heat Capacity 293.9 K, C_p=208.4 J·mol^{-1}·K^{-1}
Temperature range 89 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=27.11 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 14.0 cal·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 121.0 K, ΔH=2377 J·mol^{-1}
ΔS=19.64 J·mol^{-1}·K^{-1}
Hump in heat capacity curve at about 105 K, with excess enthalpy of 243 J·mol^{-1}.
c,I/liq 247.7 K, ΔH=2201 J·mol^{-1}
ΔS=8.89 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 1Y1&X1&1&1
Evaluation B(C_p),C(S)

C_7H_{16} (liq) 61HUF/GRO
2,2,3-Trimethylbutane
Heat Capacity 298.15 K, C_p=213.51 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=292.25 J·mol^{-1}·K^{-1}
Phase Changes
Lambda-type transitions at 87, 108 K.
c,II/c,I 121.4 K, ΔH=2242 J·mol^{-1}
ΔS=18.47 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 1Y1&X1&1&1
Evaluation A

C_7H_{16} (liq) 30HUF/PAR2
3,3-Dimethylpentane
Heat Capacity 292.9 K, C_p=211.7 J·mol^{-1}·K^{-1}
Temperature range 92 to 293 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=293.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 60.67 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 138.2 K, ΔH=7067 J·mol^{-1}
ΔS=51.14 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 2X2&1&1
Evaluation B(C_p),C(S)

C_7H_{16} (liq) 76FIN/MES
3,3-Dimethylpentane
Heat Capacity 298.15 K, C_p=214.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=305.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 132.7 K, ΔH=793.7 J·mol^{-1}
ΔS=5.98 J·mol^{-1}·K^{-1}
c,II/liq 138.20 K, ΔH=7642.5 J·mol^{-1}
ΔS=55.30 J·mol^{-1}·K^{-1}
c,I/liq 138.75 K, ΔH=6846.3 J·mol^{-1}
ΔS=49.34 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 2X2&1&1
Evaluation A

C_7H_{16} (liq) 30HUF/PAR2
2,3-Dimethylpentane
Heat Capacity 291.5 K, C_p=215.9 J·mol^{-1}·K^{-1}
Temperature range 68 to 292 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=306.3 J·mol^{-1}·K^{-1}
Extrapolation below 70 K, 69.5 J·mol^{-1}·K^{-1}. Forms glass at low temperatures. Value includes estimated zero point entropy of 17 J·mol^{-1}·K^{-1}.
Molecular Weight 100.2034
Wiswesser Line Notation 2Y1&Y1&1
Evaluation B(C_p),C(S)

C_7H_{16} (liq) 76FIN/MES
2,3-Dimethylpentane
Heat Capacity 298.15 K, C_p=218.3 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=297.1 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 2Y1&Y1&1
Evaluation A
T(glass)=82.6 K.

C_7H_{16} (liq) 30HUF/PAR2
3-Ethylpentane
Heat Capacity 294.8 K, C_p=217.6 J·mol^{-1}·K^{-1}
Temperature range 92 to 295 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=312.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 68.87 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 154.3 K, ΔH=9460 J·mol^{-1}
ΔS=61.31 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 2Y2&2
Evaluation B(C_p),C(S)

C_7H_{16} (liq) 61HUF/GRO
3-Ethylpentane
Heat Capacity 298.15 K, C_p=219.58 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=314.55 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 154.58 K, ΔH=9548 J·mol^{-1}
ΔS=61.77 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 2Y2&2
Evaluation A

C_7H_{16} (liq) 30HUF/PAR2
2,2-Dimethylpentane
Heat Capacity 294.1 K, C_p=217.1 J·mol^{-1}·K^{-1}
Temperature range 92 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=284.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 64.10 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 148.1 K, ΔH=5862 J·mol^{-1}
ΔS=39.58 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 3X1&1&1
Evaluation B(C_p),C(S)

C_7H_{16} (liq) 61HUF/GRO
2,2-Dimethylpentane
Heat Capacity 298.15 K, C_p=221.12 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=300.29 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 149.43 K, ΔH=5824 J·mol^{-1}
ΔS=38.98 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 3X1&1&1
Evaluation A

C_7H_{16} (liq) 30HUF/PAR2
3-Methylhexane
Heat Capacity 289.2 K, C_p=214.2 J·mol^{-1}·K^{-1}
Temperature range 71 to 289 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=309.6 J·mol^{-1}·K^{-1}
Extrapolation below 70 K, 70.71 J·mol^{-1}·K^{-1}. Forms glass at low temperatures. Value includes estimated zero point entropy of 17 J·mol^{-1}·K^{-1}.
Molecular Weight 100.2034
Wiswesser Line Notation 3Y2&1
Evaluation B(C_p),C(S)

C_7H_{16} (liq) 36PAR/THO
3-Methylhexane
Heat Capacity 289.2 K, C_p=216.7 J·mol^{-1}·K^{-1}
Temperature range 71 to 290 K. Glass at lower temperatures. Value is unsmoothed experimental datum.
Molecular Weight 100.2034
Wiswesser Line Notation 3Y2&1
Evaluation B

C_7H_{16} (liq) 30PAR/HUI
2-Methylhexane
Heat Capacity 292.4 K, C_p=219.2 J·mol^{-1}·K^{-1}
Temperature range 86 to 293 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=314.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K.
Phase Changes
c/liq 154.0 K, ΔH=8870 J·mol^{-1}
ΔS=57.60 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 4Y1&1
Evaluation B(C_p),C(S)

C_7H_{16} (liq) 30HUF/PAR2
2-Methylhexane
Entropy 298.1 K, $S=315.1\ J\cdot mol^{-1}\cdot K^{-1}$
Extrapolation below 90 K, 70.12 $J\cdot mol^{-1}\cdot K^{-1}$. Based on previously published specific heat data, 30PAR/HUF.
Phase Changes
c/liq 154.0 K, $\Delta H=8870\ J\cdot mol^{-1}$
$\Delta S=57.60\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 100.2034
Wiswesser Line Notation 4Y1&1
Evaluation C(S)

C_7H_{16} (liq) 61HUF/GRO
2-Methylhexane
Heat Capacity 298.15 K, $C_p=222.92\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 10 to 300 K.
Entropy 298.15 K, $S=323.34\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
Lambda-type transition at 72 K.
c/liq 154.90 K, $\Delta H=9184\ J\cdot mol^{-1}$
$\Delta S=59.29\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 100.2034
Wiswesser Line Notation 4Y1&1
Evaluation A

C_7H_{16} (liq) 24WIL/DAN
n-Heptane
Heat Capacity 303 K, $C_p=217.0\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 303 to 350 K. Equation only.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation C

C_7H_{16} (liq) 30PAR/HUF
n-Heptane
Heat Capacity 299.2 K, $C_p=222.2\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 90 to 300 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S=326.4\ J\cdot mol^{-1}\cdot K^{-1}$
Extrapolation below 90 K, 71.00 $J\cdot mol^{-1}\cdot K^{-1}$.
Phase Changes
c/liq 182.2 K, $\Delta H=14163\ J\cdot mol^{-1}$
$\Delta S=77.73\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B(C_p),C(S)

C_7H_{16} (liq) 30HUF/PAR2
n-Heptane
Entropy 298.1 K, $S=330.1\ J\cdot mol^{-1}\cdot K^{-1}$
Extrapolation below 90 K, 71.00 $J\cdot mol^{-1}\cdot K^{-1}$. Based on previously published specific heat data, 30PAR/HUF.
Phase Changes
c/liq 182.2 K, $\Delta H=14163\ J\cdot mol^{-1}$
$\Delta S=77.73\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation C(S)

C_7H_{16} (liq) 32RIC/WAL
n-Heptane
Heat Capacity 298.1 K, $C_p=224.3\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 293 to 323 K.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation C

C_7H_{16} (liq) 37VOL
n-Heptane
Heat Capacity 298 K, $C_p=223.0\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature. C_p given as 0.532 cal/deg/gram.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 39PHI
n-Heptane
Heat Capacity 300.8 K, $C_p=210.9\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation C

C_7H_{16} (liq) 39BYK
n-Heptane
Heat Capacity 298 K, $C_p=211.3\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation C

C_7H_{16} (liq) 40PIT
n-Heptane
Heat Capacity 296.5 K, $C_p=224.60\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 15 to 318 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S=328.86\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 182.52 K, $\Delta H=14040.7\ J\cdot mol^{-1}$
$\Delta S=76.93\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 47OSB/GIN
n-Heptane
Heat Capacity 298.15 K, $C_p=224.85\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 278 to 318 K.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 53GIN/FUR
n-Heptane
Heat Capacity 298.15 K, $C_p=224.74\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 25 to 520 K.
Phase Changes
c/liq 182.56 K, $\Delta H=14022\ J\cdot mol^{-1}$
$\Delta S=76.81\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A
See correction in 53GIN/FUR2.

C_7H_{16} (liq) 54DOU/FUR
n-Heptane
Heat Capacity 298.15 K, C_p=224.74 J·mol^{-1}·K^{-1}
Temperature range 20 to 520 K.
Entropy 298.15 K, S=327.98 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 182.56 K, ΔH=14022 J·mol^{-1}
ΔS=78.81 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 55HEL/HEI
n-Heptane
Heat Capacity 299.8 K, C_p=233.13 J·mol^{-1}·K^{-1}
Temperature range 70 to 220 °F.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 58SWI/ZIE
n-Heptane
Heat Capacity 332 K, C_p=247.3 J·mol^{-1}·K^{-1}
Mean value 22 to 96 °C.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation C

C_7H_{16} (liq) 61HUF/GRO
n-Heptane
Heat Capacity 298.15 K, C_p=224.93 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=328.57 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 182.55 K, ΔH=14037 J·mol^{-1}
ΔS=76.89 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 61MCC/MES
n-Heptane
Heat Capacity 298.15 K, C_p=224.93 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K. C_{sat}(liq)=56.582−0.14490T +5.7813×10^{-4}T^2−4.1667×10^{-7}T^3 cal·mol^{-1}·deg^{-1}.
Phase Changes
c/liq 182.55 K, ΔH=14037 J·mol^{-1}
ΔS=76.89 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 63OET
n-Heptane
Heat Capacity 298.15 K, C_p=328.61 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 182.56 K, ΔH=14030.6 J·mol^{-1}
ΔS=76.81 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B
Run as check on calorimeter. No details.

C_7H_{16} (liq) 72MIL
n-Heptane
Heat Capacity 250 K, C_p=209.6 J·mol^{-1}·K^{-1}
Temperature range 130 to 263 K.
Phase Changes
c/liq 182.56 K, ΔH=14061 J·mol^{-1}
ΔS=77.02 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 73KAL/WOY
n-Heptane
Heat Capacity 298.15 K, C_p=226.53 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 74DIA/REN
n-Heptane
Heat Capacity 298.15 K, C_p=225.3 J·mol^{-1}·K^{-1}
Temperature range 298 to 323 K.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 75GRI/RAS
n-Heptane
Heat Capacity 298 K, C_p=223.4 J·mol^{-1}·K^{-1}
Temperature range 300 to 463 K.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 75HOL/ZIE
n-Heptane
Heat Capacity 298.15 K, C_p=224.19 J·mol^{-1}·K^{-1}
Temperature range 182 to 312 K. C_p=866.18820 −9.9628490T+0.054561085T^2−0.00013079634T^3+1. 1957392×10^{-7}T^4 J·mol^{-1}·K^{-1}.
Phase Changes
c,I/liq 182.586 K
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 75WOY/KAL
n-Heptane
Heat Capacity 303.15 K, C_p=226.53 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 76FOR/BEN2
n-Heptane
Heat Capacity 298.15 K, C_p=224.707 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 77MEI/BLO
n-Heptane
Heat Capacity 298.15 K, C_p=255.0 J·mol^{-1}·K^{-1}
Temperature range 160 to 350 K.
Phase Changes
c/liq 182.7 K, ΔH=14059 J·mol^{-1}
ΔS=77.0 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 78WOY/KAL
n-Heptane
Heat Capacity 333.15 K, C_p=226.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 79BRO/ZIE
n-Heptane
Heat Capacity 298.15 K, C_p=224.66 J·mol^{-1}·K^{-1}
Temperature range 183 to 302 K. Results as equation only.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 79CZA
n-Heptane
Heat Capacity 300 K, C_p=225.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 79GRO/HAM
n-Heptane
Heat Capacity 298.15 K, C_p=224.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 79SCH/OFF
n-Heptane
Heat Capacity 285 K, C_p=220.00 J·mol^{-1}·K^{-1}
Temperature range 90 to 285 K.
Phase Changes
c/liq 182.59 K, ΔH=14053 J·mol^{-1}
ΔS=76.96 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 80KAL/JED
n-Heptane
Heat Capacity 297.860 K, C_p=224.62 J·mol^{-1}·K^{-1}
Temperature range 185 to 300 K. Unsmoothed experimental datum.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 81GRO/ING
n-Heptane
Heat Capacity 298.15 K, C_p=224.69 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 82TAN
n-Heptane
Heat Capacity 298.15 K, C_p=224.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 82ZAR
n-Heptane
Heat Capacity 298 K, C_p=224.0 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 83KIM/TRE
n-Heptane
Heat Capacity 298.15 K, C_p=224.764 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 83TAN/ZHO
n-Heptane
Heat Capacity 300 K, C_p=225.33 J·mol^{-1}·K^{-1}
Temperature range 220 to 380 K.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 84GRO/ING
n-Heptane
Heat Capacity 298.15 K, C_p=224.71 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 84ROU/GRO
n-Heptane
Heat Capacity 298.15 K, C_p=224.78 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 85BAL/BRA
n-Heptane
Heat Capacity 298.15 K, C_p=224.781 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 85LAI/ROD
n-Heptane
Heat Capacity 298.15 K, C_p=224.781 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 85TAN/NAK
n-Heptane
Heat Capacity 298.15 K, C_p=224.731 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 87KAL/KOH
n-Heptane
Heat Capacity 293.15 K, C_p=222.88 J·mol^{-1}·K^{-1}
Temperature range 293.15, 313.15 K.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 87TAN
n-Heptane
Heat Capacity 298.15 K, C_p=224.721 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 87VAN/VAN
n-Heptane
Heat Capacity 300 K, C_p=225.14 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Phase Changes
c/liq 182.57 K, ΔH=13990 J·mol^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 87WIL/ING
n-Heptane
Heat Capacity 298.15 K, C_p=224.71 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 88AND/PAT
n-Heptane
Heat Capacity 298.15 K, C_p=224.64 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 88SAI/TAN
n-Heptane
Heat Capacity 298.15 K, C_p=224.72 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 88SHI/OGA
n-Heptane
Heat Capacity 298.15 K, C_p=224.73 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

$C_7H_{16}O$ (liq) 36EVA/EDL
4,4-Dimethyl-3-oxahexane; tert-Amyl ethyl ether
Heat Capacity 298 K, C_p=243 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.2028
Wiswesser Line Notation 2X1&1&O2
Evaluation C

$C_7H_{16}O$ (liq) 88CAC/COS
3-Ethyl-3-pentanol
Heat Capacity 298.15 K, C_p=353.91 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.2028
Wiswesser Line Notation QX2&2&2
Evaluation B

$C_7H_{16}O$ (liq) 56PAR/KEN
1-Heptanol; n-Heptyl alcohol
Heat Capacity 298.15 K, C_p=278.57 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.1 K, S=325.9 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 65.06 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 240.4 K, ΔH=18175 J·mol^{-1}
ΔS=75.60 J·mol^{-1}·K^{-1}
Molecular Weight 116.2028
Wiswesser Line Notation Q7
Evaluation B(C_p),C(S)

$C_7H_{16}O$ (liq) 59HUT/BAI
1-Heptanol; n-Heptyl alcohol
Heat Capacity 298 K, C_p=274.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.2028
Wiswesser Line Notation Q7
Evaluation C

$C_7H_{16}O$ (liq) 79GRI/YAN
1-Heptanol; n-Heptyl alcohol
Heat Capacity 302.97 K, C_p=278.9 J·mol^{-1}·K^{-1}
Temperature range 303 to 462 K. p=0.98 bar.
Molecular Weight 116.2028
Wiswesser Line Notation Q7
Evaluation B

$C_7H_{16}O$ (liq) 84ZEG/SOM
1-Heptanol; n-Heptyl alcohol
Heat Capacity 298.15 K, C_p=273.67 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.2028
Wiswesser Line Notation Q7
Evaluation C

$C_7H_{16}O$ (liq) 88NAZ/BAS
1-Heptanol; n-Heptyl alcohol
Heat Capacity 303.35 K, C_p=297.0 J·mol^{-1}·K^{-1}
Temperature range 303 to 447 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.556 kJ/kg·K. C_p data given at pressures from 0.1 to 50 MPa.
Molecular Weight 116.2028
Wiswesser Line Notation Q7
Evaluation B

$C_7H_{16}O$ (liq) 89VES/BAR
1-Heptanol; n-Heptyl alcohol
Heat Capacity 298.15 K, C_p=270.8 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K.
Molecular Weight 116.2028
Wiswesser Line Notation Q7
Evaluation A

$C_7H_{16}O$ (liq) 76CON/GIN
4-Heptanol
Heat Capacity 298 K, C_p=317.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.2028
Wiswesser Line Notation QY3&3
Evaluation B

$C_7H_{16}O_2$ (liq) 73KUS/SUU
2,5-Dioxanonane: 1-n-Butoxy-2-methoxyethane
Heat Capacity 298.15 K, C_p=282.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 132.2022
Wiswesser Line Notation 4O2O1
Evaluation B

$C_7H_{16}S$ (liq) 66GOO/DEP
1-Heptanethiol; n-Heptyl mercaptan
Heat Capacity 298.15 K. C_p=259.32 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 132.2634
Wiswesser Line Notation SH7
Evaluation A

$C_7H_{16}S$ (liq) 70FIN/MCC
1-Heptanethiol; n-Heptyl mercaptan
Heat Capacity 298.15 K, C_p=259.32 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=375.35 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 229.92 K, ΔH=25384 J·mol^{-1}
ΔS=110.40 J·mol^{-1}·K^{-1}
Molecular Weight 132.2634
Wiswesser Line Notation SH7
Evaluation A

$C_7H_{17}NSi$ (liq) 74LEB/RAB
N-(β-Trimethylsilylethyl)ethylenimine
Heat Capacity
Temperature range 50 to 300 K. Data given graphically.
Phase Changes
c/liq 176.54 K, ΔH=10623 J·mol^{-1}
ΔS=60.2 J·mol^{-1}·K^{-1}
Molecular Weight 143.3035
Wiswesser Line Notation T3NTJ A2-SI-1&1&1
Evaluation A

$C_7H_{17}NSi$ (liq) 74LEB/TSV
N-(β-Trimethylsilylethyl)ethylenimine
Heat Capacity 300 K, C_p=300.8 J·mol^{-1}·K^{-1}
Temperature range 64 to 300 K.
Entropy 300 K, S=406.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 176.54 K, ΔH=10623 J·mol^{-1}
ΔS=60.2 J·mol^{-1}·K^{-1}
Molecular Weight 143.3035
Wiswesser Line Notation T3NTJ A2-SI-1&1&1
Evaluation A
T(glass)=124.0 K. Data given for glassy state from 50 to 150 K.

$C_7H_{17}NSi$ (liq) 75LEB/TSV
N-(β-Trimethylsilylethyl)ethylenimine
Heat Capacity 300 K, C_p=300.8 J·mol^{-1}·K^{-1}
Temperature range 6 to 300 K.
Entropy 300 K, S=406.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 176.54 K, ΔH=10623 J·mol^{-1}
ΔS=60.2 J·mol^{-1}·K^{-1}
Molecular Weight 143.3035
Wiswesser Line Notation T3NTJ A2-SI-1&1&1
Evaluation A
T(glass)=124.0 K.

$(C_7H_{17}NSi)_n$ (liq) 74LEB/RAB
Poly-N-(β-trimethylsilylethyl)ethylenimine
Heat Capacity
Temperature range 50 to 300 K. Data given graphically.
Molecular Weight 143.3035
Wiswesser Line Notation /*2N&2-SI-1&1&1 &*/
Evaluation A
T(glass)=205.5 K.

$(C_7H_{17}NSi)_n$ (liq) 75LEB/TSV
Poly-N-(β-trimethylsilylethyl)ethylenimine
Heat Capacity 300 K, C_p=287.4 J·mol^{-1}·K^{-1}
Temperature range 6 to 300 K.
Entropy 300 K, S=294.1 J·mol^{-1}·K^{-1}
Molecular Weight 143.3035
Wiswesser Line Notation /*2N*2-SI-1&1&1/ &*/
Evaluation A
T(glass)=207.5 K.

$C_7H_{20}Si_2$ (c) 75GUS/KAR
Hexamethyldisilylmethane
Heat Capacity 298.15 K, C_p=357.52 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K. Data given graphically.
Entropy 298.15 K, S=515.89 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 140.70 K, ΔH=11113 J·mol^{-1}
ΔS=78.99 J·mol^{-1}·K^{-1}
liq/g 460.58 K, ΔH=40250 J·mol^{-1}
ΔS=98.99 J·mol^{-1}·K^{-1}
Molecular Weight 160.4060
Wiswesser Line Notation 1-SI-1&1&1-SI-1&1&1
Evaluation B

$C_7H_{20}Si_2$ (liq) 82GUS/KAR
Hexamethyldisilylmethane
Heat Capacity 298.15 K, C_p=357.5 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=515.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 140.70 K, ΔH=11113 J·mol^{-1}
ΔS=78.99 J·mol^{-1}·K^{-1}
Molecular Weight 160.4060
Wiswesser Line Notation 1-SI-1&1&1-SI-1&1&1
Evaluation A

C_8D_8 (liq) 85LEB/LEB
Styrene-d_8
Heat Capacity 298.15 K, C_p=201.9 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 243.74 K, ΔH=10800 J·mol^{-1}
ΔS=44.3 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation 1U1R &1/3/4/H-2 8
Evaluation B

$(C_8D_8)_n$ (gls) 83LEB/SMI
Polystyrene-d_8
Heat Capacity 298.15 K, C_p=154.7 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S=154.6 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation /*YR&1*/ &1/2-BCDEF/4/H-2 8
Evaluation A

C_8F_{16} (liq) 57YAR/KAY
Perfluorodimethylcyclohexane;
Hexadecafluorodimethylcyclohexane
Heat Capacity 298 K, C_p=405.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K. Equation only.
Molecular Weight 400.0624
Wiswesser Line Notation L6TJ AXFFF AF BF CF DF EF FF XXFFF XF XF XF XF
Evaluation C
Unspecified isomer.

$C_8F_{16}O$ (liq) 57YAR/KAY
Perfluoro-3-butyltetrahydrofuran;
Hexadecafluoro-3-butyltetrahydrofuran
Heat Capacity 298 K, C_p=431.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K. Equation only.
Molecular Weight 416.0618
Wiswesser Line Notation T5OTJ BF BF CXFFXFFXFFXFFF CF DF DF EF EF
Evaluation B

C_8F_{18} (liq) 82CAM/RE
n-Perfluorooctane
Heat Capacity
C_p is given graphically only. Temperature range 4.2 to 300 K.
Phase Changes
c,II/c,I 190–200 K, ΔH=7222 J·mol^{-1}
ΔS=35.94 J·mol^{-1}·K^{-1}
Data given for two solid-solid transitions at 190 and 200 K.
Molecular Weight 438.0592
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFXFFF
Evaluation A

$(C_8H_3D_5)_n$ (gls) 83LEB/SM
Polystyrene-d_5
Heat Capacity 298.15 K, C_p=146.6 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S=150.5 J·mol^{-1}·K^{-1}
Molecular Weight 109.1907
Wiswesser Line Notation /*YR&1*/ &2-BCDEF/H-2 5
Evaluation A

$C_8H_4Cl_2O_2$ (liq) 1881RE
Phthalyl dichloride; o-Phthalyl dichloride
Heat Capacity 298 K, C_p=248.5 J·mol^{-1}·K^{-1}
Temperature range 290 to 475 K.
Molecular Weight 203.0244
Wiswesser Line Notation GVR BVG
Evaluation D

$C_8H_4Cl_2O_2$ (c) 73SAP/MO
Isophthaloyl dichloride; m-Phthalic acid dichloride
Heat Capacity 300 K, C_p=203.9 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=240.5 J·mol^{-1}·K^{-1}
Molecular Weight 203.0238
Wiswesser Line Notation GVR CVG
Evaluation C

$C_8H_4Cl_2O_2$ (c) 73SAP/MO
Terephthaloyl dichloride; p-Phthalic acid dichloride
Heat Capacity 300 K, C_p=207.9 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=226.1 J·mol^{-1}·K^{-1}
Molecular Weight 203.0238
Wiswesser Line Notation GVR DVG
Evaluation C

$C_8H_4Cl_2O_2$ (c) 79KAR/SA
Terephthalyl dichloride; p-Phthalic acid dichloride
Heat Capacity 298.15 K, C_p=207.9 J·mol^{-1}·K^{-1}
Temperature range 60 to 298 K.
Entropy 298.15 K, S=226.1 J·mol^{-1}·K^{-1}
Molecular Weight 203.0238
Wiswesser Line Notation GVR DVG
Evaluation A

$C_8H_4Cl_2O_2$ (c) 82KAR/SHV
Terephthaloyl dichloride; p-Phthalic acid dichloride
Phase Changes
c,II/c,I 337.3 K, ΔH=2335 J·mol^{-1}
ΔS=6.90 J·mol^{-1}·K^{-1}
c,I/liq 356.1 K, ΔH=21100 J·mol^{-1}
ΔS=59.3 J·mol^{-1}·K^{-1}
Molecular Weight 203.0238
Wiswesser Line Notation GVR DVG
Evaluation B

$C_8H_4N_2$ (c) 82KAR/SHV
1,2-Dicyanobenzene; o-Phthalonitrile
Heat Capacity 298.15 K, C_p=161.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 480 K.
Entropy 298.15 K, S=192.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 414.0 K, ΔH=20000 J·mol^{-1}
ΔS=48.26 J·mol^{-1}·K^{-1}
Molecular Weight 128.1330
Wiswesser Line Notation NCR BCN
Evaluation A

$C_8H_4N_2$ (c) 84RAB/KAR
1,2-Dicyanobenzene; o-Phthalonitrile
Heat Capacity 298.15 K, C_p=161.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 500 K.
Entropy 298.15 K, S=192.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 414.0 K, ΔH=20000 J·mol^{-1}
ΔS=48.26 J·mol^{-1}·K^{-1}
Molecular Weight 128.1330
Wiswesser Line Notation NCR BCN
Evaluation A

$C_8H_4N_2$ (c) 88LEB/BYK
1,4-Dicyanobenzene; Terephthalodinitrile
Heat Capacity 298.15 K, C_p=161.2 J·mol^{-1}·K^{-1}
Temperature range 0 to 330 K.
Entropy 298.15 K, S=183.0 J·mol^{-1}·K^{-1}
Molecular Weight 128.1330
Wiswesser Line Notation NCR DCN
Evaluation A

$C_8H_4N_2O_2$ (c) 62STR/BAR
1,4-Phenylenediisocyanate; 1,4-Diisocyanatobenzene
Heat Capacity 298 K, C_p=211.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 160.1318
Wiswesser Line Notation OCNR DNCO
Evaluation D

$C_8H_4O_3$ (c) 36PAR/TOD
Phthalic anhydride
Heat Capacity 298.1 K, C_p=161.80 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 298.1 K, S=179.5 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 58.12 J·mol^{-1}·K^{-1}.
Molecular Weight 148.1178
Wiswesser Line Notation T56 BVOVJ
Evaluation B(C_p),C(S)

$C_8H_4O_3$ (c) 87BUS/MAS
Phthalic anhydride
Heat Capacity 298.15 K, C_p=160.0 J·mol^{-1}·K^{-1}
Temperature range 13 to 350 K.
Entropy 298.15 K, S=180.0 J·mol^{-1}·K^{-1}
Molecular Weight 148.1178
Wiswesser Line Notation T56 BVOVJ
Evaluation A

C_8H_5Ag (c) 80BYK/KIP
Silver phenylacetylenide
Heat Capacity 298.15 K, C_p=156.8 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=199.3 J·mol^{-1}·K^{-1}
Molecular Weight 208.9955
Wiswesser Line Notation -AG-1UU1R
Evaluation A

C_8H_5Cu (c) 79LEB/BYK
Copper phenylacetylenide
Heat Capacity 298.15 K, C_p=154.0 J·mol^{-1}·K^{-1}
Temperature range 11 to 330 K.
Entropy 298.15 K, S=173.8 J·mol^{-1}·K^{-1}
Molecular Weight 164.6735
Wiswesser Line Notation -CU-1UU1R
Evaluation A

C_8H_5Cu (c) 82BYK/LEB
Copper phenylacetylenide
Heat Capacity 298.15 K, C_p=154.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=173.6 J·mol^{-1}·K^{-1}
Molecular Weight 164.6735
Wiswesser Line Notation -CU-1UU1R
Evaluation A

$(C_8H_5D_3)_n$ (gls) 83LEB/SMI
Polystyrene-d_3
Heat Capacity 298.15 K, C_p=139.8 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S=143.5 J·mol^{-1}·K^{-1}
Molecular Weight 107.1749
Wiswesser Line Notation /*YR&1*/ &3/6/H-2 3
Evaluation A

$C_8H_5F_3O_2$ (liq) 62GOO/LAC
3-Trifluoromethylbenzoic acid; m-Trifluorotoluic acid;
α,α,α-Trifluoro-m-toluic acid
Heat Capacity 298.15 K, C_p=223.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 190.1215
Wiswesser Line Notation QVR CXGGG
Evaluation B

$C_8H_5MnO_3$ (c) 83CHH/POM
Cymantrene; Cyclopentadienyl manganese tricarboxyl
Heat Capacity 298.15 K, C_p=214.79 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=259.35 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 75–135 K, ΔS=<1 J·mol^{-1}·K^{-1}
"Abnormally" high heat capacity.
c/liq 350 K, ΔH=19300 J·mol^{-1}
ΔS=55 J·mol^{-1}·K^{-1}
Molecular Weight 204.0637
Wiswesser Line Notation L5ϕJ ϕ-MN- CO 3
Evaluation A

C_8H_6 (liq) 31SMI/AND
Phenylacetylene
Heat Capacity 298.5 K, C_p=179.5 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 102.1354
Wiswesser Line Notation 1UU1R
Evaluation C

C_8H_6 (liq) 82LEB/BYK
Phenylacetylene
Heat Capacity 298.15 K, C_p=180.10 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 480 K.
Entropy 298.15 K, S=221.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 228.04 K, ΔH=9460 J·mol^{-1}
ΔS=41.5 J·mol^{-1}·K^{-1}
Molecular Weight 102.1354
Wiswesser Line Notation 1UU1R
Evaluation A

$C_8H_6N_2$ (c) 93SAB/PEM
Phthalazine
Phase Changes
c/liq/g 364.41 K
c/liq ΔH=13320 J·mol^{-1}
c/g 298.15 K ΔH=81140 J·mol^{-1}
Molecular Weight 130.1488
Wiswesser Line Notation T66 CNNJ
Evaluation A

$C_8H_6N_2$ (c) 93SAB/PEM
Quinazoline
Phase Changes
c/liq/g 320.82 K
c/liq ΔH=16950 J·mol^{-1}
c/g 298.15 K ΔH=77590 J·mol^{-1}
Molecular Weight 130.1488
Wiswesser Line Notation T66 BN DNJ
Evaluation A

$C_8H_6N_2$ (c) 93SAB/PEM
Quinoxaline
Phase Changes
c/liq/g 305.68 K
c/liq ΔH=11800 J·mol^{-1}
c/g 298.15 K ΔH=69390 J·mol^{-1}
Molecular Weight 130.1488
Wiswesser line Notation T66 BN ENJ
Evaluation A

C_8H_6O (liq) 86CHI/NGU
2,3-Benzofuran
Heat Capacity 298.15 K, C_p=178.70 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S=215.59 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 232.000 K
c,I/liq 245.482 K
Molecular Weight 118.1348
Wiswesser Line Notation T56 BOJ
Evaluation A

$C_8H_6O_3$ (c) 92STE/CH
Benzoyl formic acid
Heat Capacity 298.15 K, C_p=192.9 J·mol^{-1}·K^{-1}
Temperature range 285 to 425 K. C/R(c)=0.025T+15.78 (285 t 338.9 K); C/R(liq)=0.0411T+17.67 (338.9 to 425 K), R=8.3145 J/K·mol.
Phase Changes
c/liq 338.9 K, ΔH=21800 J·mol^{-1}
Molecular Weight 150.1336
Wiswesser Line Notation QVVR
Evaluation A

$C_8H_6O_4$ (c) 36PAR/TOI
o-Phthalic acid; Phthalic acid
Heat Capacity 298.1 K, C_p=188.11 J·mol^{-1}·K^{-}
Temperature range 90 to 300 K.
Entropy 298.1 K, S=207.94 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 66.19 J·mol^{-1}·K^{-1}.
Molecular Weight 166.1330
Wiswesser Line Notation QVR BVQ
Evaluation B(C_p),C(S)

$C_8H_6O_4$ (c) 39SAT/SOG
o-Phthalic acid; Phthalic acid
Heat Capacity 323 K, C_p=201.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 166.1330
Wiswesser Line Notation QVR BVQ
Evaluation C
Same data in 40SAT/SOG.

$C_8H_6O_4$ (c) 41SAT/SOG
o-Phthalic acid; Phthalic acid
Heat Capacity 323 K, C_p=201.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 166.1330
Wiswesser Line Notation QVR BVQ
Evaluation C
Same data in 40SAT/SOG5.

$C_8H_6O_4$ (c) 39SAT/SOG
m-Phthalic acid; Isophthalic acid
Heat Capacity 323 K, C_p=201.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 166.1330
Wiswesser Line Notation QVR CVQ
Evaluation C
See data in 40SAT/SOG.

$C_8H_6O_4$ (c) 41SAT/SOG
m-Phthalic acid; Isophthalic acid
Heat Capacity 323 K, C_p=201.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 166.1330
Wiswesser Line Notation QVR CVQ
Evaluation C
Same data in 40SAT/SOG5.

$C_8H_6O_4$ (c) 41SAT/SOG4
p-Phthalic acid; Terephthalic acid
Heat Capacity 323 K, C_p=199.6 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 166.1330
Wiswesser Line Notation QVR DVQ
Evaluation C
Same data in 40SAT/SOG5.

C_8H_6S (c) 54FIN/GRO
Benzothiophene
Heat Capacity 298.15 K, C_p=163.01 J·mol^{-1}·K^{-1}
Temperature range 12 to 335 K.
Entropy 298.15 K, S=177.11 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 304.50 K, ΔH=11827 J·mol^{-1}
ΔS=38.84 J·mol^{-1}·K^{-1}
Molecular Weight 134.1954
Wiswesser Line Notation T56 BSJ
Evaluation A

C_8H_6S (c,I) 91CHI/KNI2
Benzothiophene
Heat Capacity 295.859 K, C_p=172.14 J·mol^{-1}·K^{-1}
Temperature range 277 to 495 K. Unsmoothed experimental datum. C_p(liq, 298.15 K, smoothed, graphical extrapolation)=188.17 J·mol^{-1}·K^{-1}.
Entropy K, S=J·mol^{-1}·K^{-1}
S(liq, 298.15 K, smoothed, graphical extrapolation)=219.05 J·mol^{-1}·K^{-1}.
Phase Changes
c,I/liq 304.48 K, ΔH=11819.1 J·mol^{-1}
ΔS=38.82 J·mol^{-1}·K^{-1}
Molecular Weight 134.1954
Wiswesser Line Notation T56 BSJ
Evaluation A

$C_8H_7ClN_2O_2$ (c) 82CUE/SOL
2-Chloroisonitrosoacetanilide
Phase Changes
c/liq 429 K, ΔH=29700 J·mol^{-1}
ΔS=69.3 J·mol^{-1}·K^{-1}
Molecular Weight 198.6085
Wiswesser Line Notation QVU1VMR BG
Evaluation D

C_8H_7N (c) 81LEB/RYA
Indole; 1-Benzo[b]pyrrole
Heat Capacity C_p=192.1 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K. Data given over temperature range.
Molecular Weight 117.1500
Wiswesser Line Notation T56 BMJ
Evaluation B

$C_8H_7N_5O_8$ (c) 73KRI/LIC
2,4,6-Trinitro-N-(methylnitro)-m-toluidene; Methyltetryl; 2,4,6,N-Tetranitro-N-methyltoluidine
Heat Capacity 298 K, C_p=326.4 J·mol^{-1}·K^{-1}
Temperature range 200 to 376 K. Equation only.
Phase Changes
c/liq 375.6 K, ΔH=19330 J·mol^{-1}
ΔS=51.5 J·mol^{-1}·K^{-1}
Molecular Weight 301.1720
Wiswesser Line Notation WNN1&R C1 BNW DNW FNW
Evaluation C

$C_8H_7N_5O_8$ (c) 73KRI/LIC
2,4,6-Trinitrophenylethyl nitramine; Ethyltetryl; 2,4,6,N-Tetranitroethylaniline
Heat Capacity 298 K, C_p=332.2 J·mol^{-1}·K^{-1}
Temperature range 200 to 369 K. Equation only.
Phase Changes
c/liq 369.0 K, ΔH=23510 J·mol^{-1}
ΔS=63.7 J·mol^{-1}·K^{-1}
Molecular Weight 301.1720
Wiswesser Line Notation WNN2&R BNW DNW FNW
Evaluation C

C_8H_8 (liq) 31SMI/AND
Styrene
Heat Capacity 298.5 K, C_p=179.9 J·mol^{-1}·K^{-1}
Temperature range 102 to 299 K. Value is unsmoothed experimental datum.
Molecular Weight 104.1512
Wiswesser Line Notation 1U1R
Evaluation C

C_8H_8 (liq) 43GUT/WES
Styrene
Entropy 298.15 K, S=237.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 242.47 K, ΔH=10950 J·mol^{-1}
ΔS=45.16 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation 1U1R
Evaluation A

C_8H_8 (liq) 46PIT/GUT
Styrene
Heat Capacity 298.15 K, C_p=182.84 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=237.57 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 242.27 K, ΔH=10949 J·mol^{-1}
ΔS=45.16 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation 1U1R
Evaluation A

C_8H_8 (liq) 50KUR
Styrene
Heat Capacity 298 K, C_p=235.6 J·mol^{-1}·K^{-1}
Temperature range 21 to 139 °C.
Molecular Weight 104.1512
Wiswesser Line Notation 1U1R
Evaluation B

C_8H_8 (liq) 61WAR/PET2
Styrene
Heat Capacity 298.16 K, C_p=182.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.16 K, S=240.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 242.27 K, ΔH=10964 J·mol^{-1}
ΔS=45.32 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation 1U1R
Evaluation A

C_8H_8 (liq) 85LEB/LEB
Styrene
Heat Capacity 298.15 K, C_p=183.2 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 242.47 K, ΔH=10950 J·mol^{-1}
ΔS=45.2 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation 1U1R
Evaluation B

C_8H_8 (c) 92WHI/WAS
Cubane; Pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane
Heat Capacity
Temperature range 30 to 400 K. Data given graphically only.
Phase Changes
c,II/c,I 395.04 K, ΔH=5940 J·mol^{-1}
ΔS=15.37 J·mol^{-1}·K^{-1}
c,I/liq 404.9 K, ΔH=8700 J·mol^{-1}
ΔS=22.7 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation L444 B4 C4 4ABCD HTJ
Evaluation A

C_8H_8 (liq) 49SCO/GRO
Cyclooctatetraene
Heat Capacity 298.15 K, C_p=185.18 J·mol^{-1}·K^{-1}
Temperature range 12 to 340 K.
Entropy 298.15 K, S=220.29 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 268.48 K, ΔH=11274.2 J·mol^{-1}
ΔS=41.493 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation L8J
Evaluation A

$(C_8H_8)_n$ (c) 61WAR/PET2
Polystyrene
Heat Capacity 298.16 K, C_p=131.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 395 K. Interpolated.
Entropy 298.16 K, S=128.6 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation /*YR&1*/
Evaluation A

$(C_8H_8)_n$ (c) 62DAI/EVA4
Polystyrene, isotactic
Heat Capacity 298.15 K, C_p=127.6 J·mol^{-1}·K^{-1}
Temperature range 20 to 310 K.
Entropy 298.15 K, S=131.4 J·mol^{-1}·K^{-1}
When extrapolated to 100% crystallinity, the entropy is 128.4 J·mol^{-1}·K^{-1}.
Molecular Weight 104.1512
Wiswesser Line Notation /*YR&1*/
Evaluation A

$(C_8H_8)_n$ (c) 65ABU/DOL
Polystyrene, atactic
Heat Capacity 298 K, C_p=124.3 J·mol^{-1}·K^{-1}
Temperature range 223 to 553 K. Value per monomer unit.
Molecular Weight 104.1512
Wiswesser Line Notation /*YR&1*/
Evaluation B
Also data above the glass transition.

$(C_8H_8)_n$ (c) 65ABU/DOL
Polystyrene, isotactic, annealed
Heat Capacity 298 K, C_p=123.8 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K. Values per monomer unit.
Molecular Weight 104.1512
Wiswesser Line Notation /*YR&1*/
Evaluation B
Also data for amorphous and semicrystalline isotactic, and above glass transition.

$(C_8H_8)_n$ (c) 65KAR/BA
Polystyrene
Heat Capacity 298.15 K, C_p=127.3 J·mol^{-1}·K^{-1}
Temperature range 305 to 525 K. Glass transition at 355 K. Values per C_8H_8 unit.
Molecular Weight 104.1512
Wiswesser Line Notation /*YR&1*/
Evaluation B

$(C_8H_8)_n$ (amorp) 65KAR/BA
Polystyrene, isotactic
Heat Capacity 298.15 K, C_p=127.5 J·mol^{-1}·K^{-1}
Temperature range 300 to 522 K. Glass transition at 360 K. Values per C_8H_8 unit.
Molecular Weight 104.1512
Wiswesser Line Notation /*YR&1*/
Evaluation B

$(C_8H_8)_n$ (amorp) 65KAR/BA
Polystyrene, atactic
Heat Capacity 298.15 K, C_p=127.7 J·mol^{-1}·K^{-1}
Temperature range 80 to 480 K. Also annealed sample, 293 to 378 K. Glass transition at about 367 K. Values per C_8H_8 unit.
Molecular Weight 104.1512
Wiswesser Line Notation /*YR&1*/
Evaluation B
NBS broad molecular weight distribution. Sample NS706.

$(C_8H_8)_n$ (c) 68CHA/BES
Polystyrene
Heat Capacity 298.15 K, C_p=127.48 J·mol^{-1}·K^{-1}
Temperature range 10 to 360 K. National Bureau of Standards sample 705.
Entropy 298.15 K, S=134.83 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation /*YR&1*/
Evaluation A

$(C_8H_8)_n$ (gls) 83LEB/SM
Polystyrene
Heat Capacity 298.15 K, C_p=127.5 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S=134.8 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation /*YR&1*/
Evaluation D

$C_8H_8N_2O_2$ (c) 82CUE/SOL
Isonitrosoacetanilide
Phase Changes
c/liq 448 K, $\Delta H = 10400$ J·mol^{-1}
$\Delta S = 23.2$ J·mol^{-1}·K^{-1}
Molecular Weight 164.1634
Wiswesser Line Notation QNU1VMR
Evaluation D

$C_8H_8N_2O_3$ (c) 41SAT/SOG
p-Nitroacetanilide
Heat Capacity 323 K, $C_p = 230.5$ J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 180.1628
Wiswesser Line Notation WNR DMV1
Evaluation C
Same data in 40SAT/SOG2.

$C_8H_8N_6O_6$ (c) 93ABD/TAH
Ammonium purpurate: Murexide
Heat Capacity 300 K, $C_p = 600$ J·mol^{-1}·K^{-1}
Temperature range 300 to 550 K. Data given graphically only. C_p value estimated from graph.
Molecular Weight 284.1878
Wiswesser Line Notation T6VMVMVJ FUN- FT6VMVMQJ EQ &ZH
Evaluation C

C_8H_8O (liq) 39PHI
Acetophenone; Methyl phenyl ketone
Heat Capacity 303.2 K, $C_p = 227.6$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 120.1506
Wiswesser Line Notation 1VR
Evaluation C

C_8H_8O (liq) 86CHI/NGU
4,5-Dihydro-2,3-benzofuran; Coumaran
Heat Capacity 298.15 K, $C_p = 188.64$ J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, $S = 226.43$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 250.890 K
Molecular Weight 120.1506
Wiswesser Line Notation T56 BOT&J
Evaluation A

C_8H_8O (liq) 93STE/CHI2
2.5-Dihydro-3.4-benzofuran; Phthalan
Heat Capacity 298.15 K, $C_p = 188.7$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 120.1506
Wiswesser Line Notation T56 COT&J
Evaluation A

$C_8H_8O_2$ (liq) 71HAL/BAL
Methyl benzoate
Heat Capacity 297 K, $C_p = 216.5$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 136.1500
Wiswesser Line Notation 1OVR
Evaluation C

$C_8H_8O_2$ (liq) 79FUC
Methyl benzoate
Heat Capacity 298.15 K, $C_p = 221.3$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 136.1500
Wiswesser Line Notation 1OVR
Evaluation B

$C_8H_8O_2$ (c) 26AND/LYN
o-Toluic acid; 2-Methylbenzoic acid
Heat Capacity 298 K, $C_p = 174.9$ J·mol^{-1}·K^{-1}
Temperature range 22 to 200 °C.
Phase Changes
c/liq 376.9 K, $\Delta H = 20170$ J·mol^{-1}
$\Delta S = 53.5$ J·mol^{-1}·K^{-1}
Molecular Weight 136.1500
Wiswesser Line Notation QVR B1
Evaluation C

$C_8H_8O_2$ (c) 26AND/LYN
m-Toluic acid; 3-Methylbenzoic acid
Heat Capacity 298 K, $C_p = 163.6$ J·mol^{-1}·K^{-1}
Temperature range 22 to 170 °C.
Phase Changes
c/liq 381.9 K, $\Delta H = 15730$ J·mol^{-1}
$\Delta S = 41.2$ J·mol^{-1}·K^{-1}
Molecular Weight 136.1500
Wiswesser Line Notation QVR C1
Evaluation C

$C_8H_8O_2$ (c) 26AND/LYN
p-Toluic acid; 4-Methylbenzoic acid
Heat Capacity 298 K, $C_p = 169.0$ J·mol^{-1}·K^{-1}
Temperature range 22 to 225 °C.
Phase Changes
c/liq 452.8 K, $\Delta H = 22720$ J·mol^{-1}
$\Delta S = 50.2$ J·mol^{-1}·K^{-1}
Molecular Weight 136.1500
Wiswesser Line Notation QVR D1
Evaluation C

$C_8H_8O_3$ (liq) 33KOL/UDO
Methyl salicylate
Heat Capacity 295.2 K, $C_p = 268.6$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 152.1494
Wiswesser Line Notation QR BVO1
Evaluation C

$C_8H_8O_3$ (liq) 34KOL/UDO2
Methyl salicylate
Heat Capacity 295.2 K, $C_p = 248.9$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 152.1494
Wiswesser Line Notation QR BVO1
Evaluation C

$C_8H_8O_3$ (c) 41SAT/SOG3
4-Methoxybenzoic acid; p-Anisic acid
Heat Capacity 323 K, $C_p = 205.0$ J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 152.1494
Wiswesser Line Notation QVR DO1
Evaluation C
Same data as 40SAT/SOG4.

$C_8H_8O_3$ (c) 92SAB/ELW3
4-Methoxybenzoic acid; p-Anisic acid
Phase Changes
c/liq 456.70 K, ΔH=28330 J·mol^{-1}
Molecular Weight 152.1494
Wiswesser Line Notation QVR DO1
Evaluation A

$C_8H_8O_3$ (c) 41SAT/SOG3
Mandelic acid
Heat Capacity 323 K, C_p=199.2 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 152.1494
Wiswesser Line Notation QVYQR
Evaluation C
Same data as 40SAT/SOG4.

$C_8H_8O_3$ (c) 78GEI/KAR2
Tetrahydrophthalic anhydride
Heat Capacity
Temperature range 12 to 390 K. Data deposited in VINITI, No. 3882-77, 5 October 1977. Includes C_p, S, ΔHm, Tm.
Molecular Weight 152.1494
Wiswesser Line Notation T666 1A M CVOVT&&J
Evaluation B (for original data)

C_8H_9NO (c) 41SAT/SOG
Acetanilide
Heat Capacity 323 K, C_p=191.6 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 135.1652
Wiswesser Line Notation 1VMR
Evaluation C
Same data in 40SAT/SOG2.

C_8H_9NO (c) 80AND/CON
Acetanilide
Phase Changes
c,I/liq 387.525 K, ΔH=21653 J·mol^{-1}
ΔS=55.87 J·mol^{-1}·K^{-1}
Molecular Weight 135.1652
Wiswesser Line Notation 1VMR
Evaluation A

C_8H_9NO (c) 86NIL/WAD2
Acetanilide
Heat Capacity 298.15 K, C_p=179.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 135.1652
Wiswesser Line Notation 1VMR
Evaluation B

$C_8H_9NO_2$ (c) 71PRI
Methyl N-phenylcarbamate
Heat Capacity 298 K, C_p=203.3 J·mol^{-1}·K^{-1}
Temperature range 200 to 390 K. Complete data deposited in VINITI, No. 2713-71, 25 March 1971.
Phase Changes
c/liq 325 K, ΔH=14548 J·mol^{-1}
ΔS=44.8 J·mol^{-1}·K^{-1}
Molecular Weight 151.1646
Wiswesser Line Notation 1OVMR
Evaluation B

$C_8H_9NO_2$ (c) 26AND/LY
o-Hydroxyacetanilide
Heat Capacity 298 K, C_p=182.4 J·mol^{-1}·K^{-1}
Temperature range 22 to 140 °C.
Phase Changes
c/liq 364.5 K, ΔH=21250 J·mol^{-1}
ΔS=58.3 J·mol^{-1}·K^{-1}
Molecular Weight 151.1646
Wiswesser Line Notation QR BMV1
Evaluation C

$C_8H_9NO_2$ (c) 80SAB/SK
N-Phenylglycine
Heat Capacity 298.15 K, C_p=176.6 J·mol^{-1}·K^{-1}
Temperature range 298.15 K. One temperature.
Phase Changes
c/g 298.15 K, ΔH=128.0 J·mol^{-1}
ΔS=0.43 J·mol^{-1}·K^{-1}
Sublimation measurements made over 350 to 380 K; da corrected to 298.15 K.
Molecular Weight 151.1646
Wiswesser Line Notation QV1MR
Evaluation A

$C_8H_9NO_2$ (c) 80SAB/SK
α-Phenylglycine(D)
Heat Capacity 298.15 K, C_p=177.4 J·mol^{-1}·K^{-1}
Temperature range 298.15 K. One temperature.
Phase Changes
c/g 298.15 K, ΔH=165 J·mol^{-1}
ΔS=0.55 J·mol^{-1}·K^{-1}
Sublimation measurements made over 435 to 455 K; da corrected to 298.15 K.
Molecular Weight 151.1646
Wiswesser Line Notation ZYRVQ
Evaluation A

$C_8H_9NO_3$ (c) 81LEB/RY
p-Nitrophenetole; p-Nitroethoxybenzene
Heat Capacity C_p=246.2 J·mol^{-1}·K^{-1}
Temperature range 298 to 328 K. Data given over temperatu range.
Molecular Weight 167.1640
Wiswesser Line Notation WNR DO2
Evaluation B

$C_8H_9NO_4$ (c) 39SAT/SOC
Ammonium acid o-phthalate
Heat Capacity 323 K, C_p=279.1 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 183.1634
Wiswesser Line Notation QVR BVQ &ZH
Evaluation C
Same data in 40 SAT/SOG.

$C_8H_9NO_4$ (c) 39SAT/SOC
Ammonium acid m-phthalate
Heat Capacity 323 K, C_p=251.5 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 183.1634
Wiswesser Line Notation QVR CVQ &ZH
Evaluation C
Same data in 40 SAT/SOG.

C_8H_{10} (liq) 24WIL/DAN
1,2-Dimethylbenzene; o-Xylene
Heat Capacity 303 K, C_p=182.4 J·mol^{-1}·K^{-1}
Temperature range 303 to 348 K. Equation only.
Molecular Weight 106.1670
Wiswesser Line Notation 1R B1
Evaluation C

C_8H_{10} (liq) 30HUF/PAR
1,2-Dimethylbenzene; o-Xylene
Heat Capacity 298.1 K, C_p=183.89 J·mol^{-1}·K^{-1}
Temperature range 90 to 295 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=248.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 60.79 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 208 K, ΔH=31 J·mol^{-1}
ΔS=0.15 J·mol^{-1}·K^{-1}
c,I/liq 247.8 K, ΔH=13037 J·mol^{-1}
ΔS=52.61 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 1R B1
Evaluation B(C_p),C(S)

C_8H_{10} (liq) 43PIT/SCO
1,2-Dimethylbenzene; o-Xylene
Heat Capacity 298.15 K, C_p=187.82 J·mol^{-1}·K^{-1}
Temperature range 14 to 301 K.
Entropy 298.15 K, S=246.02 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 247.82 K, ΔH=13598 J·mol^{-1}
ΔS=54.87 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 1R B1
Evaluation A

C_8H_{10} (liq) 47KUR
1,2-Dimethylbenzene; o-Xylene
Heat Capacity 298 K, C_p=187.0 J·mol^{-1}·K^{-1}
Temperature range 15 to 132 °C, mean C_p, three temperatures.
Molecular Weight 106.1670
Wiswesser Line Notation 1R B1
Evaluation D

C_8H_{10} (liq) 58SWI/ZIE2
1,2-Dimethylbenzene; o-Xylene
Heat Capacity 347 K, C_p=206.7 J·mol^{-1}·K^{-1}
Mean value 22 to 126 °C.
Molecular Weight 106.1670
Wiswesser Line Notation 1R B1
Evaluation C

C_8H_{10} (liq) 77FOR/BEN
1,2-Dimethylbenzene; o-Xylene
Heat Capacity 298.15 K, C_p=187.584 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 1R B1
Evaluation B

C_8H_{10} (liq) 79FOR/BEN
1,2-Dimethylbenzene; o-Xylene
Heat Capacity 298.15 K, C_p=187.653 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 1R B1
Evaluation B

C_8H_{10} (liq) 24WIL/DAN
1,3-Dimethylbenzene; m-Xylene
Heat Capacity 303 K, C_p=178.2 J·mol^{-1}·K^{-1}
Temperature range 303 to 348 K. Equation only.
Molecular Weight 106.1670
Wiswesser Line Notation 1R C1
Evaluation C

C_8H_{10} (liq) 30HUF/PAR
1,3-Dimethylbenzene; m-Xylene
Heat Capacity 275.3 K, C_p=175.3 J·mol^{-1}·K^{-1}
Temperature range 96 to 275 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=252.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 66.94 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 166 K, ΔH=208 J·mol^{-1}
ΔS=1.25 J·mol^{-1}·K^{-1}
c,I/liq 219.6 K, ΔH=11443 J·mol^{-1}
ΔS=52.11 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 1R C1
Evaluation B(C_p),C(S)

C_8H_{10} (liq) 43PIT/SCO
1,3-Dimethylbenzene; m-Xylene
Heat Capacity 298.15 K, C_p=183.18 J·mol^{-1}·K^{-1}
Temperature range 14 to 320 K.
Entropy 298.15 K, S=253.80 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 225.27 K, ΔH=11569 J·mol^{-1}
ΔS=51.36 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 1R C1
Evaluation A

C_8H_{10} (liq) 47KUR
1,3-Dimethylbenzene; m-Xylene
Heat Capacity 298 K, C_p=184.5 J·mol^{-1}·K^{-1}
Temperature range 16 to 132 °C, mean C_p, three temperatures.
Molecular Weight 106.1670
Wiswesser Line Notation 1R C1
Evaluation C

C_8H_{10} (liq) 58SWI/ZIE2
1,3-Dimethylbenzene; m-Xylene
Heat Capacity 336 K, C_p=199.2 J·mol^{-1}·K^{-1}
Mean value 21 to 106 °C.
Molecular Weight 106.1670
Wiswesser Line Notation 1R C1
Evaluation C

C_8H_{10} (liq) 77FOR/BEN
1,3-Dimethylbenzene; m-Xylene
Heat Capacity 298.15 K, C_p=181.482 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 1R C1
Evaluation B

C_8H_{10} (liq) 79FOR/BEN
1,3-Dimethylbenzene; m-Xylene
Heat Capacity 298.15 K, C_p=181.550 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 1R C1
Evaluation B

C_8H_{10} (liq) 93GRO/ROU
1.3-Dimethylbenzene: m-Xylene
Heat Capacity 298.15 K, C_p=184.63 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 1R C1
Evaluation B

C_8H_{10} (liq) 24WIL/DAN
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 303 K, C_p=176.6 J·mol^{-1}·K^{-1}
Temperature range 303 to 348 K. Equation only.
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation C

C_8H_{10} (liq) 30HUF/PAR
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 299.0 K, C_p=180.3 J·mol^{-1}·K^{-1}
Temperature range 92 to 299 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=253.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 65.19 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 286.3 K, ΔH=16933 J·mol^{-1}
ΔS=59.14 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation B(C_p),C(S)

C_8H_{10} (liq) 43PIT/SCO
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 298.15 K, C_p=183.76 J·mol^{-1}·K^{-1}
Temperature range 14 to 360 K.
Entropy 298.15 K, S=243.51 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 286.39 K, ΔH=17113 J·mol^{-1}
ΔS=59.75 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation A

C_8H_{10} (liq) 47KU
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 298 K, C_p=184.9 J·mol^{-1}·K^{-1}
Temperature range 15 to 132 °C, mean C_p, three temperatures
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation D

C_8H_{10} (liq) 47COR/G
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 298 K, C_p=181.6 J·mol^{-1}·K^{-1}
Temperature range 273 to 573 K.
Phase Changes
c/liq 286.3 K, ΔH=17100 J·mol^{-1}
ΔS=59.73 J·mol^{-1}·K
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation A

C_8H_{10} (liq) 58SWI/ZI
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 336 K, C_p=198.7 J·mol^{-1}·K
Mean value 21 to 106 °C.
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation C

C_8H_{10} (liq) 71HYD/SU
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 298.15 K, C_p=181.7 J·mol^{-1}·K
Temperature range 298; 313 K.
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation B

C_8H_{10} (liq) 77FOR/BI
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 298.15 K, C_p=181.794 J·mol^{-1}·K
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation B

C_8H_{10} (liq) 77WIL/GI
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 298.15 K, C_p=181.55 J·mol^{-1}·K
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation B

C_8H_{10} (liq) 79FOR/B
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 298.15 K, C_p=181.937 J·mol^{-1}·K
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation B

C_8H_{10} (liq) 79OTT/GOA
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 298.15 K, C_p=181.9 J·mol^{-1}·K^{-1}
Temperature range 288.15 to 328.15 K.
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation B

C_8H_{10} (liq) 86TAR/AIC
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 298.15 K, C_p=183.65 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation B

C_8H_{10} (liq) 88MES/FIN
1,4-Dimethylbenzene; p-Xylene
Heat Capacity 298.15 K, C_p=182.219 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=247.154 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 286.405 K, ΔH=17117.46 J·mol^{-1}
ΔS=59.77 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation A

C_8H_{10} (liq) 1881REI
Ethylbenzene
Heat Capacity 298 K, C_p=184.5 J·mol^{-1}·K^{-1}
Temperature range 292 to 425 K.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation D

C_8H_{10} (liq) 24WIL/DAN
Ethylbenzene
Heat Capacity 303 K, C_p=181.6 J·mol^{-1}·K^{-1}
Temperature range 303 to 343 K. Equation only.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation C

C_8H_{10} (liq) 30IIUГ/PAR
Ethylbenzene
Heat Capacity 297.4 K, C_p=181.6 J·mol^{-1}·K^{-1}
Temperature range 93 to 305 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=256.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 61.09 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 178.0 K, ΔH=9163 J·mol^{-1}
ΔS=51.48 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation B(C_p),C(S)

C_8H_{10} (liq) 31BLA/LEI
Ethylbenzene
Heat Capacity 298.15 K, C_p=186.6 J·mol^{-1}·K^{-1}
Temperature range 286 to 368 K. Heat capacity reported as 0.420 cal·g^{-1}·K^{-1} at 25 °C.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation B

C_8H_{10} (liq) 31SMI/AND
Ethylbenzene
Heat Capacity 298.5 K, C_p=183.7 J·mol^{-1}·K^{-1}
Temperature range 102 to 299 K. Value is unsmoothed experimental datum.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation C

C_8H_{10} (liq) 34KOL/UDO
Ethylbenzene
Heat Capacity 302.8 K, C_p=178.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation C

C_8H_{10} (liq) 34KOL/UDO2
Ethylbenzene
Heat Capacity 302.7 K, C_p=178.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation C

C_8H_{10} (liq) 44GUT/SPI
Ethylbenzene
Heat Capacity 298.15 K, C_p=185.81 J·mol^{-1}·K^{-1}
Temperature range 13 to 305 K.
Entropy 298.15 K, S=255.01 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 178.17 K, ΔH=9163 J·mol^{-1}
ΔS=51.43 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation A

C_8H_{10} (liq) 45SCO/BRI
Ethylbenzene
Heat Capacity 298.15 K, C_p=186.04 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Phase Changes
c/liq 178.15 K, ΔH=9181.8 J·mol^{-1}
ΔS=51.54 J·mol^{-1}·K^{-1}
liq/g 294.01 K, ΔH=42490 J·mol^{-1}
ΔS=144.5 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation A

C_8H_{10} (liq) 47KUR
Ethylbenzene
Heat Capacity 298 K, C_p=185.8 J·mol^{-1}·K^{-1}
Temperature range 15 to 18 °C, mean C_p, four temperatures.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation D

C_8H_{10} (liq) 48TSC
Ethylbenzene
Heat Capacity 295 K, C_p=161 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation C

C_8H_{10} (liq) 76FOR/BEN
Ethylbenzene
Heat Capacity 298.15 K, C_p=185.78 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation B

C_8H_{10} (liq) 77FOR/BEN
Ethylbenzene
Heat Capacity 298.15 K, C_p=185.559 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation B

C_8H_{10} (liq) 79AND/GRI
Ethylbenzene
Heat Capacity 293.31 K, C_p=184.8 J·mol^{-1}·K^{-1}
Temperature range 293 to 393 K. Unsmoothed experimental datum given as 1.741 kJ/kg·K.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation B

C_8H_{10} (liq) 79FOR/BEN
Ethylbenzene
Heat Capacity 298.15 K, C_p=185.572 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 2R
Evaluation B

$C_8H_{10}N_2O$ (c) 40CAM/CAM
p-Nitrosodimethylaniline
Heat Capacity 293 K, C_p=206.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 150.1798
Wiswesser Line Notation ONR DN1&1
Evaluation C

$C_8H_{10}N_4O_2$ (c) 79BOT/CAM
Caffeine, anhydrous
Heat Capacity 298.15 K, C_p=232 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c,II/c,I 414 K, ΔH=4030 J·mol^{-1}
ΔS=28.6 J·mol^{-1}·K^{-1}
Low temperature β to a high temperature α transition.
c,I/liq 509.3 K, ΔH=21600 J·mol^{-1}
ΔS=42.4 J·mol^{-1}·K^{-1}
Molecular Weight 194.1926
Wiswesser Line Notation T56 BN DN FNVNVJ B1 F1 H1
Evaluation B

$C_8H_{10}N_4O_2$ (c) 80CES/ST
Caffeine
Heat Capacity 298 K, C_p=173.2 J·mol^{-1}·K^{-1}
Temperature range 300 to 392 K. Unsmoothed experimental dat and equation given. C_p=41.4+0.104(T−298) cal·mol^{-1}·K^{-}
Data given at 298 K is an extrapolation by the author.
Phase Changes
c,II/c,I 426 K, ΔH=940 J·mol^{-1}
ΔS=2.2 J·mol^{-1}·K^{-1}
α to β form.
c,I/liq 512 K, ΔH=5600 J·mol^{-1}
ΔS=10.9 J·mol^{-1}·K^{-1}
β to liquid.
Molecular Weight 194.1926
Wiswesser Line Notation T56 BN DN FNVNVJ B1 F1 H1
Evaluation B
Data given for β form. β form is obtained by high temperatu sublimation.

$C_8H_{10}O$ (liq) 75FEN/HA
Ethyl phenyl ether
Heat Capacity 298.15 K, C_p=228.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 122.1664
Wiswesser Line Notation 2OR
Evaluation B

$C_8H_{10}O$ (liq) 75NIC/WA
2-Phenylethanol
Heat Capacity 298.15 K, C_p=252.64 J·mol^{-1}·K
One temperature.
Molecular Weight 122.1664
Wiswesser Line Notation Q2R
Evaluation B

$C_8H_{10}O$ (c) 82POE/FA
2,3-Dimethylphenol
Phase Changes
c/liq 346.0 K, ΔH=21024 J·mol^{-1}
ΔS=60.76 J·mol^{-1}·K^{-}
Molecular Weight 122.1664
Wiswesser Line Notation QR B1 C1
Evaluation A

$C_8H_{10}O$ (c) 82POE/FAN
2,4-Dimethylphenol
Phase Changes
c/liq 299.0 K
Molecular Weight 122.1664
Wiswesser Line Notation QR B1 D1
Evaluation A

$C_8H_{10}O$ (c) 82POE/FAN
2,5-Dimethylphenol
Phase Changes
c/liq 348.0 K, $\Delta H = 23376\ J\cdot mol^{-1}$
$\Delta S = 67.17\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 122.1664
Wiswesser Line Notation QR B1 E1
Evaluation A

$C_8H_{10}O$ (c) 82POE/FAN
2,6-Dimethylphenol
Phase Changes
c/liq 318.9 K, $\Delta H = 18897\ J\cdot mol^{-1}$
$\Delta S = 59.26\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 122.1664
Wiswesser Line Notation QR B1 F1
Evaluation A

$C_8H_{10}O$ (c) 82POE/FAN
3,4-Dimethylphenol
Phase Changes
c/liq 334.0 K, $\Delta H = 18127\ J\cdot mol^{-1}$
$\Delta S = 54.27\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 122.1664
Wiswesser Line Notation QR C1 D1
Evaluation A

$C_8H_{10}O$ (c) 57MAS
3,5-Dimethylphenol
Phase Changes
c/liq 336.59 K, $\Delta H = 17422\ J\cdot mol^{-1}$
Molecular Weight 122.1664
Wiswesser Line Notation QR C1 E1
Evaluation A

$C_8H_{10}O$ (c) 82POE/FAN
3,5-Dimethylphenol
Phase Changes
c/liq 336.8 K, $\Delta H = 17997\ J\cdot mol^{-1}$
$\Delta S = 53.38\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 122.1664
Wiswesser Line Notation QR C1 E1
Evaluation A

$C_8H_{10}O$ (c) 75NIC/WAD
4-Ethylphenol
Heat Capacity 298.15 K, $C_p = 206.9\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 122.1664
Wiswesser Line Notation QR D2
Evaluation B

$C_8H_{10}O_2$ (liq) 75NIC/WAD
2-Phenoxyethanol
Heat Capacity 298.15 K, $C_p = 294.63\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 138.1658
Wiswesser Line Notation Q2OR
Evaluation B

$C_8H_{10}O_3$ (c) 83GEI/NUR
cis-Cyclohexane-1,2-dicarboxylic anhydride
Heat Capacity 298.15 K, $C_p = 207.4\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 12 to 330 K.
Entropy 298.15 K, $S = 202.4\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c,III/c,II 304 K, $\Delta H = 5594\ J\cdot mol^{-1}$
$\Delta S = 18.41\ J\cdot mol^{-1}\cdot K^{-1}$
Conformational transition.
c,II/c,I 310.5 K, $\Delta H = 845\ J\cdot mol^{-1}$
$\Delta S = 2.72\ J\cdot mol^{-1}\cdot K^{-1}$
Conformational transition.
Molecular Weight 154.1652
Wiswesser Line Notation T56 BVOVTJ -C
Evaluation A

$C_8H_{11}N$ (liq) 1881REI
N,N-Dimethylaniline
Heat Capacity 298 K, $C_p = 212.1\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 292 to 478 K.
Molecular Weight 121.1816
Wiswesser Line Notation 1N1&R
Evaluation D

$C_8H_{11}N$ (liq) 02LOU
N,N-Dimethylaniline
Heat Capacity 375 K, $C_p = 243\ J\cdot mol^{-1}\cdot K^{-1}$
Mean value 21 to 186 °C.
Molecular Weight 121.1816
Wiswesser Line Notation 1N1&R
Evaluation D

$C_8H_{11}N$ (liq) 16BRA
N,N-Dimethylaniline
Heat Capacity 283 K, $C_p = 212.1\ J\cdot mol^{-1}\cdot K^{-1}$
Mean value, 0 to 20 °C.
Molecular Weight 121.1816
Wiswesser Line Notation 1N1&R
Evaluation C

$C_8H_{11}N$ (liq) 34KOL/UDO
N,N-Dimethylaniline
Heat Capacity 302.4 K, $C_p = 214.6\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 121.1816
Wiswesser Line Notation 1N1&R
Evaluation C

$C_8H_{11}N$ (liq) 34KOL/UDO2
N,N-Dimethylaniline
Heat Capacity 302.3 K, $C_p = 214.6\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 121.1816
Wiswesser Line Notation 1N1&R
Evaluation C

$C_8H_{11}N$ (liq) 34RAD/JUL
N,N-Dimethylaniline
Heat Capacity 289 K, C_p=209.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 121.1816
Wiswesser Line Notation 1N1&R
Evaluation C

$C_8H_{11}N$ (c) 87MEI/DOG
1-Norbornyl cyanide; 1-Cyanobicyclo[2.2.1]heptane
Heat Capacity 298.15 K, C_p=196.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 121.1816
Wiswesser Line Notation L55 A TJ BCN
Evaluation C

$C_8H_{11}N$ (c) 87MEI/DOG
1-Norbornyl isonitrile; 1-Isocyanobicylco[2.2.1]heptane
Heat Capacity 298.15 K, C_p=172.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 121.1816
Wiswesser Line Notation L55 A TJ BNC
Evaluation C

$C_8H_{11}N$ (c) 62SER/KOL
2-Cyanobicyclo[2.2.1]heptane(exo)
Heat Capacity 280 K, C_p=200.03 J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Entropy 298.15 K, S=230.58 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 237.7 K, ΔH=7929 J·mol^{-1}
ΔS=33.35 J·mol^{-1}·K^{-1}
c,I/liq 300.27 K, ΔH=2943 J·mol^{-1}
ΔS=9.83 J·mol^{-1}·K^{-1}
Molecular Weight 121.1816
Wiswesser Line Notation L55 A TJ CCN -EXO
Evaluation A

$C_8H_{11}N$ (c) 70KOL/SER
2-Cyanobicyclo[2.2.1]heptane(exo)
Heat Capacity 285 K, C_p=200.0 J·mol^{-1}·K^{-1}
Temperature range 12 to 340 K.
Entropy 298.15 K, S=241.7 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 237.7 K, ΔH=7929 J·mol^{-1}
ΔS=33.4 J·mol^{-1}·K^{-1}
c,I/liq 298.8 K, ΔH=2943.4 J·mol^{-1}
ΔS=9.83 J·mol^{-1}·K^{-1}
Molecular Weight 121.1816
Wiswesser Line Notation L55 A TJ CCN -EXO
Evaluation A

$C_8H_{11}N$ (c) 62SER/KOL
2-Cyanobicyclo[2.2.1]heptane(endo)
Heat Capacity 298.15 K, C_p=193.89 J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Entropy 298.15 K, S=223.80 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 177.35 K, ΔH=2095 J·mol^{-1}
ΔS=11.80 J·mol^{-1}·K^{-1}
c,I/liq 331.67 K, ΔH=2961 J·mol^{-1}
ΔS=8.91 J·mol^{-1}·K^{-1}
Molecular Weight 121.1816
Wiswesser Line Notation L55 A TJ CCN -ENDO
Evaluation A

$C_8H_{11}N$ (c) 70KOL/SE
2-Cyanobicyclo[2.2.1]heptane(endo)
Heat Capacity 298.15 K, C_p=193.93 J·mol^{-1}·K^{-}
Temperature range 12 to 340 K.
Entropy 298.15 K, S=224.68 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 177.3 K, ΔH=2251.8 J·mol^{-1}
ΔS=12.70 J·mol^{-1}·K^{-}
c,I/liq 331.2 K, ΔH=2961.0 J·mol^{-1}
ΔS=8.94 J·mol^{-1}·K^{-1}
Molecular Weight 121.1816
Wiswesser Line Notation L55 A TJ CCN -ENDO
Evaluation A

$C_8H_{11}N$ (liq) 91SVO/ZAI
2,3,6-Trimethylpyridine
Heat Capacity 300.60 K, C_p=220.0 J·mol^{-1}·K^{-}
Temperature range 300 to 328 K. C_p(liq)=410.64 −1.517
+2.9366×10^{-3}T^2 J/K·mol (300 to 328 K).
Molecular Weight 121.1816
Wiswesser Line Notation T6NJ B1 C1 F1
Evaluation B

$C_8H_{11}N$ (liq) 57M
2,4,6-Collidine; 2,4,6-Trimethylpyridine
Phase Changes
c/liq 228.96 K, ΔH=9535 J·mol^{-1}
Molecular Weight 121.1816
Wiswesser Line Notation T6NJ B1 D1 F1
Evaluation A

$C_8H_{11}N$ (liq) 91SVO/ZAI
2,4,6-Collidine; 2,4,6-Trimethylpyridine
Heat Capacity 300.60 K, C_p=215.1 J·mol^{-1}·K^{-}
Temperature range 300 to 328 K. C_p(liq)=81.418+0.44263T J
·mol (300 to 328 K).
Molecular Weight 121.1816
Wiswesser Line Notation T6NJ B1 D1 F1
Evaluation B

$C_8H_{11}N$ (liq) 75NIC/W
2-Phenylethylamine
Heat Capacity 298.15 K, C_p=239.24 J·mol^{-1}·K
One temperature.
Molecular Weight 121.1816
Wiswesser Line Notation Z2R
Evaluation B

$C_8H_{11}N$ (liq) 86STE/C
2,6-Dimethylaniline
Heat Capacity 298.15 K, C_p=238.86 J·mol^{-1}·K
Temperature range 10 to 450 K.
Entropy 298.15 K, S=251.35 J·mol^{-1}·K^{-}
Phase Changes
c/liq 284.598 K
Molecular Weight 121.1816
Wiswesser Line Notation ZR B1 F1
Evaluation A

$C_8H_{11}NO_3$ (c) 89KHO/ISK
2-Methyl-3-hydroxy-4,5-dihydroxymethylpyridine
Heat Capacity 298.15 K, C_p=244.46 J·mol^{-1}·K^{-1}
One temperature.
Entropy 298.15 K, S=278.59 J·mol^{-1}·K^{-1}
Molecular Weight 169.1798
Wiswesser Line Notation T6NJ B1 CQ D1Q E1Q
Evaluation B

$C_8H_{11}NO_3$ (c) 90KHO/ISK
2-Methyl-3-hydroxy-4,5-dihydroxymethylpyridine
Heat Capacity 300 K, C_p=237.40 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 300 K, S=271.77 J·mol^{-1}·K^{-1}
Molecular Weight 169.1798
Wiswesser Line Notation T6NJ B1 CQ D1Q E1Q
Evaluation A

C_8H_{12} (c,I) 70WON/WES
Bicyclo[2.2.2]octene-2
Heat Capacity 298.15 K, C_p=156.73 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S=210.46 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 110.50 K, ΔH=188 J·mol^{-1}
ΔS=1.33 J·mol^{-1}·K^{-1}
Second order transition.
c,II/c,I 176.47 K, ΔH=5648 J·mol^{-1}
ΔS=24.52 J·mol^{-1}·K^{-1}
ΔH and ΔS obtained separately by graphical integration of observed C_p (or total enthalpy input) subtracting contributions from extrapolated normal C_p, ΔH, ΔS and T not self-consistent.
c,I/liq 389.75 K, ΔH=5381 J·mol^{-1}
ΔS=14.39 J·mol^{-1}·K^{-1}
ΔH and ΔS obtained separately by graphical integration of observed C_p (or total enthalpy input) subtracting contributions from extrapolated normal C_p, ΔH, ΔS and T not self-consistent.
Molecular Weight 108.1828
Wiswesser Line Notation L66 A B AUTJ
Evaluation A(C_p), B(Phase changes)

C_8H_{12} (liq) 75LEB/LEB
Cycloocta-1,5-diene
Heat Capacity 298.15 K, C_p=198.9 J·mol^{-1}·K^{-1}
Temperature range 6 to 320 K.
Entropy 298.15 K, S=250.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 194.3 K, ΔH=−393 J·mol^{-1}
c,I/liq 203.983 K, ΔH=9828 J·mol^{-1}
ΔS=48.24 J·mol^{-1}·K^{-1}
Molecular Weight 108.1828
Wiswesser Line Notation L8 AU EUTJ
Evaluation A

C_8H_{12} (liq) 75LEB/TSV2
Cycloocta-1,5-diene
Heat Capacity 298.15 K, C_p=208.1 J·mol^{-1}·K^{-1}
Temperature range 10.6 to 322.7 K. Data deposited in VINITI, No. 1324-75, 15 May 1975.
Entropy 298.15 K, S=264.3 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 194.34 K, ΔH=−381 J·mol^{-1}
Irreversible exothermic transition.
c,I/liq 203.983 K, ΔH=9828 J·mol^{-1}
ΔS=48.24 J·mol^{-1}·K^{-1}
Molecular Weight 108.1828
Wiswesser Line Notation L8 AU EUTJ
Evaluation A

$(C_8H_{12})_n$ (liq) 76LEB/LIT
Polyoctadiene
Heat Capacity 298.15 K, C_p=205.4 J·mol^{-1}·K^{-1}
Temperature range 15 to 328 K. Data deposited in VINITI No. 2097-76, 10 June 1976.
Entropy 298.15 K, S=220.5 J·mol^{-1}·K^{-1}
Entropy at zero kelvin of amorphous polyoctadiene was assumed to be equal to the sum of the configurational entropy and the entropy of mixing the cis and the trans forms. $S_0°$=15.7 J·mol^{-1}·K^{-1}.
Phase Changes
c,I/gls 168.5 K
Heat capacity increment following conversion to glass is 41.3 J·mol^{-1}·K^{-1}.
c,I/liq 255 K, ΔH=270 J·mol^{-1}
ΔS=1.06 J·mol^{-1}·K^{-1}
Temperature range of anomaly, probably due to fusion of crystal of the cis-form, is 100–255 K.
Molecular Weight 108.1828
Wiswesser Line Notation /*L8 AU EUTJ*/
Evaluation B

$C_8H_{12}BrN$ (c) 89VAN/WHI
2-Phenylethylammonium bromide
Phase Changes
c,II/c,I 347 K, ΔH=6680 J·mol^{-1}
ΔS=2.31 J·mol^{-1}·K^{-1}
Molecular Weight 202.0935
Wiswesser Line Notation Z2R &EH
Evaluation A

$C_8H_{12}ClN$ (c) 89VAN/WHI
2-Phenylethylammonium chloride
Phase Changes
c,III/c,II 389 K, ΔH=7590 J·mol^{-1}
ΔS=2.35 J·mol^{-1}·K^{-1}
c,II/c,I 432 K, ΔH=3230 J·mol^{-1}
ΔS=0.90 J·mol^{-1}·K^{-1}
Molecular Weight 157.6425
Wiswesser Line Notation Z2R &GH
Evaluation A

$C_8H_{12}N_2$ (c) 70MUR/BRE2
Tetramethylsuccinonitrile
Phase Changes
c,II/c,I 345 K, ΔH=18104 J·mol^{-1}
ΔS=52.63 J·mol^{-1}·K^{-1}
c,I/liq 442 K, ΔH=7146 J·mol^{-1}
ΔS=16.19 J·mol^{-1}·K^{-1}
Molecular Weight 136.1962
Wiswesser Line Notation NCX1&1&X1&1&CN
Evaluation A

$C_8H_{12}N_2O_2$ (liq) 62STR/BAR
1,6-Hexamethylene diisocyanate; 1,6-Diisocyanatohexane
Heat Capacity 298 K, C_p=299.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 136.1962
Wiswesser Line Notation OCN6NCO
Evaluation D

$C_8H_{12}N_2O_2$ (liq) 83BYK/LEB2
1,6-Hexamethylene diisocyanate; 1,6-Diisocyanatohexane
Heat Capacity 298.15 K, C_p=294.0 J·mol^{-1}·K^{-1}
Temperature range 0 to 330 K.
Phase Changes
c/liq 206.06 K, ΔH=18640 J·mol^{-1}
ΔS=90.46 J·mol^{-1}·K^{-1}
Molecular Weight 136.1962
Wiswesser Line Notation OCN6NCO
Evaluation A

$C_8H_{12}N_2O_2$ (liq) 85LEB/BYK2
1,6-Hexamethylene diisocyanate; 1,6-Diisocyanatohexane
Heat Capacity 298.15 K, C_p=294.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=420.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 206.064 K, ΔH=18640 J·mol^{-1}
ΔS=90.46 J·mol^{-1}·K^{-1}
Molecular Weight 136.1962
Wiswesser Line Notation OCN6NCO
Evaluation A

$(C_8H_{12}N_2O_2)_n$ (gls) 85LEB/BYK2
1,6-Hexamethylene diisocyanate polycyclotrimer
Heat Capacity 298.15 K, C_p=222.7 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=242.0 J·mol^{-1}·K^{-1}
Molecular Weight 168.1950
Wiswesser Line Notation /T6NVNVNVJ A6NV&* C6NV&* E6NV&*/ 1/3
Evaluation A
T(glass)=334 K.

$C_8H_{12}N_2O_3$ (c) 89VAN/WHI
2-Phenylethylammonium nitrate
Phase Changes
c,III/c,II 320 K, ΔH=7280 J·mol^{-1}
ΔS=2.73 J·mol^{-1}·K^{-1}
c,II/c,I 370 K, ΔH=1050 J·mol^{-1}
ΔS=0.42 J·mol^{-1}·K^{-1}
Molecular Weight 184.1944
Wiswesser Line Notation Z2R &WNQ
Evaluation A

$C_8H_{12}N_2O_4$ (c) 39SAT/SOG2
Ammonium o-phthalate
Heat Capacity 323 K, C_p=294.1 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 200.1938
Wiswesser Line Notation QVR BVQ &ZH 2
Evaluation C
Same data in 40SAT/SOG.

$C_8H_{12}N_2O_4$ (c) 39SAT/SOG2
Ammonium m-phthalate; Ammonium isophthalate
Heat Capacity 323 K, C_p=285.3 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 200.1938
Wiswesser Line Notation QVR CVQ &ZH 2
Evaluation C
Same data in 40SAT/SOG.

$C_8H_{12}N_4$ (c) 81LEB/RY
2,2′-Azodiisobutyrodinitrile; Dinitrile-2,2′-azodiisobutyric acid
Heat Capacity 298.12 K, C_p=238.1 J·mol^{-1}·K^{-1}
Temperature range 296 to 334 K.
Molecular Weight 164.2096
Wiswesser Line Notation NCX1&1&NUNX1&1&CN
Evaluation B

$C_8H_{12}N_4$ (c) 84LEB/GU
2,2′-Azodiisobutyrodinitrile; Dinitrile-2,2′-azodiisobutyric acid
Heat Capacity 298 K, C_p=237.55 J·mol^{-1}·K^{-1}
Temperature range 296 to 335 K.
Phase Changes
c/liq 378 K
Molecular Weight 164.2096
Wiswesser Line Notation NCX1&1&NUNX1&1&CN
Evaluation B
$\Delta\Delta H$ sublimation=76600 J·mol^{-1}, temperature range=288 313 K.

$C_8H_{12}N_6$ (c) 73KAR/SAI
Terephthalic bisamidrazone
Heat Capacity 298 K, C_p=276.8 J·mol^{-1}·K^{-1}
Temperature range 20 to 298 K.
Entropy 298 K, S=255.2 J·mol^{-1}·K^{-1}
Molecular Weight 192.2230
Wiswesser Line Notation ZYUNZR DYUNZZ
Evaluation B

$C_8H_{12}S_6$ (c) 62CHA/WI
1.3.5.7-Tetramethyl-2.4.6.8.9.10-hexathiaadamantane
Heat Capacity 298.15 K, C_p=301.62 J·mol^{-1}·K
Temperature range 5 to 300 K.
Entropy 298.15 K, S=321.12 J·mol^{-1}·K^{-1}
Molecular Weight 300.5428
Wiswesser Line Notation T66 B6/B-H/DI A B- C 1B I AS B-S (ES GS ISTJ B1 D1 F1 H1
Evaluation A

C_8H_{14} -(liq) 90STE/C
2,5-Dimethylhexa-2,4-diene
Heat Capacity 298.15 K. C_p=459.0 J·mol^{-1}·K^{-1}
One temperature. Authors give C_p/R=55.2. This value appears t large by a factor of two. Actual C_p should be around 229.5 J/n ·K.
Molecular Weight 110.1986
Wiswesser Line Notation 1Y1&U2UY1&1
Evaluation B

C_8H_{14} (liq) 70CHA/M(
cis-Bicyclo[4.2.0]octane
Heat Capacity 345 K, C_p=258.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 110.1986
Wiswesser Line Notation L46TJ -C
Evaluation B

C_8H_{14} (liq) 64SER/GOR
2-Methylbicyclo[2.2.1]heptane(exo)
Heat Capacity 298.15 K, C_p=185.8 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=246.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 164.10 K, ΔH=8381.8 J·mol^{-1}
ΔS=51.0 J·mol^{-1}·K^{-1}
Includes effects of transition just below melting point.
Molecular Weight 110.1986
Wiswesser Line Notation L55 ATK C1 -EXO
Evaluation A

C_8H_{14} (liq) 64SER/GOR
2-Methylbicyclo[2.2.1]heptane(endo)
Heat Capacity 298.15 K, C_p=184.3 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=238.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 152.42 K, ΔH=4707.0 J·mol^{-1}
ΔS=30.88 J·mol^{-1}·K^{-1}
c,I/liq 278.25 K, ΔH=1620.5 J·mol^{-1}
ΔS=5.8 J·mol^{-1}·K^{-1}
Molecular Weight 110.1986
Wiswesser Line Notation L55 ATK C1 -ENDO
Evaluation A

C_8H_{14} (liq) 70CHA/MCC
cis-Bicyclo[3.3.0]octane
Heat Capacity 308 K, C_p=212.4 J·mol^{-1}·K^{-1}
Temperature range 308, 334 K.
Molecular Weight 110.1986
Wiswesser Line Notation L55TJ -C
Evaluation B

C_8H_{14} (liq) 70CHA/MCC
trans-Bicyclo[3.3.0]octane
Heat Capacity 308 K, C_p=180.3 J·mol^{-1}·K^{-1}
Temperature range 308, 334 K.
Molecular Weight 110.1986
Wiswesser Line Notation L55TJ -T
Evaluation B

C_8H_{14} (liq) 79FUC/PEA
Allylcyclopentane
Heat Capacity 298.15 K, C_p=202.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 110.1986
Wiswesser Line Notation L5TJ A2U1
Evaluation B

C_8H_{14} (c,I) 70WON/WES
Bicyclo[2.2.2]octane
Heat Capacity 298.15 K, C_p=157.69 J·mol^{-1}·K^{-1}
Temperature range 5 to 470 K.
Entropy 298.15 K, S=209.95 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 164.25 K, ΔH=4586 J·mol^{-1}
ΔS=27.87 J·mol^{-1}·K^{-1}
ΔH and ΔS obtained separately by graphical integration of observed C_p (or total enthalpy input) subtracting contributions from extrapolated normal C_p, ΔH, ΔS and T not self-consistent.
c,I/liq 447.48 K, ΔH=8347 J·mol^{-1}
ΔS=18.74 J·mol^{-1}·K^{-1}
ΔH and ΔS obtained separately by graphical integration of observed C_p (or total enthalpy input) subtracting contributions from extrapolated normal C_p, ΔH, ΔS and T not self-consistent.
Molecular Weight 110.1986
Wiswesser Line Notation L66 A BTJ
Evaluation A(C_p), B(Phase changes)

C_8H_{14} (liq) 79FUC/PEA
Ethylidenecyclohexane
Heat Capacity 298.15 K, C_p=203.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 110.1986
Wiswesser Line Notation L6YTJ AU2
Evaluation B

C_8H_{14} (liq) 78LEB/LEB
Cyclooctene
Heat Capacity 298.15 K, C_p=207.8 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=254.5 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 100 K
Glass transition.
c,II/c,I 190 K, ΔH=635 J·mol^{-1}
ΔS=3.34 J·mol^{-1}·K^{-1}
c,I/liq 259.15 K, ΔH=1813 J·mol^{-1}
ΔS=7.02 J·mol^{-1}·K^{-1}
Molecular Weight 110.1986
Wiswesser Line Notation L8UTJ
Evaluation A

$(C_8H_{14})_n$ (c) 78LEB/LEB
Polyoctenylene
Heat Capacity 298.15 K, C_p=198.1 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S=203.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 180 K, ΔH=6336 J·mol^{-1}
ΔS=35.2 J·mol^{-1}·K^{-1}
Glass transition.
c,I/liq 308 K, ΔH=16760 J·mol^{-1}
ΔS=54.4 J·mol^{-1}·K^{-1}
Molecular Weight 110.1986
Wiswesser Line Notation /L8TJ A* B*/
Evaluation A

$C_8H_{14}N_2O_2$ (c) 91ABA/DEL
N-Acetylproline-N'-methylamide(DL);
1-Acetyl-N-methyl-2-pyrrolidine carboxamide(DL)
Heat Capacity 298 K, C_p=232.45 J·mol^{-1}·$^{-1}$
Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 170.2188
Wiswesser Line Notation T5NTJ AV1 BVM1 -DL
Evaluation C

$C_8H_{14}N_2O_2$ (c) 91ABA/DEL
N-Acetylproline-N'-methylamide(L);
1-Acetyl-N-methyl-2-pyrrolidine carboxamide(L)
Heat Capacity 298 K, C_p=222.90 J·mol^{-1}·K^{-1}
Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 170.2108
Wiswesser Line Notation T5NTJ AV1 BVM1 -L
Evaluation C

$C_8H_{14}N_6O_{10}$ (c) 71HAL
1,7-Diacetoxy-2,4,6-trinitro-2,4,6-triazaheptane
Phase Changes
c/liq 422.5 K, ΔH=38493 J·mol^{-1}
Molecular Weight 354.2328
Wiswesser Line Notation T7N CN ENTJ ANW CNW EMW FOV1 GOV1
Evaluation C

$C_8H_{14}O$ (liq) 84BAG/BAE
6-Methyl-5-hepten-2-one
Heat Capacity 298.35 K, C_p=267.9 J·mol^{-1}·K^{-1}
Temperature range 273 to 343 K. C_p(liq)=0.24752+0.010420T -1.4×10^{-5}T^2 kJ/kg·K (273 to 343 K).
Molecular Weight 126.1980
Wiswesser Line Notation 1YU3V1
Evaluation B

$C_8H_{14}O$ (liq) 88BAG/GUR
6-Methyl-5-hepten-2-one
Heat Capacity 298.35 K, C_p=268.8 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 126.1980
Wiswesser Line Notation 1YU3V1
Evaluation B

$C_8H_{14}O$ (liq) 70WES/WON
3-Oxabicyclo[3.2.2]nonane
Heat Capacity 298.15 K, C_p=185.06 J·mol^{-1}·K^{-1}
Temperature range 5 to 477 K.
Entropy 298.15 K, S=236.27 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 208.5 K, ΔH=7017 J·mol^{-1}
ΔS=34.39 J·mol^{-1}·K^{-1}
Transition region 160 to 220 K, maximum at 208.5 K. Entropy change obtained by difference of integrated heat input and lattice (extrapolated C_p) contribution.
c,I/liq 448.43 K, ΔH=6753 J·mol^{-1}
ΔS=15.06 J·mol^{-1}·K^{-1}
Molecular Weight 126.1980
Wiswesser Line Notation T67 A B EOTJ
Evaluation A

$C_8H_{14}O_2$ (liq) 52ERD/JAG
Butyl 2-methylpropenoate; Butyl methacrylate
Heat Capacity 293 K, C_p=270.70 J·mol^{-1}·K^{-1}
Temperature range 20 to 40 °C.
Molecular Weight 142.1974
Wiswesser Line Notation 4OVY1&U1
Evaluation C

$C_8H_{14}O_2$ (liq) 85KAR/ABD
Butyl 2-methylpropenoate; Butyl methacrylate
Heat Capacity 298.15 K, C_p=273.7 J·mol^{-1}·K^{-1}
Temperature range 196 to 350 K. C_p (J·kg^{-1}·K^{-1}) =1344.3+1.9467 T. C_p data calculated from equation.
Phase Changes
c/liq 196.8 K
Molecular Weight 142.1974
Wiswesser Line Notation 4OVY1&U1
Evaluation B

$C_8H_{14}O_2$ (liq) 85KAR/ABD
Butyl 2-methylpropenoate; Butyl methacrylate
Phase Changes
c/liq 196.8 K, ΔH=13947 J·mol^{-1}
ΔS=70.87 J·mol^{-1}·K^{-1}
Molecular Weight 142.1974
Wiswesser Line Notation 4OVY1&U1
Evaluation A

$C_8H_{14}O_2$ (liq) 85KAR/SA
Butyl 2-methyl-2-propenoate; Butyl methacrylate
Heat Capacity 298.15 K, C_p=273.8 J·mol^{-1}·K^{-1}
Temperature range 90 to 350 K. C_p(c)=248.85+4.98T J/kg·K (9 to 192 K); C_p(liq)=1344.27+1.95T J/kg·K (196.8 to 350 K) C_p data calculated from equation.
Phase Changes
c/liq 196.8 K
Molecular Weight 142.1974
Wiswesser Line Notation 4OVY1&U1
Evaluation B

$C_8H_{14}O_4$ (liq) 33KOL/UDC
Diethyl succinate
Heat Capacity 292.6 K, C_p=338.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 174.1962
Wiswesser Line Notation 2OV2VO2
Evaluation C

$C_8H_{14}O_4$ (liq) 34KOL/UDO
Diethyl succinate
Heat Capacity 292.6 K, C_p=338.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 174.1962
Wiswesser Line Notation 2OV2VO2
Evaluation C

$C_8H_{14}O_4$ (liq) 79FU
Diethyl succinate
Heat Capacity 298.15 K, C_p=330.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 174.1962
Wiswesser Line Notation 2OV2VO2
Evaluation B

$C_8H_{14}O_4$ (liq) 86NIL/WAD
Ethyleneglycoldipropanoate
Heat Capacity 298.15 K, C_p=331.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 174.1962
Wiswesser Line Notation 2VO2OV2
Evaluation A

$C_8H_{14}O_4$ (c) 74CIN/BER
Suberic acid
Phase Changes
c,II/c,I 407.0 K, ΔH=9033 J·mol^{-1}
ΔS=22.22 J·mol^{-1}·K^{-1}
c,I/liq 415.5 K, ΔH=29162 J·mol^{-1}
ΔS=70.21 J·mol^{-1}·K^{-1}
Molecular Weight 174.1962
Wiswesser Line Notation QV6VQ
Evaluation B

$C_8H_{14}O_4$ (c) 70MUR/BRE2
Tetramethylsuccinic acid
Phase Changes
c,II/c,I 383 K, ΔH=13432 J·mol^{-1}
ΔS=35.27 J·mol^{-1}·K^{-1}
c,I/liq 464 K, ΔH=6472 J·mol^{-1}
ΔS=13.97 J·mol^{-1}·K^{-1}
Molecular Weight 174.1962
Wiswesser Line Notation QVX1&1&X1&1&VQ
Evaluation A

$C_8H_{15}N$ (c) 63BAR/WES
3-Azabicyclo[3.2.2]nonane
Heat Capacity 310 K, C_p=239.03 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K. Transition too close to 298.15 K to allow meaningful value of C_p.
Entropy 310 K, S=245.73 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 297.78 K, ΔH=14481 J·mol^{-1}
ΔS=48.63 J·mol^{-1}·K^{-1}
Molecular Weight 125.2132
Wiswesser Line Notation T67 A B HMTJ
Evaluation A

$C_8H_{15}N$ (c) 64WUL/WES
3-Azabicyclo[3.2.2]nonane
Heat Capacity 350 K, C_p=237.8 J·mol^{-1}·K^{-1}
Temperature range 330 to 490 K.
Phase Changes
c,I/liq 467.12 K, ΔH=6916 J·mol^{-1}
ΔS=14.81 J·mol^{-1}·K^{-1}
Molecular Weight 125.2132
Wiswesser Line Notation T67 A B HMTJ
Evaluation A

$C_8H_{15}NO_2$ (liq) 85KAR/ABD2
Dimethylaminoethyl methacrylate
Phase Changes
c/liq 237.7 K, ΔH=16852 J·mol^{-1}
ΔS=70.90 J·mol^{-1}·K^{-1}
Molecular Weight 157.2120
Wiswesser Line Notation 1UY1&VO2N1&1
Evaluation A

$C_8H_{15}O_2Tl$ (c) 76MEI/SEY
Thallium octanoate
Phase Changes
liq/liq 494 K, ΔH=2720 J·mol^{-1}
ΔS=5.44 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
c,I/liq 403 K, ΔH=4686 J·mol^{-1}
ΔS=11.7 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 347.5753
Wiswesser Line Notation OV7 .TL
Evaluation B

$C_8H_{15}O_2Tl$ (c) 89ROU/TUR
Thallium octanoate
Heat Capacity 305 K, C_p=294 J·mol^{-1}·K^{-1}
Temperature range 305 to 490 K.
Phase Changes
c,IV/c,III 268.7 K, ΔH=166 J·mol^{-1}
ΔS=0.58 J·mol^{-1}·K^{-1}
c,III/c,II 289.8 K, ΔH=3783 J·mol^{-1}
ΔS=13.05 J·mol^{-1}·K^{-1}
c,II/c,I 294.3 K, ΔH=2162 J·mol^{-1}
ΔS=7.32 J·mol^{-1}·K^{-1}
c,I/liq 411.0 K, ΔH=5670 J·mol^{-1}
ΔS=13.80 J·mol^{-1}·K^{-1}
Solid-mesophase.
liq/liq 494.7 K, ΔH=2993 J·mol^{-1}
ΔS=6.07 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
Molecular Weight 347.5753
Wiswesser Line Notation OV7 .TL
Evaluation A

C_8H_{16} (liq) 36PAR/TOD2
2,4,4-Trimethyl-1-pentene
Heat Capacity 296.0 K, C_p=235.35 J·mol^{-1}·K^{-1}
Temperature range 81 to 296 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=306.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 59.75 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 178.9 K, ΔH=8765 J·mol^{-1}
ΔS=48.99 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation 1X1&1&1Y1&U1
Evaluation B(C_p),C(S)
Low boiling isomer.

C_8H_{16} (liq) 36PAR/TOD2
2,4,4-Trimethyl-1-pentene
Heat Capacity 298.6 K, C_p=240.20 J·mol^{-1}·K^{-1}
Temperature range 81 to 296 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=311.7 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 62.51 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 166 K, ΔH=6795 J·mol^{-1}
ΔS=40.9 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation 1X1&1&1Y1&U1
Evaluation B(C_p),C(S)
High boiling isomer.

C_8H_{16} (liq) 30PAR/HUF2
2,4,4-Trimethyl-2-pentene
Heat Capacity 296.0 K, C_p=233.5 J·mol^{-1}·K^{-1}
Temperature range 92 to 296 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=298.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 63.76 J·mol^{-1}·K^{-1}.
Molecular Weight 112.2144
Wiswesser Line Notation 1X1&1&1UY1&1
Evaluation B(C_p),C(S)

C_8H_{16} (liq) 1881REI
2-Octene
Heat Capacity 298 K, C_p=239.3 J·mol^{-1}·K^{-1}
Temperature range 291 to 365 K.
Molecular Weight 112.2144
Wiswesser Line Notation 6U2
Evaluation D
Uncertain isomeric structure.

C_8H_{16} (liq) 57MCC/FIN2
1-Octene
Heat Capacity 298.15 K, C_p=241.21 J·mol^{-1}·K^{-1}
Temperature range 11 to 360 K.
Entropy 298.15 K, S=360.45 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 171.46 K, ΔH=15313 J·mol^{-1}
ΔS=89.31 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation 7U1
Evaluation A

C_8H_{16} (liq) 65MES/TOD2
n-Propylcyclopentane
Heat Capacity 298.15 K, C_p=216.27 J·mol^{-1}·K^{-1}
Temperature range 12 to 370 K.
Entropy 298.15 K, S=310.83 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 155.79 K, ΔH=10033 J·mol^{-1}
ΔS=64.44 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation L5TJ A3
Evaluation A

C_8H_{16} (liq) 49HUF/TOD
1,1-Dimethylcyclohexane
Heat Capacity 298.15 K, C_p=209.24 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=267.23 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 153.15 K, ΔH=5984.4 J·mol^{-1}
ΔS=39.00 J·mol^{-1}·K^{-1}
c,I/liq 239.81 K, ΔH=2025 J·mol^{-1}
ΔS=8.44 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation L6TJ A1 A1
Evaluation A

C_8H_{16} (liq) 89VOS/SLO
1,2-Dimethylcyclohexane
Heat Capacity 325.2 K, C_p=173.9 J·mol^{-1}·K^{-1}
Temperature range 325.2 to 461.2 K. Unsmoothed experimental datum.
Molecular Weight 112.2144
Wiswesser Line Notation L6TJ A1 B1
Evaluation C

C_8H_{16} (liq) 49HUF/TOD
1-trans-2-Dimethylcyclohexane
Heat Capacity 298.15 K, C_p=209.41 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=273.22 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 184.99 K, ΔH=10491.8 J·mol^{-1}
ΔS=56.72 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation L6TJ A1 B1 -A&A -B&B
Evaluation A

C_8H_{16} (liq) 49HUF/TOD
1-cis-2-Dimethylcyclohexane
Heat Capacity 298.15 K, C_p=210.20 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=274.14 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 172.5 K, ΔH=8256.7 J·mol^{-1}
ΔS=47.86 J·mol^{-1}·K^{-1}
c,I/liq 223.28 K, ΔH=1645.1 J·mol^{-1}
ΔS=7.37 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation L6TJ A1 B1 -A&AB
Evaluation A

C_8H_{16} (liq) 49HUF/TOD
1-trans-3-Dimethylcyclohexane
Heat Capacity 298.15 K, C_p=212.84 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=276.27 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 183.06 K, ΔH=9865.9 J·mol^{-1}
ΔS=53.89 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation L6TJ A1 C1 -A&A -B&C
Evaluation A

C_8H_{16} (liq) 49HUF/TOD
1-cis-3-Dimethylcyclohexane
Heat Capacity 298.15 K, C_p=209.37 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=272.63 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 197.59 K, ΔH=10820.2 J·mol^{-1}
ΔS=54.77 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation L6TJ A1 C1 -A&AC
Evaluation A

C_8H_{16} (liq) 49HUF/TOD
1-trans-4-Dimethylcyclohexane
Heat Capacity 298.15 K, C_p=210.25 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=268.03 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 236.22 K, ΔH=12331.1 J·mol^{-1}
ΔS=52.21 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation L6TJ A1 D1 -A&A -B&D
Evaluation A

C_8H_{16} (liq) 49HUF/TOD
1-cis-4-Dimethylcyclohexane
Heat Capacity 298.15 K, C_p=212.09 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=271.12 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 185.73 K, ΔH=9306.9 J·mol^{-1}
ΔS=50.11 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation L6TJ A1 D1 -A&AD
Evaluation A

C_8H_{16} (liq) 49HUF/TOD
Ethylcyclohexane
Heat Capacity 298.15 K, C_p=211.79 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K. S=280.91 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 161.84 K, ΔH=8333.3 J·mol^{-1}
ΔS=51.49 J·mol^{-1}·K^{-1}
Molecular Weight 122.2144
Wiswesser Line Notation L6TJ A2
Evaluation A

C_8H_{16} (liq) 49PAR/MOO
Ethylcyclohexane
Heat Capacity 298.15 K, C_p=214.2 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.15 K, S=281.6 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 57.74 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 161.4 K, ΔH=8276 J·mol^{-1}
ΔS=51.3 J·mol^{-1}·K^{-1}
Molecular Weight 122.2144
Wiswesser Line Notation L6TJ A2
Evaluation B(C_p),C(S)

C_8H_{16} (liq) 56FIN/SCO
Cyclooctane
Heat Capacity 298.15 K, C_p=215.48 J·mol^{-1}·K^{-1}
Temperature range 12 to 330 K.
Entropy 298.15 K, S=262.00 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 166.5 K, ΔH=6305.7 J·mol^{-1}
ΔS=37.87 J·mol^{-1}·K^{-1}
c,II/c,I 183.8 K, ΔH=478.2 J·mol^{-1}
ΔS=2.60 J·mol^{-1}·K^{-1}
c,I/liq 287.98 K, ΔH=2409.6 J·mol^{-1}
ΔS=8.37 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation L8TJ
Evaluation A

C_8H_{16} (liq) 75JOL/BOI
Cyclooctane
Heat Capacity 298.15 K, C_p=214.24 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 112.2144
Wiswesser Line Notation L8TJ
Evaluation B

C_8H_{16} (liq) 79FOR/DAR
Cyclooctane
Heat Capacity 298.15 K, C_p=215.461 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 112.2144
Wiswesser Line Notation L8TJ
Evaluation B

C_8H_{16} (liq) 79WIL/FAR
Cyclooctane
Heat Capacity 298.15 K, C_p=214.53 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 112.2144
Wiswesser Line Notation L8TJ
Evaluation B

C_8H_{16} (liq) 85TAN
Cyclooctane
Heat Capacity 298.15 K, C_p=215.53 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 112.2144
Wiswesser Line Notation L8TJ
Evaluation A

C_8H_{16} (liq) 88SHI/OGA2
Cyclooctane
Heat Capacity 298.15 K, C_p=215.78 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 112.2144
Wiswesser Line Notation L8TJ
Evaluation A

$C_8H_{16}N_2O_2$ (c) 91ABA/DEL
N-Acetylvaline-N′-methylamide(DL); 2-(Acetylamino)-N, 3-dimethylbutanamide(DL)
Heat Capacity 298 K, C_p=259.16 J·mol^{-1}·K^{-1}
Data extrapolated to 298. K from values obtained at higher temperatures.
Molecular Weight 172.2266
Wiswesser Line Notation 1VMYY1&1&VM1 -DL
Evaluation C

$C_8H_{16}N_2O_2$ (c) 91ABA/DEL
N-Acetylvaline-N′-methylamide(L);
2-(Acetylamino)-N,3-dimethylbutanamide(L)
Heat Capacity 298 K, C_p=245.92 J·mol^{-1}·K^{-1}
Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 172.2266
Wiswesser Line Notation 1VMYY1&1&VM1 -L
Evaluation C

$C_8H_{16}N_2O_2$ (c) 91ABA/DEL
N-Acetylnorvaline-N′-methylamide(DL); 2-(Acetylamino)-N-methylpentanamide(DL)
Heat Capacity 298 K, C_p=239.69 J·mol^{-1}·K^{-1}
Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 172.2266
Wiswesser Line Notation 3XVM1&MV1 -DL
Evaluation C

$C_8H_{16}N_2O_2$ (c) 88FER/DEL
N-Acetyl-D-leucine amide
Phase Changes
c/liq 404.0 K, $\Delta H = 20200\ J\cdot mol^{-1}$
$\Delta S = 50.0\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 172.2266
Wiswesser Line Notation ZVY4&MV1
Evaluation A

$C_8H_{16}N_2O_3$ (c) 41HUF
Leucylglycine(DL)
Heat Capacity 297.1 K, $C_p = 255.64\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 86 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, $S = 281.2\ J\cdot mol^{-1}\cdot K^{-1}$
Extrapolation below 90 K, $82.47\ J\cdot mol^{-1}\cdot K^{-1}$.
Molecular Weight 188.2260
Wiswesser Line Notation QV1MVYZ1Y1&1-DL
Evaluation A(C_p),C(S)

$C_8H_{16}N_2O_3$ (c) 89KUL/KOZ
α-Alanylvaline(DL)
Heat Capacity 298 K, $C_p = 240.0\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 298 to 348 K.
Molecular Weight 188.2260
Wiswesser Line Notation ZY1&VMYVQY1&1
Evaluation C

$C_8H_{16}N_2O_3$ (c) 90BAD/KUL
Alanylvaline(DL)
Heat Capacity 298 K, $C_p = 240\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 298, 313, 333, 348 K.
Molecular Weight 188.2260
Wiswesser Line Notation ZY1&VMY&Y1&1&VQ -DL
Evaluation D

$C_8H_{16}O$ (liq) 1881REI
2-Octanone; Methyl hexyl ketone
Heat Capacity 298 K, $C_p = 274.5\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 291 to 463 K.
Molecular Weight 128.2138
Wiswesser Line Notation 6V1
Evaluation D

$C_8H_{16}O$ (liq) 65OET
2-Octanone; Methyl hexyl ketone
Heat Capacity 298.15 K, $C_p = 273.26\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 13 to 330 K.
Entropy 298.15 K, $S = 373.84\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 252.86 K, $\Delta H = 24419\ J\cdot mol^{-1}$
$\Delta S = 96.57\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 128.2138
Wiswesser Line Notation 6V1
Evaluation A

$C_8H_{16}O$ (liq) 80DYA/VA
Octanal; Caprylaldehyde
Heat Capacity
Temperature range 50 to 350 K.
Phase Changes
c,l/liq 247.72 K, $\Delta H = 25860\ J\cdot mol^{-1}$
$\Delta S = 104.4\ J\cdot mol^{-1}\cdot K^{-1}$
98.01 mol% purity.
Molecular Weight 128.2138
Wiswesser Line Notation VH7
Evaluation B
Manuscript deposited in Cent. Sci. Res. Inst. Tech. En; Petrochemicals, July 27, 1979.

$C_8H_{16}O$ (liq) 82DYA/VA
Octanal; Caprylaldehyde
Entropy 298.15 K, $S = 365.4\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq $\Delta H = 26130\ J\cdot mol^{-1}$
Molecular Weight 128.2138
Wiswesser Line Notation VH7
Evaluation B

$C_8H_{16}O$ (liq) 84VAS/PE
Octanal; Caprylaldehyde
Heat Capacity 298.15 K, $C_p = 259.58\ J\cdot mol^{-1}\cdot K^{-}$
Temperature range 10 to 350 K.
Entropy 298.15 K, $S = 365.45\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 247.72 K
Molecular Weight 128.2138
Wiswesser Line Notation VH7
Evaluation A

$C_8H_{16}O_2$ (liq) 84GUS/SH
Isoamyl propionate
Heat Capacity 298.15 K, $C_p = 285.2\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 205 to 348 K. Unsmoothed experiment datum. Interpolated to 298.15 K.
Molecular Weight 144.2132
Wiswesser Line Notation 2VO2Y
Evaluation C

$C_8H_{16}O_2$ (liq) 84VAS/PE
Butyl butanoate
Heat Capacity 300 K, $C_p = 281.9\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 180 to 370 K.
Phase Changes
c/liq 181.68 K, $\Delta H = 14930\ J\cdot mol^{-1}$
$\Delta S = 82.2\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 144.2132
Wiswesser Line Notation 4OV3
Evaluation A

$C_8H_{16}O_2$ (liq) 83GUS/KI
Amyl propionate; Pentyl propionate
Heat Capacity 277.11 K, $C_p = 239.5\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 200 to 360 K. Unsmoothed experiment datum. C_p given as $1.661\ J\cdot g^{-1}\cdot K^{-1}$.
Molecular Weight 144.2132
Wiswesser Line Notation 5OV2
Evaluation B

$C_8H_{16}O_2$ (liq) 84GUS/SHU
Amyl propionate; Pentyl propionate
Heat Capacity 298.15 K, C_p=245.2 J·mol^{-1}·K^{-1}
Temperature range 205 to 348 K. Unsmoothed experimental datum. Interpolated to 298.15 K.
Molecular Weight 144.2132
Wiswesser Line Notation 5OV2
Evaluation C

$C_8H_{16}O_2$ (liq) 84VAS/PET
Hexyl ethanoate
Heat Capacity 300 K, C_p=282.8 J·mol^{-1}·K^{-1}
Temperature range 210 to 370 K.
Phase Changes
c/liq 212.10 K, ΔH=19830 J·mol^{-1}
ΔS=93.5 J·mol^{-1}·K^{-1}
Molecular Weight 144.2132
Wiswesser Line Notation 6OV1
Evaluation A

$C_8H_{16}O_2$ (liq) 79FUC
Methyl heptanoate; Methyl oenanthoate; Methyl enanthoate
Heat Capacity 298.15 K, C_p=285.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 144.2132
Wiswesser Line Notation 6VO1
Evaluation B

$C_8H_{16}O_2$ (liq) 24GAR/RAN
Octanoic acid; Caprylic acid
Heat Capacity 305 K, C_p=304.6 J·mol^{-1}·K^{-1}
Temperature range 0 to 46 °C. Mean value 18 to 46 °C.
Phase Changes
c/liq 289.5 K, ΔH=21380 J·mol^{-1}
ΔS=73.9 J·mol^{-1}·K^{-1}
Molecular Weight 144.2132
Wiswesser Line Notation QV7
Evaluation B

$C_8H_{16}O_2$ (liq) 82SCH/MIL2
Octanoic acid; Caprylic acid
Heat Capacity 298.15 K, C_p=297.92 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Phase Changes
c,I/liq 289.66 K, ΔH=21350 J·mol^{-1}
ΔS=73.71 J·mol^{-1}·K^{-1}
Molecular Weight 144.2132
Wiswesser Line Notation QV7
Evaluation B

$C_8H_{17}Cl$ (liq) 93SHE
1-Chlorooctane; n-Octyl chloride
Heat Capacity 298.15 K, C_p=274.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 148.6753
Wiswesser Line Notation G8
Evaluation B

$C_8H_{17}NO_2$ (c) 83SKO/SAB
8-Aminooctanoic acid
Heat Capacity 298 K, C_p=251.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 159.2278
Wiswesser Line Notation Z7VQ
Evaluation B

C_8H_{18} (c) 30PAR/HUF
2,2,3,3-Tetramethylbutane
Heat Capacity 295.4 K, C_p=232.2 J·mol^{-1}·K^{-1}
Temperature range 89 to 295 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=256.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 64.68 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 148.1 K, ΔH=2008 J·mol^{-1}
ΔS=13.56 J·mol^{-1}·K^{-1}
Molecular Weight 114.2302
Wiswesser Line Notation 1X1&1&X1&1&1
Evaluation B(C_p),C(S)

C_8H_{18} (c) 52SCO/DOU
2,2,3,3-Tetramethylbutane
Heat Capacity 301.60 K, C_p=239.62 J·mol^{-1}·K^{-1}
Temperature range 12 to 374 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=273.76 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 152.5 K, ΔH=2000 J·mol^{-1}
ΔS=13.11 J·mol^{-1}·K^{-1}
c,I/liq 373.9 K, ΔH=7540 J·mol^{-1}
ΔS=20.17 J·mol^{-1}·K^{-1}
Molecular Weight 114.2302
Wiswesser Line Notation 1X1&1&X1&1&1
Evaluation A

C_8H_{18} (liq) 30PAR/HUF
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 295.2 K, C_p=233.9 J·mol^{-1}·K^{-1}
Temperature range 88 to 295 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=314.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 66.53 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 165.3 K, ΔH=9042 J·mol^{-1}
ΔS=54.70 J·mol^{-1}·K^{-1}
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation B(C_p),C(S)

C_8H_{18} (liq) 40PIT
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 301.9 K, C_p=241.00 J·mol^{-1}·K^{-1}
Temperature range 15 to 318 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=328.03 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 165.79 K, ΔH=9211.5 J·mol^{-1}
ΔS=55.56 J·mol^{-1}·K^{-1}
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation A

C_8H_{18} (liq) 47OSB/GIN
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p=238.57 J·mol^{-1}·K^{-1}
Temperature range 283 to 318 K.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation A

C_8H_{18} (liq) 50AUE/SAG
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 300 K, C_p=233.7 J·mol^{-1}·K^{-1}
Temperature range 300 to 366 K. C_p given as 0.4980 Btu(lb)$^{-1}$ (°R)$^{-1}$ at 80 °F.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation B

C_8H_{18} (liq) 73SUB/RAS
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p=237.8 J·mol^{-1}·K^{-1}
Temperature range 298 to 323 K.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation B

C_8H_{18} (liq) 74RAJ/SUB
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p=237.8 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 323.15 K.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation B

C_8H_{18} (liq) 76FOR/BEN2
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p=238.871 J·mol^{-1}·K^{-1}
Average of three values.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation A

C_8H_{18} (liq) 87KAL/KOH
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 293.15 K, C_p=237.85 J·mol^{-1}·K^{-1}
Temperature range 293.15, 313.15 K.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation B

C_8H_{18} (liq) 88COS/HUU
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p=242.49 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation B

C_8H_{18} (liq) 88PER/AIC
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p=242.49 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation A

C_8H_{18} (liq) 88SHI/OGA
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p=239.71 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation A

C_8H_{18} (liq) 47OSB/GIN
2,5-Dimethylhexane
Heat Capacity 298.15 K, C_p=249.20 J·mol^{-1}·K^{-1}
Temperature range 278 to 318 K.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&2Y1&1
Evaluation A

C_8H_{18} (liq) 41PIT/SCC
2,3,4-Trimethylpentane
Heat Capacity 293.79 K, C_p=246.23 J·mol^{-1}·K^{-1}
Temperature range 14 to 325 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=329.32 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 163.63 K, ΔH=9268 J·mol^{-1}
ΔS=56.64 J·mol^{-1}·K^{-1}
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&Y1&Y1&1
Evaluation B

C_8H_{18} (liq) 47OSB/GIN
2,3,4-Trimethylpentane
Heat Capacity 298.15 K, C_p=247.32 J·mol^{-1}·K^{-1}
Temperature range 278 to 318 K.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&Y1&Y1&1
Evaluation A

C_8H_{18} (liq) 47OSB/GIN
2,3,3-Trimethylpentane
Heat Capacity 298.15 K, C_p=245.56 J·mol^{-1}·K^{-1}
Temperature range 278 to 318 K.
Molecular Weight 114.2302
Wiswesser Line Notation 2X1&1&Y1&1
Evaluation A

C_8H_{18} (liq) 47OSB/GIN
3,3-Dimethylhexane
Heat Capacity 298.15 K, C_p=246.60 J·mol^{-1}·K^{-1}
Temperature range 278 to 318 K.
Molecular Weight 114.2302
Wiswesser Line Notation 3X2&1&1
Evaluation A

C_8H_{18} (liq) 47OSB/GIN
4-Methylheptane
Heat Capacity 298.15 K, C_p=251.08 J·mol^{-1}·K^{-1}
Temperature range 278 to 318 K.
Molecular Weight 114.2302
Wiswesser Line Notation 3Y3&1
Evaluation A

C_8H_{18} (liq) 47OSB/GIN
3-Methylheptane
Heat Capacity 298.15 K, C_p=249.66 J·mol^{-1}·K^{-1}
Temperature range 293 to 318 K.
Molecular Weight 114.2302
Wiswesser Line Notation 4Y2&1
Evaluation A

C_8H_{18} (liq) 73FIN/MES
3-Methylheptane
Heat Capacity 298.15 K, C_p=250.20 J·mol^{-1}·K^{-1}
Temperature range 10 to 380 K.
Entropy 298.15 K, S=362.6 J·mol^{-1}·K^{-1}
Thermodynamic properties calculated from a Debye function at 10 K.
Phase Changes
c,l/liq 152.6574 K, ΔH=11694 J·mol^{-1}
ΔS=7.665 J·mol^{-1}·K^{-1}
Molecular Weight 114.2302
Wiswesser Line Notation 4Y2&1
Evaluation A

C_8H_{18} (liq) 47OSB/GIN
2-Methylheptane
Heat Capacity 298.15 K, C_p=251.58 J·mol^{-1}·K^{-1}
Temperature range 283 to 318 K.
Molecular Weight 114.2302
Wiswesser Line Notation 5Y1&1
Evaluation A

C_8H_{18} (liq) 71MES/FIN
2-Methylheptane
Heat Capacity 298.15 K, C_p=252.00 J·mol^{-1}·K^{-1}
Temperature range 11 to 370 K.
Entropy 298.15 K, S=356.39 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 64.19 K, ΔH=11920 J·mol^{-1}
ΔS=72.60 J·mol^{-1}·K^{-1}
Molecular Weight 114.2302
Wiswesser Line Notation 5Y1&1
Evaluation A

C_8H_{18} (liq) 30PAR/HUF
n-Octane
Heat Capacity 293.7 K, C_p=247.7 J·mol^{-1}·K^{-1}
Temperature range 85 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=359.8 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 77.19 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 215.6 K, ΔH=20092 J·mol^{-1}
ΔS=93.19 J·mol^{-1}·K^{-1}
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B(C_p),C(S)

C_8H_{18} (liq) 31HUF/PAR
n-Octane
Heat Capacity 298.3 K, C_p=251.5 J·mol^{-1}·K^{-1}
Temperature range 92 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=359.8 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 75.73 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 215.8 K, ΔH=20652 J·mol^{-1}
ΔS=95.7 J·mol^{-1}·K^{-1}
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B(C_p),C(S)

C_8H_{18} (liq) 47OSB/GIN
n-Octane
Heat Capacity 298.15 K, C_p=253.89 J·mol^{-1}·K^{-1}
Temperature range 293 to 318 K.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation A

C_8H_{18} (liq) 51CON/SAG
n-Octane
Heat Capacity 299.8 K, C_p=253.93 J·mol^{-1}·K^{-1}
Temperature range 80 to 200 °F.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 54FIN/GRO2
n-Octane
Heat Capacity 298.15 K, C_p=254.14 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=361.20 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 216.38 K, ΔH=20740 J·mol^{-1}
ΔS=95.85 J·mol^{-1}·K^{-1}
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation A

C_8H_{18} (liq) 75GRI/RAS
n-Octane
Heat Capacity 298 K, C_p=253.2 J·mol^{-1}·K^{-1}
Temperature range 305 to 463 K.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 80SHA/LYU
n-Octane
Heat Capacity 298.15 K, C_p=252.92 J·mol^{-1}·K^{-1}
Temperature range 65 to 300 K.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation A

C_8H_{18} (liq) 81GRO/ING
n-Octane
Heat Capacity 298.15 K, C_p=254.07 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 82ZAR
n-Octane
Heat Capacity 298 K, C_p=252.4 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 84GRI/AND
n-Octane
Heat Capacity 297.54 K, C_p=252.4 J·mol^{-1}·K^{-1}
Temperature range 297 to 410 K. Unsmoothed experimental datum given as 2.210 KJ/kg·K.
Molecular Weight 114.2303
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 84ROU/GRO
n-Octane
Heat Capacity 298.15 K, C_p=254.02 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 85LAI/GRO
n-Octane
Heat Capacity 298.15 K, C_p=254.18 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 85LAI/ROD
n-Octane
Heat Capacity 298.15 K, C_p=253.72 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 86BEN/DAR3
n-Octane
Heat Capacity 298.15 K. C_p=254.11 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 86TAR/AIC
n-Octane
Heat Capacity 298.15 K, C_p=255.68 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 88AND/PAT
n-Octane
Heat Capacity 298.15 K, C_p=255.68 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 88PER/AIC
n-Octane
Heat Capacity 298.15 K, C_p=255.68 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation A

C_8H_{18} (liq) 91BAN/GAR
n-Octane
Heat Capacity 318.15 K, C_p=262.20 J·mol^{-1}·K^{-1}
Temperature range 318 to 373 K. p=0.1 MPa.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 91TRE/COS
n-Octane
Heat Capacity 298.15 K, C_p=255.68 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 93CZA
n-Octane
Heat Capacity 299 K, C_p=254.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

$(C_8H_{14})_n$ (amorph) 92GRE
Poly(vinyl cyclohexane)
Phase Changes
c/liq 678 K, ΔH=5600 J·mol^{-1}
Molecular Weight 110.1986
Wiswesser Line Notation /*1YR&*/
Evaluation A
T(glass)=353 K.

$C_8H_{18}N_2$ (c) 80BYS
1,1-Dimethylazoethane
Phase Changes
c,II/c,I 242.6 K, $\Delta H = 4890\ J\cdot mol^{-1}$
$\Delta S = 20.2\ J\cdot mol^{-1}\cdot K^{-1}$
c,I/liq 258.6 K, $\Delta H = 10280\ J\cdot mol^{-1}$
$\Delta S = 39.7\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 142.2443
Wiswesser Line Notation *1X1&1&NUNX1&1&1*
Evaluation A

$C_8H_{18}N_2O$ (c) 80BYS
1,1-Dimethylazoxyethane
Phase Changes
c,II/c,I 268.0 K, $\Delta H = 8340\ J\cdot mol^{-1}$
$\Delta S = 31.1\ J\cdot mol^{-1}\cdot K^{-1}$
c,I/liq 288.4 K, $\Delta H = 11520\ J\cdot mol^{-1}$
$\Delta S = 39.9\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 158.2437
Wiswesser Line Notation 1X1&1&NO&UNX1&1&1
Evaluation A

$C_8H_{18}N_2O$ (c) 81BYS
Di-tert-butyldiazene-N-oxide
Heat Capacity 298.15 K, $C_p = 316.3\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 290 to 310 K.
Phase Changes
c,I/liq 288.4 K
liq/g 298.15 K, $\Delta H = 51702\ J\cdot mol^{-1}$
$\Delta S = 173.4\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 158.2437
Wiswesser Line Notation 1X1&1&NO&UNX1&1&1
Evaluation A

$C_8H_{18}N_2O_2$ (c) 84LEB/GUT
Bis-hydroxyethylpiperazine
Heat Capacity 298 K, $C_p = 250.68\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 293 to 311 K.
Phase Changes
c/liq 405 K, $\Delta H = 25900\ J\cdot mol^{-1}$
$\Delta S = 64.0\ J\cdot mol^{-1}\cdot K^{-1}$
liq/g 551 K
Molecular Weight 174.2424
Wiswesser Line Notation T6N DNTJ A2Q D2Q
Evaluation B
$\Delta\Delta H$ sublimation $= 104100\ J\cdot mol^{-1}$, temperature range = 334 to 356 K.

$C_8H_{18}O$ (liq) 75FEN/HAR
Di-tert-butyl ether; 2,2,4,4-Tetramethyl-3-oxapentane
Heat Capacity 298.15 K, $C_p = 276.1\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 130.2296
Wiswesser Line Notation 1X1&1&OX1&1&1
Evaluation B

$C_8H_{18}O$ (liq) 87COB/CAS
Di-n-butyl ether
Heat Capacity 298.15 K, $C_p = 278.16\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature. Average of two measurements.
Molecular Weight 130.2296
Wiswesser Line Notation 4O4
Evaluation B

$C_8H_{18}O$ (liq) 87BUS/MAS
2-Ethylhexanol
Heat Capacity 298.15 K, $C_p = 317.5\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 13 to 350 K.
Entropy 298.15 K, $S = 347.0\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 130.2296
Wiswesser Line Notation Q1Y4&2
Evaluation A

$C_8H_{18}O$ (liq) 31CLI/AND
2-Methyl-1-heptanol
Heat Capacity 298.5 K, $C_p = 313.0\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 102 to 311 K. Value is unsmoothed experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation Q1Y5&1
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/AND
5-Methyl-1-heptanol
Heat Capacity 298.5 K, $C_p = 304.2\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 102 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation Q4Y2&1
Evaluation C

$C_8H_{18}O$ (liq) 78RYB/EME
6-Methyl-1-heptanol; Isooctyl alcohol
Heat Capacity 303.15 K, $C_p = 327.8\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 293.15 to 353.15 K. C_p given as 2517 $J\cdot kg^{-1}\cdot K^{-1}$.
Molecular Weight 130.2296
Wiswesser Line Notation Q5Y1&1
Evaluation C

$C_8H_{18}O$ (liq) 1881REI
1-Octanol; n-Octyl alcohol; Capryl alcohol
Heat Capacity 298 K, $C_p = 324.3\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 291 to 470 K.
Molecular Weight 130.2296
Wiswesser Line Notation Q8
Evaluation D

$C_8H_{18}O$ (liq) 31CLI/AND
1-Octanol; n-Octyl alcohol; Capryl alcohol
Heat Capacity 286.0 K, $C_p = 284.5\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 102 to 286 K. Value is unsmoothed experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation Q8
Evaluation C

$C_8H_{18}O$ (liq) 59HUT/BAI
1-Octanol; n-Octyl alcohol; Capryl alcohol
Heat Capacity 298 K, $C_p = 312.1\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 130.2296
Wiswesser Line Notation Q8
Evaluation C

$C_8H_{18}O$ (liq) 79GRI/YAN
1-Octanol; n-Octyl alcohol; Capryl alcohol
Heat Capacity 310.67 K, C_p=318.3 J·mol^{-1}·K^{-1}
Temperature range 310 to 452 K. p=0.98 bar.
Molecular Weight 130.2296
Wiswesser Line Notation Q8
Evaluation B

$C_8H_{18}O$ (liq) 84ZEG/SOM
1-Octanol; n-Octyl alcohol; Capryl alcohol
Heat Capacity 298.15 K, C_p=305.55 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.2296
Wiswesser Line Notation Q8
Evaluation C

$C_8H_{18}O$ (liq) 86NAZ/BAS2
1-Octanol; n-Octyl alcohol; Capryl alcohol
Heat Capacity 303.2 K, C_p=329.5 J·mol^{-1}·K^{-1}
Temperature range 303.2 to 448 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.53 kJ/kg·K.
Molecular Weight 130.2296
Wiswesser Line Notation Q8
Evaluation B

$C_8H_{18}O$ (liq) 89VES/BAR
1-Octanol; n-Octyl alcohol; Capryl alcohol
Heat Capacity 298.15 K, C_p=304.0 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K.
Molecular Weight 130.2296
Wiswesser Line Notation Q8
Evaluation A

$C_8H_{18}O$ (liq) 31CLI/AND
4-Methyl-4-heptanol
Heat Capacity 298.5 K, C_p=367.4 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QX3&3&1
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/AND
2-Methyl-2-heptanol
Heat Capacity 298.5 K, C_p=337.6 J·mol^{-1}·K^{-1}
Temperature range 102 to 311 K. Value is unsmoothed experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QX5&1&1
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/AND
4-Methyl-2-heptanol
Heat Capacity 298.5 K, C_p=312.5 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QY1&1Y3&1
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/ANI
5-Methyl-2-heptanol
Heat Capacity 298.5 K, C_p=296.2 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothe experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QY1&2Y2&1
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/ANI
6-Methyl-2-heptanol
Heat Capacity 298.5 K, C_p=315.1 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothe experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QY1&3Y1&1
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/ANI
3-Methyl-2-heptanol
Heat Capacity 298.5 K, C_p=297.5 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothe experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QY1&Y4&1
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/ANI
6-Methyl-3-heptanol
Heat Capacity 298.5 K, C_p=310.5 J·mol^{-1}·K^{-1}
Temperature range 102 to 323 K. Value is unsmoothe experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QY2&2Y1&1
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/ANI
4-Methyl-3-heptanol
Heat Capacity 298.5 K, C_p=309.2 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothe experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QY2&Y3&1
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/ANI
2-Methyl-4-heptanol
Heat Capacity 298.5 K, C_p=331.8 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothe experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QY3&1Y1&1
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/ANI
4-Octanol
Heat Capacity 298.5 K, C_p=337.6 J·mol^{-1}·K^{-1}
Temperature range 102 to 311 K. Value is unsmoothe experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QY4&3
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/AND
3-Octanol
Heat Capacity 298.5 K, C_p=338.5 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QY5&2
Evaluation C

$C_8H_{18}O$ (liq) 31CLI/AND
2-Octanol
Heat Capacity 298.5 K, C_p=330.1 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 130.2296
Wiswesser Line Notation QY6&1
Evaluation C

$C_8H_{18}O_2$ (liq) 93GIM/AUD
Di-tert-butyl peroxide
Heat Capacity
Temperature range 293 to 353 K. C_p(liq)−1.20+2.77e^{-3}T(K) J/K·g (20 to 80 °C).
Molecular Weight 146.2290
Wiswesser Line Notation 1X1&1&OO1X1&1
Evaluation B

$C_8H_{18}O_2$ (liq) 73KUS/SUU
4,7-Dioxadecane; 1,2-Di-n-propoxyethane
Heat Capacity 298.15 K, C_p=309.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 146.2290
Wiswesser Line Notation 3O2O3
Evaluation B

$C_8H_{18}O_3$ (liq) 78ROU/PER2
3,6,9-Trioxaundecane; Bis(2-ethoxyethyl) ether
Heat Capacity 298.1 K, C_p=347.5 J·mol^{-1}·K^{-1}
Temperature range 283 to 313 K.
Molecular Weight 162.2284
Wiswesser Line Notation 2O2O2O2
Evaluation B

$C_8H_{18}O_3$ (liq) 87COB/CAS
2-(2-Butoxyethoxy)ethanol
Heat Capacity 298.15 K, C_p=354.89 J·mol^{-1}·K^{-1}
One temperature. Average of two measurements.
Molecular Weight 162.2284
Wiswesser Line Notation Q2O2O4
Evaluation B

$C_8H_{18}O_4$ (liq) 66BEA/CLE
2,5,8,11-Tetraoxadodecane; Triglyme
Heat Capacity 298.15 K, C_p=368.2 J·mol^{-1}·K^{-1}
Temperature range 90 to 350 K.
Entropy 298.15 K, S=492.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K. 103.8 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 229.3 K, ΔH=23715 J·mol^{-1}
ΔS=103.4 J·mol^{-1}·K^{-1}
Molecular Weight 178.2278
Wiswesser Line Notation 1O2O2O2O1
Evaluation A(C_p),C(S)

$C_8H_{18}O_4$ (liq) 91TRE/COS
2,5,8,11-Tetraoxadodecane; Triglyme
Heat Capacity 298.15 K, C_p=367.78 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 178.2278
Wiswesser Line Notation 1O2O2O2O1
Evaluation B

$C_8H_{18}O_5$ (liq) 79STE/TAM
Tetraethylene glycol; 1,11-Dihydroxy-3,6,9-trioxaundecane
Heat Capacity 298 K, C_p=419.2 J·mol^{-1}·K^{-1}
Temperature range 273 to 533 K.
Molecular Weight 194.2272
Wiswesser Line Notation Q2O2O2O2Q
Evaluation B

$C_8H_{18}O_5$ (liq) 82ZAR
Tetraethylene glycol; 1,11-Dihydroxy-3,6,9-trioxaundecane
Heat Capacity 298 K, C_p=428.8 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 194.2272
Wiswesser Line Notation Q2O2O2O2Q
Evaluation B

$C_8H_{18}S$ (liq) 61MCC/FIN
5-Thianonane; Di-n-butyl sulfide
Heat Capacity 298.15 K, C_p=284.34 J·mol^{-1}·K^{-1}
Temperature range 11 to 370 K.
Entropy 298.15 K, S=405.09 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 198.13 K, ΔH=19426 J·mol^{-1}
ΔS=98.05 J·mol^{-1}·K^{-1}
Molecular Weight 146.2902
Wiswesser Line Notation 4S4
Evaluation A

$C_8H_{18}S$ (liq) 82TUT/GAB
1-Octanethiol; n-Octyl mercaptan
Heat Capacity 300 K, C_p=300.24 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K. C_p=282.50+3.340×10^{-2}T+8.582×10^{-5}T^2.
Molecular Weight 146.2902
Wiswesser Line Notation SH8
Evaluation C

$C_8H_{19}Al$ (liq) 91SHE/RAB
Diisobutylaluminum hydride
Heat Capacity 298.15 K, C_p=321.7 J·mol^{-1}·K^{-1}
Temperature range 5 to 303 K.
Entropy 298.15 K, S=347.0 J·mol^{-1}·K^{-1}
Molecular Weight 142.2196
Wiswesser Line Notation 1Y1&1-ALH-1Y1&1
Evaluation A
T(glass)=144.5 K.

$C_8H_{19}Cl_2NSiZn$ (liq) 76EVS/LEB
N-(β-Trimethylsilylethyl)azetidine, zinc chloride complex
Heat Capacity 298.15 K, C_p=607.1 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K. Deposited in VINITI, No. 3824-75, 26 December 1975.
Entropy 298.15 K, S=575.1 J·mol^{-1}·K^{-1}
Molecular Weight 312.7758
Wiswesser Line Notation T4NTJ A2-SI-1&1&1 &.ZN..G2
Evaluation B
Complex assumed 1:1.

$(C_8H_{19}Cl_2NSiZn)_n$ (liq) 76EVS/LEB
Poly-N-(β-trimethylsilylethyl)azetidine, zinc chloride complex
Heat Capacity 298.15 K, C_p=568.8 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K. Deposited in VINITI, No. 3824-75, 26 December 1975.
Entropy 298.15 K, S=542.2 J·mol^{-1}·K^{-1}
Molecular Weight 312.7758
Wiswesser Line Notation /*3N*2-SI-1&1&1 &.ZN..G2/
Evaluation B
Complex assumed 1:1.

$C_8H_{19}N$ (liq) 01KAH
Diisobutyl amine
Heat Capacity C_p=129.2 J·mol^{-1}·K^{-1}
Temperature range 294.15 to 403.15 K. Heat capacity is an average value over the temperature range.
Molecular Weight 129.2448
Wiswesser Line Notation 2YMY2
Evaluation D

$C_8H_{19}N$ (liq) 93STE/CHI2
n-Octylamine
Heat Capacity 298.15 K, C_p=309.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 129.2448
Wiswesser Line Notation Z8
Evaluation A

$C_8H_{19}NSi$ (liq) 75LEB/RAB
N-(β-Trimethylsilylethyl)trimethylenimine
Heat Capacity 298.15 K, C_p=304.6 J·mol^{-1}·K^{-1}
Temperature range 7 to 305 K.
Entropy 298.15 K, S=398.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 199.43 K, ΔH=12900 J·mol^{-1}
ΔS=64.6 J·mol^{-1}·K^{-1}
Molecular Weight 157.3303
Wiswesser Line Notation T4NTJ A2-SI-1&1&1
Evaluation A
T(glass)=126.7 K.

$C_8H_{19}NSi$ (liq) 77LEB/RAB5
N-(β-Trimethylsilylethyl)trimethylenimine
Heat Capacity 298.15 K, C_p=304.6 J·mol^{-1}·K^{-1}
Temperature range 7 to 305 K.
Entropy 298.15 K, S=398.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 199.43 K, ΔH=12900 J·mol^{-1}
ΔS=64.6 J·mol^{-1}·K^{-1}
Molecular Weight 157.3303
Wiswesser Line Notation T4NTJ A2-SI-1&1&1
Evaluation A
T(glass)=126.7 K.

$(C_8H_{19}NSi)_n$ (liq) 76LEB/EVS
Poly-N-(β-trimethylsilylethyl)azetidine
Heat Capacity 298 K, C_p=318.0 J·mol^{-1}·K^{-1}
Temperature range 65 to 305 K. Deposited in VINITI. No. 3786-75. 26 December 1975.
Entropy 298 K, S=315.7 J·mol^{-1}·K^{-1}
Molecular Weight 157.3303
Wiswesser Line Notation /*3N*2-SI-1&1&1/
Evaluation B
T(glass)=204.0 K.

$C_8H_{20}BrN$ (c) 74BUR/VER
Tetraethylammonium bromide
Heat Capacity 298 K, C_p=246.9 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
Phase Changes
c/liq 447 K, ΔH=20300 J·mol^{-1}
ΔS=45 J·mol^{-1}·K^{-1}
Molecular Weight 210.1567
Wiswesser Line Notation 2K2&2&2 E
Evaluation B

$C_8H_{20}Br_4FeN$ (c) 88NAV/PUE
Tetraethylammonium tetrabromoferrate
Heat Capacity 298.15 K, C_p=369.4 J·mol^{-1}·K^{-1}
Temperature range 50 to 300 K.
Entropy 298.15 K, S=415.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 236.1 K, ΔH=2428 J·mol^{-1}
ΔS=10.2 J·mol^{-1}·K^{-1}
Molecular Weight 505.7157
Wiswesser Line Notation 2K2&2&2 .FE G4
Evaluation A

$C_8H_{20}Cl_4FeN$ (c) 88NAV/PUE
Tetraethylammonium tetrachloroferrate
Heat Capacity 298.15 K, C_p=374.8 J·mol^{-1}·K^{-1}
Temperature range 1.4 to 300 K.
Entropy 298.15 K, S=490.2 J·mol^{-1}·K^{-1}
Phase Changes
c,V/c,IV 2.93 K
Neel point, lambda transition.
c,IV/c,III 234.7 K, ΔH=2203 J·mol^{-1}
ΔS=8.06 J·mol^{-1}·K^{-1}
First order transition.
c,III/c,II 217.5 K
c,II/c,I 226.6 K, ΔH=2295 J·mol^{-1}
ΔS=11.4 J·mol^{-1}·K^{-1}
First order transition.
Molecular Weight 327.9117
Wiswesser Line Notation 2K2&2&2 .FE G4
Evaluation A

$C_8H_{20}Ge$ (liq) 54STA/WAR
Tetraethylgermane; Germanium tetraethyl
Phase Changes
c/liq 180.47 K, ΔH=12406 J·mol^{-1}
ΔS=68.74 J·mol^{-1}·K^{-1}
Molecular Weight 188.8360
Wiswesser Line Notation 2-GE-2&2&2
Evaluation B

$C_8H_{20}Ge$ (liq) 72MAS/RAB
Tetraethylgermane; Germanium tetraethyl
Heat Capacity 298.15 K, C_p=309.6 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Phase Changes
c/liq 180.3 K, ΔH=12615 J·mol^{-1}
ΔS=70.0 J·mol^{-1}·K^{-1}
Molecular Weight 188.8360
Wiswesser Line Notation 2-GE-2&2&2
Evaluation B

$C_8H_{20}Ge$ (liq) 85RAB/SHE
Tetraethylgermane; Germanium tetraethyl
Heat Capacity 298.15 K, C_p=294.7 J·mol^{-1}·K^{-1}
Temperature range 8 to 300 K.
Entropy 298.15 K, S=428.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 179.99 K, ΔH=12312 J·mol^{-1}
ΔS=68.00 J·mol^{-1}·K^{-1}
Molecular Weight 188.8360
Wiswesser Line Notation 2-GE-2&2&2
Evaluation A

$C_8H_{20}IN$ (c) 73JOH/MAR
Tetraethylammonium iodide
Heat Capacity 298.15 K, C_p=254.4 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=311.3 J·mol^{-1}·K^{-1}
Molecular Weight 257.1572
Wiswesser Line Notation 2 K2&2&2 &I
Evaluation A

$C_8H_{20}IN$ (c) 88NAG/SAK
Tetraethylammonium iodide
Heat Capacity 298.15 K, C_p=254 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 257.1572
Wiswesser Line Notation 2K2&2&2 &I
Evaluation B

$C_8H_{20}N_4$ (liq) 88BOB/KAM
N [(2 Aminoethyl)2 aminoethyl]piperazine
Heat Capacity 333 K, C_p=391 J·mol^{-1}·K^{-1}
Temperature range 333 to 473 K.
Molecular Weight 172.2728
Wiswesser Line Notation T6M DNTJ D2M2Z
Evaluation D

$C_8H_{20}N_4$ (liq) 88BOB/KAM
N,N′-Di-(2-aminoethyl)piperazine
Heat Capacity 333 K, C_p=407 J·mol^{-1}·K^{-1}
Temperature range 333 to 473 K.
Molecular Weight 172.2728
Wiswesser Line Notation T6N DNTJ A2Z D2Z
Evaluation D

$C_8H_{20}O_4Si$ (liq) 85NKI/CHA
Tetraethyl silicate; Ethyl silicate
Heat Capacity 298.15 K, C_p=352.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 208.3291
Wiswesser Line Notation 2O-SI-O2&O2&O2
Evaluation B

$C_8H_{20}O_4Si$ (liq) 92VAN/COR
Tetraethyl silicate; Ethyl silicate
Heat Capacity 298.15 K, C_p=364.4 J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K. C_p/R(liq)=2.49615×10^5(T/K)$^{-2}$+70.8549×10^{-3}+19.9007 (193 to 362 K), where R=8.3144 J/K·mol.
Entropy 298.15 K, S=533.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 187.72 K, ΔH=13200 J·mol^{-1}
ΔS=70.32 J·mol^{-1}·K^{-1}
c,I/liq 190.97 K, ΔH=11140 J·mol^{-1}
ΔS=58.33 J·mol^{-1}·K^{-1}
Molecular Weight 208.3291
Wiswesser Line Notation 2O-SI-O2&O2&O2
Evaluation A

$C_8H_{20}Pb$ (liq) 54STA/WAR
Tetraethyl lead
Phase Changes
c/liq 142.94 K, ΔH=8791 J·mol^{-1}
ΔS=61.50 J·mol^{-1}·K^{-1}
Molecular Weight 323.4460
Wiswesser Line Notation 2-PB-2&2&2
Evaluation B

$C_8H_{20}Pb$ (liq) 56SCO/GOO
Tetraethyl lead
Heat Capacity 298.15 K, C_p=310.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 323.4460
Wiswesser Line Notation 2-PB-2&2&2
Evaluation B

$C_8H_{20}Pb$ (liq) 89RAB/NIS2
Tetraethyl lead
Heat Capacity 298.15 K, C_p=307.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 315 K.
Entropy 298.15 K, S=464.6 J·mol^{-1}·K^{-1}
Phase Changes
c,III/liq 90.8 K
Glass/supercooled liquid transition.
c,II/liq 141.4 K, ΔH=9110 J·mol^{-1}
ΔS=64.43 J·mol^{-1}·K^{-1}
c,I/liq 139.41 K, ΔH=9091 J·mol^{-1}
ΔS=65.21 J·mol^{-1}·K^{-1}
Molecular Weight 323.4460
Wiswesser Line Notation 2-PB-2&2&2
Evaluation A

$C_8H_{20}Si$ (liq) 54STA/WAR
Tetraethyl silicon; Tetraethylsilane
Phase Changes
c/liq 189.36 K, ΔH=13012 J·mol^{-1}
ΔS=68.70 J·mol^{-1}·K^{-1}
Molecular Weight 144.3315
Wiswesser Line Notation 2-SI-2&2&2
Evaluation B

$C_8H_{20}Si$ (liq) 72MAS/RAB
Tetraethyl silicon; Tetraethylsilane
Heat Capacity 298.15 K, $C_p = 298.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 60 to 300 K.
Phase Changes
c/liq 190.6 K, $\Delta H = 13410\ J \cdot mol^{-1}$
$\Delta S = 70.4\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 144.3315
Wiswesser Line Notation 2-SI-2&2&2
Evaluation B

$C_8H_{20}Si$ (liq) 92STE/CHI
Tetraethyl silicon; Tetraethylsilane
Heat Capacity 298.15 K, $C_p = 297.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 315 to 595 K.
Molecular Weight 144.3315
Wiswesser Line Notation 2-SI-2&2&2
Evaluation A

$C_8H_{20}Sn$ (liq) 54STA/WAR
Tetraethyl tin
Phase Changes
c/liq 142.14 K, $\Delta H = 9146\ J \cdot mol^{-1}$
$\Delta S = 64.35\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 234.9360
Wiswesser Line Notation 2-SN-2&2&2
Evaluation B

$C_8H_{20}Sn$ (liq) 72MAS/RAB
Tetraethyl tin
Heat Capacity 298.15 K, $C_p = 301.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 60 to 300 K.
Phase Changes
c,II/c,I 121.4 K, $\Delta H = -1090\ J \cdot mol^{-1}$
Metastable transition.
c,I/liq 141.9 K, $\Delta H = 8929\ J \cdot mol^{-1}$
$\Delta S = 62.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 234.9360
Wiswesser Line Notation 2-SN-2&2&2
Evaluation B

$C_8H_{20}TeZn$ (liq) 91LEB/KUL
Diethylzinc diethyltellurim complex
Heat Capacity 298.15 K, $C_p = 399.01\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 13 to 306 K.
Entropy 298.15 K, $S = 556.98\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 120.0 K, $\Delta H = 165.3\ J \cdot mol^{-1}$
$\Delta S = 1.37\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 108 to 120 K.
c,I/liq 187.90 K, $\Delta H = 16496\ J \cdot mol^{-1}$
$\Delta S = 87.80\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 299.1470
Wiswesser Line Notation 2-ZN-2 &2-TE-2
Evaluation A

$C_8H_{23}N_5$ (liq) 88BOB/KAM
Tetraethylenepentamine
Heat Capacity 333 K, $C_p = 460\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 333 to 513 K.
Molecular Weight 189.3032
Wiswesser Line Notation Z2M2M2M2Z
Evaluation D

$C_8H_{24}Ag_{13}I_{15}N_2$ (c) 85LIN/ARM
Bis-(tetramethylammonium iodide) tridecasilver iodide
Heat Capacity 282.93 K, $C_p = 1076\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 79 to 283 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 150 K, $\Delta S = 5.34\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 3454.1425
Wiswesser Line Notation 1K1&1&1&1 2 .AG I 13
Evaluation A

$C_8H_{24}Br_4CuN$ (c) 89LOP/RUI
Bis-(tetramethylammonium) tetrabromo cuprate
Heat Capacity
Temperature range 60 to 343 K. Data given graphically.
Phase Changes
c,IV/c,III 242.8 K, $\Delta H = 1538\ J \cdot mol^{-1}$
$\Delta S = 5.82\ J \cdot mol^{-1} \cdot K^{-1}$
c,III/c,II 249.35 K, $\Delta H = 9.56\ J \cdot mol^{-1}$
$\Delta S = 0.033\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I 270.70 K, $\Delta H = 3742\ J \cdot mol^{-1}$
$\Delta S = 15.46\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 517.4463
Wiswesser Line Notation 1K1&1&1 2 .CU E4
Evaluation A

$C_8H_{24}Br_4N_2Zn$ (c) 92IGA/RUI
Tetramethylammonium tetrabromozincate(II)
Heat Capacity 302.315 K, $C_p = 453.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 170 to 370 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 287.20 K, $\Delta H = 4074\ J \cdot mol^{-1}$
$\Delta S = 16.2\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 533.2870
Wiswesser Line Notation 1K1&1&1 -ZN- E4
Evaluation B

$C_8H_{24}CdI_4N_2$ (c) 91KAL/BOR
Bis-(tetramethylammonium) tetraiodocadmate
Phase Changes
c,II/c,I 233 K, $\Delta H = 1950\ J \cdot mol^{-1}$
$\Delta S = 8.4\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 7683190
Wiswesser Line Notation 1K1&1&1 2 -CD- I4
Evaluation B

$C_8H_{24}Cl_4FeN_2$ (c) 88RUI/LOP
Bis-(tetramethylammonium) tetrachloroferrate
Heat Capacity 300 K, $C_p = 424\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 60 to 350 K. Data given graphically. C_p datum is graphical estimate.
Phase Changes
c,IV/c,III 240.0 K, $\Delta H = 859.6\ J \cdot mol^{-1}$
$\Delta S = 3.68\ J \cdot mol^{-1} \cdot K^{-1}$
c,III/c,II 266.8 K, $\Delta H = 238.5\ J \cdot mol^{-1}$
$\Delta S = 0.90\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I 281.0 K, $\Delta H = 2179.9\ J \cdot mol^{-1}$
$\Delta S = 8.34\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 345.9500
Wiswesser Line Notation 1K1&1&1 2 -FE- G4
Evaluation B

$C_8H_{24}Cl_4MnN_2$ (c) 75BOC/ARR

Tetrachlorobis(butylammonium) manganate

Phase Changes

c,II/c,I	371 K,	ΔH=2.4 J·mol^{-1}
		ΔS=0.007 J·mol^{-1}·K^{-1}

Molecular Weight 345.0410

Wiswesser Line Notation 4ZH 2 -MN- G4

Evaluation A

$C_8H_{24}Cl_4MnN_2$ (c) 88ZUB/LOP

Bis-(tetramethylammonium) tetrachloromanganate

Heat Capacity 300 K, C_p=424 J·mol^{-1}·K^{-1}

Temperature range 50 to 330 K. Data given graphically and estimated from graph.

Phase Changes

c,V/c,IV	175.63 K,	ΔH=308 J·mol^{-1}
		ΔS=1.75 J·mol^{-1}·K^{-1}
c,IV/c,III	268.65 K,	ΔH=233 J·mol^{-1}
		ΔS=0.83 J·mol^{-1}·K^{-1}
c,III/c,II	292.3 K,	ΔH=5.8 J·mol^{-1}
		ΔS=0.02 J·mol^{-1}·K^{-1}
c,II/c,I	292.6 K,	ΔH=2079 J·mol^{-1}
		ΔS=7.98 J·mol^{-1}·K^{-1}

Molecular Weight 345.0410

Wiswesser Line Notation 1K1&1&1 2 -MN- G4

Evaluation A

$C_8H_{24}Cl_4N_2Zn$ (c) 90STR/TAR

Bis-(tetramethylammonium) tetrachlorozincate

Heat Capacity 300 K, C_p=424 J·mol^{-1}·K^{-1}

Temperature range 80 to 360 K. Data given graphically. C_p value estimated from baseline of graph.

Phase Changes

c,IX/c,VII	159 K,	ΔH=448 J·mol^{-1}
		ΔS=2.82 J·mol^{-1}·K^{-1}
c,VIII/c,VII	165 K,	ΔH=80 J·mol^{-1}
		ΔS=0.48 J·mol^{-1}·K^{-1}
c,VII/c,VI	177.75 K,	ΔH=180 J·mol^{-1}
		ΔS=1.02 J·mol^{-1}·K^{-1}
c,VI/c,V	276.95 K,	ΔH=145 J·mol^{-1}
		ΔS=0.52 J·mol^{-1}·K^{-1}
c,V/c,IV	281.0 K,	ΔH=132 J·mol^{-1}
		ΔS=0.47 J·mol^{-1}·K^{-1}

Molecular Weight 355.4830

Wiswesser Line Notation 1K1&1&1 2 -ZN- G4

Evaluation A(transitions)

c,IV/c,III 296.6 168 0.56; c,III/c,II 325.95 192 0.59; c,II/c,I 328.95 235 0.73.

$C_8H_{24}O_4Si_4$ (liq) 75MEK/KAR2

Octamethylcyclotetrasiloxane

Heat Capacity

Temperature range 13 to 310 K.

Entropy	298.15 K,	S=623.0 J·mol^{-1}·K^{-1}
Phase Changes		
c,II/c,I	253–258 K,	ΔH=4866 J·mol^{-1}
c,I/liq	290.55 K,	ΔH=23765 J·mol^{-1}
		ΔS=81.80 J·mol^{-1}·K^{-1}

Molecular Weight 296.6172

Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI-OTJ A1 A1 C1 C1 E1 E1 G1 G1

Evaluation A

$C_8H_{24}O_4Si_4$ (liq) 81MEK/KAR

Octamethylcyclotetrasiloxane

Heat Capacity 298.15 K, C_p=509.6 J·mol^{-1}·K^{-1}

Temperature range 13 to 390 K. Data given graphically.

Entropy 298.15 K, S=623.0 J·mol^{-1}·K^{-1}

Phase Changes

c/liq	290.25 K,	ΔH=23765 J·mol^{-1}
		ΔS=81.80 J·mol^{-1}·K^{-1}

Molecular Weight 296.6172

Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI-OTJ A1 A1 C1 C1 E1 E1 G1 G1

Evaluation A

$C_8H_{28}N_4Si_4$ (c) 81MEK/KAR

Octamethylcyclotetrasilazane

Heat Capacity 298.15 K, C_p=570 J·mol^{-1}·K^{-1}

Temperature range 13 to 390 K. Data given graphically.

Entropy 298.15 K, S=599.6 J·mol^{-1}·K^{-1}

Phase Changes

c/liq	367.67 K,	ΔH=25050 J·mol^{-1}
		ΔS=66.5 J·mol^{-1}·K^{-1}

Molecular Weight 292.6780

Wiswesser Line Notation T8-SI-M-SI-M-SI-M-SI-MTJ A1 A1 C1 C1 E1 E1 G1 G1

Evaluation A

$C_9Fe_2O_9$ (c) 89SEL/SHE

Nonadecacarbonyl diiron

Heat Capacity 298.15 K, C_p=373.1 J·mol^{-1}·K^{-1}

Temperature range 7 to 300 K.

Entropy 298.15 K, S=451.1 J·mol^{-1}·K^{-1}

Molecular Weight 363.7876

Wiswesser Line Notation CO 9 .FE

Evaluation A

$C_9H_4O_5$ (c) 78MAR/CIO2

Trimellitic anhydride

Heat Capacity 298.15 K, C_p=248.9 J·mol^{-1}·K^{-1}

Temperature range 298 to 540 K.

Phase Changes

c/liq	385 K,	ΔH=10464 J·mol^{-1}
		ΔS=27.2 J·mol^{-1}·K^{-1}

Molecular Weight 192.1276

Wiswesser Line Notation T56 BVOVJ GVQ

Evaluation D

$C_9H_6CrO_2S$ (c) 81CIIII/POM

Benzene chromium dicarbonyl thiocarbonyl

Heat Capacity 298.15 K, C_p=226.66 J·mol^{-1}·K^{-1}

Temperature range 5 to 300 K.

Entropy 298.15 K, S=292.8 J·mol^{-1}·K^{-1}

Molecular Weight 230.2012

Wiswesser Line Notation L6ϕJ ϕ-CR– CO 2 &CS

Evaluation A

$C_9H_6CrO_3$ (c) 78POM/CHH

Benzene chromium tricarbonyl

Heat Capacity 298.15 K, C_p=151.3 J·mol^{-1}·K^{-1}

Temperature range 120 to 300 K. Data given graphically. C_p=38.17+2.37×10^{-1}T+3.77×10^{-4}T^2+3.38×10^{-7}T^3 J·mol^{-1}·K^{-1} (120 to 300 K). C_p value calculated from equation.

Molecular Weight 214.1406

Wiswesser Line Notation L6ϕJ ϕ-CR– CO 3

Evaluation C

$C_9H_6CrO_3$ (c) 81CHH/POM
Benzene chromium tricarbonyl
Heat Capacity 298.15 K, C_p=238.1 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=267.4 J·mol^{-1}·K^{-1}
Molecular Weight 214.1406
Wiswesser Line Notation L6ϕJ ϕ-CR– CO 3
Evaluation A
C_p data does not agree with earlier work reported in 78POM/CHH.

$C_9H_6N_2O_2$ (liq) 62STR/BAR
2,4-Tolylenediisocyanate; 1-Methyl-2,4-diisocyanatobenzene
Heat Capacity 298 K, C_p=287.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 174.1586
Wiswesser Line Notation OCNR B1 ENCO
Evaluation D

$C_9H_6O_2$ (c) 91ELW/SAB
Coumarin
Phase Changes
c/liq 342.14 K, ΔH=19140 J·mol^{-1}
Molecular Weight 146.1452
Wiswesser Line Notation T66 BOVJ
Evaluation A

$C_9H_6O_2$ (c) 92SAB/ELW4
Coumarin
Phase Changes
c/liq 342.14 K, ΔH=19140 J·mol^{-1}
c/g 298.15 K, ΔH=83090 J·mol^{-1}
Molecular Weight 146.1452
Wiswesser Line Notation T66 BOVJ
Evaluation A

$C_9H_6O_2$ (c) 88SAB/ELW
Chromone
Heat Capacity 298.15 K, C_p=176.8 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 330.27 K, ΔH=17310 J·mol^{-1}
liq/g 298.15 K, ΔH=81290 J·mol^{-1}
Molecular Weight 146.1452
Wiswesser Line Notation T66 BV EOJ
Evaluation A

C_9H_7Cu (c) 82BYK/LEB
Copper benzylacetylenide
Heat Capacity 298.15 K, C_p=178.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=197.6 J·mol^{-1}·K^{-1}
Molecular Weight 178.7003
Wiswesser Line Notation -CU-1UU2R
Evaluation A

C_9H_7N (liq) 16BRA
Quinoline
Heat Capacity 283 K, C_p=190.4 J·mol^{-1}·K^{-1}
Mean value, 0 to 20 °C.
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation C

C_9H_7N (liq) 34KOL/UD
Quinoline
Heat Capacity 302.5 K, C_p=192.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation C

C_9H_7N (liq) 34KOL/UDC
Quinoline
Heat Capacity 302.4 K, C_p=192.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation C

C_9H_7N (liq) 34RAD/JU
Quinoline
Heat Capacity 290 K, C_p=164.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation C

C_9H_7N (liq) 36PAR/TO
Quinoline
Heat Capacity 298.1 K, C_p=199.20 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 298.1 K, S=217.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 54.94 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 258.4 K, ΔH=10799 J·mol^{-1}
ΔS=41.79 J·mol^{-1}·K^{-1}
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation B(C_p),C(S)

C_9H_7N (liq) 51TSC/KF
Quinoline
Heat Capacity 298 K, C_p=203.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation C

C_9H_7N (liq) 57MA
Quinoline
Phase Changes
c/liq 257.93 K, ΔH=10724 J·mol^{-1}
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation A

C_9H_7N (liq) 86STE/CH
Quinoline
Heat Capacity 298.15 K, C_p=194.90 J·mol^{-1}·K^{-1}
Temperature range 6 to 450 K.
Entropy 298.15 K, S=219.69 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 220.093 K
c,I/liq 258.369 K
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation A

C_9H_7N (liq) 88STE/ARC
Quinoline
Heat Capacity 298.15 K, $C_p = 194.89\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 500 K.
Entropy 298.15 K, $S = 219.72\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 220.000 K, $\Delta H = 68.18\ J \cdot mol^{-1}$
$\Delta S = 0.310\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 258.369 K, $\Delta H = 10662.90\ J \cdot mol^{-1}$
$\Delta S = 41.27\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation A

C_9H_7N (liq) 90JAL/ROB
Quinoline
Phase Changes
liq/liq 290 K
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation B
Isochoric heat capacity was measured from 267 to 313 K.

C_9H_7N (liq) 88STE/ARC
Isoquinoline
Heat Capacity 298.15 K, $C_p = 196.16\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 500 K. Values calculated from graphically extrapolated heat capacity values.
Entropy 298.15 K, $S = 215.98\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,III/c,II 221.000 K, $\Delta H = 0.00\ J \cdot mol^{-1}$
c,II/c,I 275.000 K, $\Delta H = 0.00\ J \cdot mol^{-1}$
c,I/liq 299.620 K, $\Delta H = 13544.17\ J \cdot mol^{-1}$
$\Delta S = 45.20\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 129.1610
Wiswesser Line Notation T66 CNJ
Evaluation A

C_9H_7N (c) 86STE/CHI
Isoquinoline
Heat Capacity 298.15 K, $C_p = 177.68\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 400 K.
Entropy 298.15 K, $S = 171.06\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,III/c,II 219.600 K
c,II/c,I 275.000 K
c,I/liq 299.616 K
Molecular Weight 129.1610
Wiswesser Line Notation T66 CNJ
Evaluation A

C_9H_7NO (c) 81LEB/RYA
3-Indole aldehyde
Heat Capacity $C_p = 220.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 298 to 458 K. Data given over temperature range.
Molecular Weight 145.1604
Wiswesser Line Notation T56 BMJ DVH
Evaluation B

$C_9H_7NO_4$ (c) 41SAT/SOG
o-Nitrocinnamic acid
Heat Capacity 323 K, $C_p = 240.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 193.1586
Wiswesser Line Notation WNR B1U1VQ
Evaluation C
Same data in 40SAT/SOG2.

$C_9H_7NO_4$ (c) 41SAT/SOG
m-Nitrocinnamic acid
Heat Capacity 323 K, $C_p = 240.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 193.1586
Wiswesser Line Notation WNR C1U1VQ
Evaluation C
Same data in 40SAT/SOG2.

$C_9H_7NO_4$ (c) 41SAT/SOG
p-Nitrocinnamic acid
Heat Capacity 323 K, $C_p = 238.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 193.1586
Wiswesser Line Notation WNR D1U1VQ
Evaluation C
Same data in 40SAT/SOG2.

C_9H_8 (liq) 59STU/SIN
Indene
Heat Capacity 298.15 K, $C_p = 186.94\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 15 to 320 K.
Entropy 298.15 K, $S = 215.35\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 271.70 K, $\Delta H = 10201\ J \cdot mol^{-1}$
$\Delta S = 37.55\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 116.1622
Wiswesser Line Notation L56BHJ
Evaluation A

C_9H_8 (liq) 61STU/SIN
Indene
Heat Capacity 298.15 K, $C_p = 186.94\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 15 to 320 K.
Entropy 298.15 K, $S = 214.18\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 271.70 K, $\Delta H = 10201\ J \cdot mol^{-1}$
Molecular Weight 116.1622
Wiswesser Line Notation L56BHJ
Evaluation A

$C_9H_8ClN_3O_3$ (c) 89KHO/ISK
2-Methyl-3-nitro-4-methoxymethyl-5-cyano-6-chloropyridine
Heat Capacity 298.15 K, $C_p = 270.0\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Entropy 298.15 K, $S = 339.97\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 241.6335
Wiswesser Line Notation T6NJ BG CCN D1O1 ENW F1
Evaluation B

$C_9H_8FeN_2O_3$ (c) 90BUS/TEL
N-allylpyrazole tricarbonyliron
Heat Capacity 298.15 K, C_p=284.5 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=309.5 J·mol^{-1}·K^{-1}
Molecular Weight 248.0208
Wiswesser Line Notation T5NMJ B2U1 .FE CO 3
Evaluation A

$C_9H_8MnO_3P$ (c) 82POI/SOU
3,4-Dimethylphospholyl manganese tricarbonyl;
Dimethyl- 3,4-phosphacymantrene
Phase Changes
c,II/c,I 275 K, ΔH=190 J·mol^{-1}
ΔS=0.69 J·mol^{-1}·K^{-1}
c,I/liq 300 K, ΔH=19300 J·mol^{-1}
ΔS=64 J·mol^{-1}·K^{-1}
Molecular Weight 250.0722
Wiswesser Line Notation T5PJ C1 D1 &MN CO 3
Evaluation A

$C_9H_8O_2$ (c) 39SAT/SOG2
Cinnamic acid
Heat Capacity 323 K. C_p=197.5 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 148.1610
Wiswesser Line Notation QV1U1R
Evaluation C

$C_9H_8O_2$ (c) 86SIN/KUM
Cinnamic acid
Phase Changes
c/liq 406.15 K, ΔH=22626 J·mol^{-1}
Molecular Weight 148.1610
Wiswesser Line Notation QV1U1R
Evaluation A

$C_9H_8O_3$ (c) 83GEI/SAL
endo-Bicyclo[2.2.1]-5-heptene-2,3-dicarboxylic acid anhydride
Heat Capacity 298.15 K, C_p=183.3 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=189.5 J·mol^{-1}·K^{-1}
Molecular Weight 164.1604
Wiswesser Line Notation T555/FJ 2AE J BVOV IUTJ
Evaluation A
There is an extended hump in the C_p curve between 50 and 150 K.

$C_9H_9Cl_3$ (c) 72LAG
1,2,3-Trichloro-4,5,6-trimethylbenzene
Heat Capacity 298.15 K, C_p=252.34 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 298.15 K, S=314.93 J·mol^{-1}·K^{-1}
Molecular Weight 223.5291
Wiswesser Line Notation GR BG CG D1 E1 F1
Evaluation B
Second order transition between 140 and 270 K.

$C_9H_9Cl_3$ (c) 90FUJ/AT
1,3,5-Trichloro-2,4,6-trimethylbenzene
Heat Capacity 300 K, C_p=232.39 J·mol^{-1}·K^{-}
Temperature range 3 to 327 K. Unsmoothed experimental datur
Phase Changes
c,IV/c,III 158.7 K, ΔH=142 J·mol^{-1}
Anomaly splits into two peaks depending on sample history.
163.5 K, ΔH=87 J·mol^{-1}
c,III/c,II 314 K
Superheating effect.
Molecular Weight 223.5291
Wiswesser Line Notation GR B1 CG D1 EG F1
Evaluation A

C_9H_9FeN (c) 84CHH/PO
Azaferrocene
Heat Capacity 298.15 K, C_p=183.4 J·mol^{-1}·K^{-1}
Temperature range 70 to 290 K.
Entropy 298.15 K, S=211.8 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,I′ 200 K, ΔH=3000 J·mol^{-1}
ΔS=15.0 J·mol^{-1}·K^{-1}
c,II/c,I′ 218 K, ΔH=−3800 J·mol^{-1}
ΔS=−17.4 J·mol^{-1}·K^{-}
Molecular Weight 187.0238
Wiswesser Line Notation T5NϕJ ϕ-FE– ϕL5ϕJ
Evaluation A
Metastable phase.

C_9H_9FeN (c) 84CHH/PO
Azaferrocene
Heat Capacity 298.15 K, C_p=177.0 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=170.30 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 278.5 K, ΔH=650 J·mol^{-1}
ΔS=2.4 J·mol^{-1}·K^{-1}
c,II/c,I 289.5 K, ΔH=6748 J·mol^{-1}
ΔS=23.6 J·mol^{-1}·K^{-1}
Molecular Weight 187.0238
Wiswesser Line Notation T5NϕJ ϕ-FE– ϕL5ϕJ
Evaluation A
Stable phase.

C_9H_9FeP (c) 84CHH/PO
Phosphaferrocene
Phase Changes
c,II/c,I 266 K, ΔH=7330 J·mol^{-1}
ΔS=27.6 J·mol^{-1}·K^{-1}
Molecular Weight 203.9909
Wiswesser Line Notation T5PϕJ ϕ-FE– ϕL5ϕJ
Evaluation A
Stable phase. A metastable phase transition is reported at T=21 K.

C_9H_9NO (c) 83ZAM/K
α-Methoxybenzyl cyanide
Heat Capacity 298.15 K, C_p=153.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 147.1762
Wiswesser Line Notation NCYR&O1
Evaluation B

$(C_9H_9NO)_n$ (c) 91ROL
Poly-L-phenylalanine
Heat Capacity 300 K, C_p=169.7 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 147.1762
Wiswesser Line Notation /*VY1R&M*/ -L
Evaluation B

$(C_9H_9NO)_n$ (c) 93ROL/XEN
Poly-L-phenylalanine
Heat Capacity 300 K, C_p=169.7 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 147.1762
Wiswesser Line Notation /*VY1R&M*/ -L
Evaluation B

$C_9H_9NO_2$ (c) 41SAT/SOG2
m-Aminocinnamic acid
Heat Capacity 323 K, C_p=227.6 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 163.1756
Wiswesser Line Notation ZR C1U1VQ
Evaluation C
Same data at 40SAT/SOG3.

$(C_9H_9NO_2)_n$ (c) 91ROL
Poly-L-tyrosine
Heat Capacity 300 K, C_p=183.6 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 163.1756
Wiswesser Line Notation /*VY1R DQ &M*/ -L
Evaluation B

$(C_9H_9NO_2)_n$ (c) 93ROL/XEN
Poly-L-tyrosine
Heat Capacity 300 K, C_p=183.6 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 163.1756
Wiswesser Line Notation /*VY1R DQ &M*/ -L
Evaluation B

$C_9H_9NO_3$ (c) 41HUF
Hippuric acid; Benzoylglycine
Heat Capacity 298.4 K, C_p=214.35 J·mol^{-1}·K^{-1}
Temperature range 85 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=239.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 77.32 J·mol^{-1}·K^{-1}.
Molecular Weight 179.1750
Wiswesser Line Notation QV1MVR
Evaluation A(C_p),C(S)

$C_9H_9NO_3$ (liq) 61HUB/FRO
Hippuric acid; Benzoylglycine
Heat Capacity 298.15 K, C_p=217 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 179.1750
Wiswesser Line Notation QV1MVR
Evaluation B

$C_9H_9N_3O_4$ (c) 89KHO/ISK
3-Cyano-4-methoxymethyl-5-nitro-6-methyl-(2-pyridone)
Heat Capacity 298.15 K, C_p=275.80 J·mol^{-1}·K^{-1}
One temperature.
Entropy 298.15 K, S=323.69 J·mol^{-1}·K^{-1}
Molecular Weight 223.1878
Wiswesser Line Notation T6MVJ CCN D1O1 ENW F1
Evaluation B

C_9H_{10} (liq) 71LEB/RAB2
α-Methylstyrene
Heat Capacity 300 K, C_p=202.2 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, S=243.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 250.78 K, ΔH=11924 J·mol^{-1}
ΔS=47.55 J·mol^{-1}·K^{-1}
Molecular Weight 118.1780
Wiswesser Line Notation 1UY1&R
Evaluation B

C_9H_{10} (liq) 59STU/SIN
Indane
Heat Capacity 298.15 K, C_p=190.25 J·mol^{-1}·K^{-1}
Temperature range 15 to 320 K.
Entropy 298.15 K, S=234.34 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 221.77 K, ΔH=8598 J·mol^{-1}
ΔS=38.77 J·mol^{-1}·K^{-1}
Molecular Weight 118.1780
Wiswesser Line Notation L56T&J
Evaluation A

C_9H_{10} (liq) 61STU/SIN
Indane
Heat Capacity 298.15 K, C_p=190.25 J·mol^{-1}·K^{-1}
Temperature range 15 to 320 K. Premelting occurs at 170 K to melting.
Entropy 298.15 K, S=234.35 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 73.82 K, ΔH=781 J·mol^{-1}
ΔS=10.57 J·mol^{-1}·K^{-1}
c,I/liq 221.77 K, ΔH=8598 J·mol^{-1}
ΔS=38.77 J·mol^{-1}·K^{-1}
Molecular Weight 118.1780
Wiswesser Line Notation L56T&J
Evaluation A

$(C_9H_{10})_n$ (c) 71LEB/RAB2
Poly(α-methylstyrene)
Heat Capacity 300 K, C_p=149.2 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, S=134.7 J·mol^{-1}·K^{-1}
Molecular Weight 118.1780
Wiswesser Line Notation /*1X*1&R/
Evaluation B

$C_9H_{10}N_2O_2$ (c) 89KHO/ISK
3-Cyano-4-methoxymethyl-6-methyl-(2-pyridone)
Heat Capacity 298.15 K, C_p=211.76 J·mol^{-1}·K^{-1}
One temperature.
Entropy 298.15 K, S=269.23 J·mol^{-1}·K^{-1}
Molecular Weight 178.1902
Wiswesser Line Notation T6MVJ CCN D1O1 F1
Evaluation B

$C_9H_{10}N_2O_3$ (c) 82CUE/SOL
2-Methoxyisonitrosoacetanilide
Phase Changes
c/liq 422 K, $\Delta H = 27800\ J\cdot mol^{-1}$
$\Delta S = 65.9\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 194.1896
Wiswesser Line Notation QNU1VMR BO1
Evaluation D

$C_9H_{10}N_2O_3$ (c) 82CUE/SOL
4-Methoxyisonitrosoacetanilide
Phase Changes
c/liq 459 K, $\Delta H = 8300\ J\cdot mol^{-1}$
$\Delta S = 18.1\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 194.1896
Wiswesser Line Notation QNU1VMR DO1
Evaluation D

$C_9H_{10}O$ (liq) 86CHI/NGU
Chroman
Heat Capacity 298.15 K, $C_p = 214.00\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 10 to 450 K.
Entropy 298.15 K, $S = 246.03\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 269.836 K
Molecular Weight 134.1774
Wiswesser Line Notation T66 BOT&J
Evaluation A

$C_9H_{10}O$ (liq) 90CHI/ARC
Chroman
Heat Capacity 298.15 K, $C_p = 213.966\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 10 to 500 K.
Entropy 298.15 K, $S = 246.018\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 269.836 K, $\Delta H = 16255.37\ J\cdot mol^{-1}$
$\Delta S = 60.242\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 134.1774
Wiswesser Line Notation T66 BOT&J
Evaluation A

$C_9H_{10}O$ (liq) 86CHI/NGU
Isochroman
Heat Capacity 298.15 K, $C_p = 217.81\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 10 to 450 K.
Entropy 298.15 K, $S = 247.04\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 277.503 K
Molecular Weight 134.1774
Wiswesser Line Notation T66 COT&J
Evaluation A

$C_9H_{10}O$ (liq) 90CHI/ARC
Isochroman
Heat Capacity 298.15 K, $C_p = 217.774\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 10 to 500 K.
Entropy 298.15 K, $S = 247.024\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 277.503 K, $\Delta H = 16747.59\ J\cdot mol^{-1}$
$\Delta S = 60.351\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 134.1774
Wiswesser Line Notation T66 COT&J
Evaluation A

$C_9H_{10}O_2$ (liq) 33KOL/UDC
Benzyl ethanoate; Benzyl acetate
Heat Capacity 292.7 K, $C_p = 250.2\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation 1VO1R
Evaluation C

$C_9H_{10}O_2$ (liq) 34KOL/UDO
Benzyl ethanoate; Benzyl acetate
Heat Capacity 292.7 K, $C_p = 250.2\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation 1VO1R
Evaluation C

$C_9H_{10}O_2$ (liq) 39PH
Benzyl ethanoate; Benzyl acetate
Heat Capacity 306.0 K, $C_p = 154.0\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation 1VO1R
Evaluation C

$C_9H_{10}O_2$ (liq) 79FUC
Benzyl ethanoate; Benzyl acetate
Heat Capacity 298.15 K, $C_p = 148.5\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation 1VO1R
Evaluation B

$C_9H_{10}O_2$ (liq) 33KOL/UDC
Ethyl benzoate
Heat Capacity 292.7 K, $C_p = 241.8\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation 2OVR
Evaluation C

$C_9H_{10}O_2$ (liq) 34KOL/UDO
Ethyl benzoate
Heat Capacity 292.7 K, $C_p = 241.8\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation 2OVR
Evaluation C

$C_9H_{10}O_2$ (liq) 36KUR/VO
Ethyl benzoate
Heat Capacity 290 K, $C_p = 282.8\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation 2OVR
Evaluation D

$C_9H_{10}O_2$ (liq) 79FUC
Ethyl benzoate
Heat Capacity 298.15 K, $C_p = 246.0\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation 2OVR
Evaluation B

$C_9H_{10}O_2$ (c) 1889EYK
Phenylpropionic acid
Phase Changes
c/liq 321.6 K, $\Delta H = 15564\ J \cdot mol^{-1}$
$\Delta S = 48.4\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 150.1768
Wiswesser Line Notation QV2R
Evaluation C

$C_9H_{10}O_2$ (c) 84COL/JIM2
2,3-Dimethylbenzoic acid
Heat Capacity 299.65 K, $C_p = 216.3\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation QVR B1 C1
Evaluation B

$C_9H_{10}O_2$ (c) 84COL/JIM2
2,4-Dimethylbenzoic acid
Heat Capacity 299.65 K, $C_p = 192.2\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation QVR B1 D1
Evaluation B

$C_9H_{10}O_2$ (c) 84COL/JIM2
2,5-Dimethylbenzoic acid
Heat Capacity 299.65 K, $C_p = 202.7\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation QVR B1 E1
Evaluation B

$C_9H_{10}O_2$ (c) 84COL/JIM2
2,6-Dimethylbenzoic acid
Heat Capacity 299.65 K, $C_p = 204.2\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation QVR B1 F1
Evaluation B

$C_9H_{10}O_2$ (c) 84COL/JIM2
o-Ethylbenzoic acid
Heat Capacity 298.15 K, $C_p = 208.7\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature. C_p given as $1.39\ J \cdot K^{-1} \cdot g^{-1}$.
Molecular Weight 150.1768
Wiswesser Line Notation QVR B2
Evaluation B

$C_9H_{10}O_2$ (c) 84COL/JIM2
3,4-Dimethylbenzoic acid
Heat Capacity 299.65 K, $C_p = 199.7\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation QVR C1 D1
Evaluation B

$C_9H_{10}O_2$ (c) 84COL/JIM2
3,5-Dimethylbenzoic acid
Heat Capacity 299.15 K, $C_p = 192.2\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 150.1768
Wiswesser Line Notation QVR C1 E1
Evaluation B

$C_9H_{10}O_2$ (c) 84COL/JIM2
m-Ethylbenzoic acid
Heat Capacity 298.15 K, $C_p = 199.7\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature. C_p given as $1.33\ J\ K^{-1}\ g^{-1}$.
Molecular Weight 150.1768
Wiswesser Line Notation QVR C2
Evaluation B

$C_9H_{10}O_2$ (c) 84COl/JIM2
p-Ethylbenzoic acid
Heat Capacity 298.15 K, $C_p = 207.2\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature. C_p given as $1.38\ J \cdot K^{-1} \cdot g^{-1}$.
Molecular Weight 150.1768
Wiswesser Line Notation QVR D2
Evaluation B

$C_9H_{10}O_2$ (c) 87LES/LIC
Phenyl glycidyl ether
Heat Capacity 298 K, $C_p = 278.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 225 to 400 K.
Molecular Weight 150.1768
Wiswesser Line Notation T3OTJ B1OR
Evaluation B

$C_9H_{10}O_2$ (liq) 88LEB/BYK2
Phenyl glycidyl ether
Heat Capacity 298.15 K, $C_p = 276.0\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 330 K.
Entropy 298.15 K, $S = 274.9\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 276.79 K
Molecular Weight 150.1768
Wiswesser Line Notation T3OTJ B1OR
Evaluation A
Data also given for the vitreous state from 5 to 189 K, and for the supercooled liquid from 200 to 276.79 K.

$C_9H_{10}O_3$ (c) 78GEI/KAR
3-Methyltetrahydrophthalic anhydride
Heat Capacity
C_p data not given. Temperature range 12 to 360 K. Data deposited VINITI, No. 3381-77, 5 Oct 1977. Includes C_p, S, ΔH fusion, Tm.
Molecular Weight 166.1762
Wiswesser Line Notation TS6 BVOV AUJG F1
Evaluation B(for original data)

$C_9H_{11}N$ (liq) 89STE/CHI
1,2,3,4-Tetrahydroquinoline
Heat Capacity 298.15 K, C_p=236.04 J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, S=240.36 J·mol^{-1}·K^{-1}
Phase Changes
c,IV/c,III 61.7 K
c,III/c,II 114.75 K
c,II/c,I 231.8 K
c,I/liq 289.913 K, ΔH=11813 J·mol^{-1}
ΔS=40.75 J·mol^{-1}·K^{-1}
Molecular Weight 133.1926
Wiswesser Line Notation T66 BNT&J
Evaluation A

$C_9H_{11}N$ (liq) 86STE/CHI
5,6,7,8-Tetrahydroquinoline
Heat Capacity 298.15 K, C_p=217.33 J·mol^{-1}·K^{-1}
Temperature range 6 to 450 K.
Entropy 298.15 K, S=248.69 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 222.634 K
Molecular Weight 133.1926
Wiswesser Line Notation T66 BN&TJ
Evaluation A

$C_9H_{11}N$ (liq) 89STE/CHI
5,6,7,8-Tetrahydroquinoline
Heat Capacity 298.15 K, C_p=217.41 J·mol^{-1}·K^{-1}
Temperature range 5 to 440 K.
Entropy 298.15 K, S=248.73 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II
T(glass) near 160 K. Glass to metastable form.
c,II/c,I
near 210 K. First order transition, metastable to stable crystalline form.
c,I/liq 222.634 K, ΔH=9071.7 J·mol^{-1}
ΔS=40.75 J·mol^{-1}·K^{-1}
Molecular Weight 133.1926
Wiswesser Line Notation T66 BN&TJ
Evaluation A

$C_9H_{11}NO_2$ (c) 71PRI
Ethyl N-phenylcarbamate
Heat Capacity 298 K, C_p=227.2 J·mol^{-1}·K^{-1}
Temperature range 200 to 390 K. Complete data deposited VINITI. No. 2713-71, 25 March 1971.
Phase Changes
c/liq 326 K. ΔH=16272 J·mol^{-1}
ΔS=49.9 J·mol^{-1}·K^{-1}
Molecular Weight 165.1914
Wiswesser Line Notation 2OVMR
Evaluation B

$C_9H_{11}NO_2$ (c) 39SAT/SOG
Ammonium cinnamate
Heat Capacity 323 K, C_p=252.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 165.1914
Wiswesser Line Notation QV1U1R &ZH
Evaluation C
Same data in 40SAT/SOG.

$C_9H_{11}NO_2$ (c) 63COL/HU
Phenylalanine(L)
Heat Capacity 298.15 K, C_p=203.01 J·mol^{-1}·K^{-1}
Temperature range 11 to 305 K.
Entropy 298.15 K, S=213.64 J·mol^{-1}·K^{-1}
Molecular Weight 165.1914
Wiswesser Line Notation QVYZ1R -L
Evaluation A

$C_9H_{11}NO_2$ (c) 75SPI/WAI
Phenylalanine(L)
Heat Capacity 298.15 K, C_p=203.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 165.1914
Wiswesser Line Notation QVYZ1R -L
Evaluation B

$C_9H_{11}NO_3$ (c) 37HUF/EL
Tyrosine(L)
Heat Capacity 294.6 K, C_p=214.30 J·mol^{-1}·K^{-1}
Temperature range 87 to 295 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=221.8 J·mol^{-1}·K^{-1}
Extrapolation below 90 K. 64.56 J·mol^{-1}·K^{-1}.
Molecular Weight 181.1908
Wiswesser Line Notation QVYZ1R DQ -L
Evaluation B(C_p),C(S)

$C_9H_{11}NO_3$ (c) 63COL/HU
Tyrosine(L)
Heat Capacity 298.15 K, C_p=216.44 J·mol^{-1}·K^{-1}
One temperature.
Entropy 298.15 K, S=214.01 J·mol^{-1}·K^{-1}
Molecular Weight 181.1908
Wiswesser Line Notation QVYZ1R DQ -L
Evaluation A

$C_9H_{11}NO_4$ (c) 40CAM/CA
Salicylic acid-acetamide complex; Acetamide-salicylic acid comple
Heat Capacity 293 K, C_p=169.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 197.1902
Wiswesser Line Notation QVR BQ &ZV1
Evaluation C

C_9H_{12} (liq) 55TAY/JOH
1,2,3-Trimethylbenzene
Heat Capacity 298.15 K, C_p=216.44 J·mol^{-1}·K^{-1}
Temperature range 19 to 301 K.
Entropy 298.15 K, S=267.94 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 218.70 K, ΔH=658.6 J·mol^{-1}
ΔS=3.01 J·mol^{-1}·K^{-1}
c,II/c,I 230.27 K, ΔH=1336.0 J·mol^{-1}
ΔS=5.80 J·mol^{-1}·K^{-1}
c,I/liq 247.81 K, ΔH=8180.1 J·mol^{-1}
ΔS=33.01 J·mol^{-1}·K^{-1}
Molecular Weight 120.1938
Wiswesser Line Notation 1R B1 C1
Evaluation A

C_9H_{12} (liq) 31HUF/PAR
1,2,4-Trimethylbenzene; Pseudocumene
Heat Capacity 297.3 K, C_p=212.1 J·mol^{-1}·K^{-1}
Temperature range 94 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=283.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 69.79 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 228.6 K, ΔH=12648 J·mol^{-1}
ΔS=55.3 J·mol^{-1}·K^{-1}
Molecular Weight 120.1938
Wiswesser Line Notation 1R B1 D1
Evaluation B(C_p),C(S)

C_9H_{12} (liq) 47KUR
1,2,4-Trimethylbenzene; Pseudocumene
Heat Capacity 298 K, C_p=213.0 J·mol^{-1}·K^{-1}
Temperature range 15 to 168 °C, mean C_p, five temperatures.
Molecular Weight 120.1938
Wiswesser Line Notation 1R B1 D1
Evaluation D

C_9H_{12} (liq) 55HEL/HEI
1,2,4-Trimethylbenzene; Pseudocumene
Heat Capacity 299.8 K, C_p=210.41 J·mol^{-1}·K^{-1}
Temperature range 80 to 220 °F.
Molecular Weight 120.1938
Wiswesser Line Notation 1R B1 D1
Evaluation B

C_9H_{12} (liq) 57PUT/KIL
1,2,4-Trimethylbenzene; Pseudocumene
Heat Capacity 298.15 K, C_p=214.97 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=283.38 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 229.33 K, ΔH=13190 J·mol^{-1}
ΔS=57.53 J·mol^{-1}·K^{-1}
Molecular Weight 120.1938
Wiswesser Line Notation 1R B1 D1
Evaluation A

C_9H_{12} (liq) 79AND/GRI
1,2,4-Trimethylbenzene; Pseudocumene
Heat Capacity 295.99 K, C_p=212.1 J·mol^{-1}·K^{-1}
Temperature range 293 to 430 K. Unsmoothed experimental datum given as 1.765 kJ/kg·K.
Molecular Weight 120.1938
Wiswesser Line Notation 1R B1 D1
Evaluation B

C_9H_{12} (liq) 87WIL/ING
1,2,4-Trimethylbenzene; Pseudocumene
Heat Capacity 298.15 K, C_p=213.11 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 120.1938
Wiswesser Line Notation 1R B1 D1
Evaluation B

C_9H_{12} (liq) 1881REI
1,3,5-Trimethylbenzene; Mesitylene
Heat Capacity 298 K, C_p=211.3 J·mol^{-1}·K^{-1}
Temperature range 292 to 403 K.
Molecular Weight 120.1938
Wiswesser Line Notation 1R C1 E1
Evaluation D

C_9H_{12} (liq) 47KUR
1,3,5-Trimethylbenzene; Mesitylene
Heat Capacity 298 K, C_p=213.0 J·mol^{-1}·K^{-1}
Temperature range 15 to 155 °C, mean C_p, five temperatures.
Molecular Weight 120.1938
Wiswesser Line Notation 1R C1 E1
Evaluation D

C_9H_{12} (liq) 55HEL/HEI
1,3,5-Trimethylbenzene; Mesitylene
Heat Capacity 299.8 K, C_p=201.46 J·mol^{-1}·K^{-1}
Temperature range 80 to 220 °F.
Molecular Weight 120.1938
Wiswesser Line Notation 1R C1 E1
Evaluation B

C_9H_{12} (liq) 55TAY/KIL
1,3,5-Trimethylbenzene; Mesitylene
Heat Capacity 298.15 K, C_p=209.33 J·mol^{-1}·K^{-1}
Temperature range 20 to 305 K.
Entropy 298.15 K, S=273.55 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 228.42 K, ΔH=9514.8 J·mol^{-1}
ΔS=41.65 J·mol^{-1}·K^{-1}
Metastable melting points at 221.46 K and 223.35 K.
Molecular Weight 120.1938
Wiswesser Line Notation 1R C1 E1
Evaluation A

C_9H_{12} (liq) 68REC
1,3,5-Trimethylbenzene; Mesitylene
Heat Capacity 298 K, C_p=206.5 J·mol^{-1}·K^{-1}
Temperature range 24 to 40 °C. Equation only.
Molecular Weight 120.1938
Wiswesser Line Notation 1R C1 E1
Evaluation C

C_9H_{12} (liq) 77FOR/BEN
1,3,5-Trimethylbenzene; Mesitylene
Heat Capacity 298.15 K, C_p=207.686 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 120.1938
Wiswesser Line Notation 1R C1 E1
Evaluation B

C_9H_{12} (liq) 79AND/GRI
1,3,5-Trimethylbenzene; Mesitylene
Heat Capacity 294.99 K, C_p=205.5 J·mol^{-1}·K^{-1}
Temperature range 295 to 424 K. Unsmoothed experimental datum given as 1.710 kJ/kg·K.
Molecular Weight 120.1938
Wiswesser Line Notation 1R C1 E1
Evaluation B

C_9H_{12} (liq) 79WIL/FAR
1,3,5-Trimethylbenzene; Mesitylene
Heat Capacity 298.15 K, C_p=207.66 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 120.1938
Wiswesser Line Notation 1R C1 E1
Evaluation B

C_9H_{12} (liq) 93GRO/ROU
1,3,5-Trimethylbenzene; Mesitylene
Heat Capacity 298.15 K, C_p=207.85 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 120.1938
Wiswesser Line Notation 1R C1 E1
Evaluation B

C_9H_{12} (liq) 34KOL/UDO
Isopropylbenzene; Cumene
Heat Capacity 302.0 K, C_p=198.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 120.1938
Wiswesser Line Notation 1Y1&R
Evaluation C

C_9H_{12} (liq) 34KOL/UDO2
Isopropylbenzene; Cumene
Heat Capacity 302.0 K, C_p=198.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 120.1938
Wiswesser Line Notation 1Y1&R
Evaluation C

C_9H_{12} (liq) 47KUR
Isopropylbenzene; Cumene
Heat Capacity 298 K, C_p=213.0 J·mol^{-1}·K^{-1}
Temperature range 16 to 153 °C, mean C_p, four temperatures.
Molecular Weight 120.1938
Wiswesser Line Notation 1Y1&R
Evaluation D

C_9H_{12} (liq) 52SCH/SAG
Isopropylbenzene; Cumene
Heat Capacity 299.8 K, C_p=209.41 J·mol^{-1}·K^{-1}
Temperature range 300 to 366 K.
Molecular Weight 120.1938
Wiswesser Line Notation 1Y1&R
Evaluation B

C_9H_{12} (liq) 73KIS/SU
Isopropylbenzene; Cumene
Heat Capacity 298.15 K, C_p=215.40 J·mol^{-1}·K^{-1}
Temperature range 14 to 314 K. Glass, 14 to 126 K.
Entropy 298.15 K, S=277.57 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 177.13 K, ΔH=7326 J·mol^{-1}
ΔS=41.36 J·mol^{-1}·K^{-1}
Molecular Weight 120.1938
Wiswesser Line Notation 1Y1&R
Evaluation A

C_9H_{12} (liq) 79AND/GR
Isopropylbenzene; Cumene
Heat Capacity 295.96 K, C_p=214.4 J·mol^{-1}·K^{-1}
Temperature range 296 to 413 K. Unsmoothed experimental datu given as 1.784 kJ/kg·K.
Molecular Weight 120.1938
Wiswesser Line Notation 1Y1&R
Evaluation B

C_9H_{12} (liq) 48TS
n-Propylbenzene
Heat Capacity 295 K, C_p=184 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 120.1938
Wiswesser Line Notation 3R
Evaluation C

C_9H_{12} (liq) 65MES/TO
n-Propylbenzene
Heat Capacity 298.15 K, C_p=214.72 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=287.78 J·mol^{-1}·K^{-1}
Phase Changes
c,II/liq 171.67 K, ΔH=8498 J·mol^{-1}
ΔS=49.50 J·mol^{-1}·K^{-1}
c,I/liq 173.60 K, ΔH=9268 J·mol^{-1}
ΔS=53.39 J·mol^{-1}·K^{-1}
Metastable crystals.
Molecular Weight 120.1938
Wiswesser Line Notation 3R
Evaluation A

$C_9H_{12}O$ (liq) 75NIC/WA
3-Phenylpropanol
Heat Capacity 298.15 K, C_p=280.74 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 136.1932
Wiswesser Line Notation Q3R
Evaluation B

$C_9H_{12}O$ (liq) 88BAG/GU
2,3,6-Trimethylphenol
Heat Capacity 298.15 K, C_p=224.7 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 136.1932
Wiswesser Line Notation QR B1 C1 F1
Evaluation B
Name shown in 88BAG/GUR as 2,5,6-trimethylphenol

$C_9H_{12}O_2$ (liq) 88BAG/GUR
Trimethylhydroquinone
Heat Capacity 313.65 K, C_p=217.6 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 152.1926
Wiswesser Line Notation QR B1 C1 DQ E1
Evaluation B

$C_9H_{12}O$ (c) 91KHO/ISK
2,4,6-Trimethylphenol; Mesitol
Heat Capacity 298.15 K, C_p=213.12 J·mol^{-1}·K^{-1}
Temperature range 90 to 320 K. C_p(c)=−460.08(T/100)$^{-2}$ +1250.90(T/100)$^{-1}$−1258.35+682.09(T/100)−138.79(T/100)^2 +11.79(T/100)^3 J/mol·K.
Entropy 298.15 K, S=215.13 J·mol^{-1}·K^{-1}
Molecular Weight 136.1932
Wiswesser Line Notation QR B1 D1 F1
Evaluation B

$C_9H_{13}N$ (liq) 02LOU
2,N,N-Trimethylaniline
Heat Capacity 370 K, C_p=280 J·mol^{-1}·K^{-1}
Mean value 21 to 184 °C.
Molecular Weight 135.2084
Wiswesser Line Notation 1N1&R B1
Evaluation D

$C_9H_{13}N$ (liq) 75NIC/WAD
3-Phenylpropylamine
Heat Capacity 298.15 K, C_p=265.59 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 135.2084
Wiswesser Line Notation Z3R
Evaluation B

$C_9H_{13}NO_3$ (c) 89KHO/ISK
2-Methyl-3-hydroxy-4-methoxymethyl-5-hydroxylmethylpyridine
Heat Capacity 298.15 K, C_p=231.20 J·mol^{-1}·K^{-1}
One temperature.
Entropy 298.15 K, S=277.60 J·mol^{-1}·K^{-1}
Molecular Weight 183.2066
Wiswesser Line Notation T6NJ B1 CQ D1O1 E1Q
Evaluation B

$C_9H_{14}BrN$ (c) 89VAN/WHI
3-Phenylpropylammonium bromide
Phase Changes

c,III/c,II	337 K,	ΔH=10800 J·mol^{-1}
		ΔS=3.63 J·mol^{-1}·K^{-1}
c,II/c,I	402 K,	ΔH=110 J·mol^{-1}
		ΔS=0.03 J·mol^{-1}·K^{-1}

Molecular Weight 216.1203
Wiswesser Line Notation Z3R &EH
Evaluation A

$C_9H_{14}ClN$ (c) 89VAN/WHI
3-Phenylpropylammonium chloride
Phase Changes

c,III/c,II	343 K,	ΔH=6220 J·mol^{-1}
		ΔS=2.18 J·mol^{-1}·K^{-1}
c,II/c,I	368 K,	ΔH=4240 J·mol^{-1}
		ΔS=1.39 J·mol^{-1}·K^{-1}

Molecular Weight 171.6693
Wiswesser Line Notation Z3R &GH
Evaluation A

$C_9H_{14}O$ (liq) 84BAG/BAE
2,5,6-Trimethyl-2-cyclohexen-1-one
Heat Capacity 298.15 K, C_p=258.1 J·mol^{-1}·K^{-1}
Temperature range 273 to 343 K. C_p(liq)=1.03481+0.003008T kJ/kg·K (273 to 343 K).
Molecular Weight 138.2090
Wiswesser Line Notation L6 BU CVTJ B1 E1 F1
Evaluation B

$C_9H_{14}O$ (liq) 88BAG/GUR
2,5,6-Trimethyl-2-cyclohexen-1-one
Heat Capacity 298.15 K, C_p=258.4 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 138.2090
Wiswesser Line Notation L6 BU CVTJ B1 E1 F1
Evaluation B

$C_9H_{14}O$ (c) 91WHI/PER
Bicyclo[3.3.1]nonan-9-one
Heat Capacity
Temperature range 34 to 305 K. Unsmoothed experimental data given. Transition at 300.5 makes the C_p value at 298.15 anomalous.
Phase Changes

c,II/c,I	300.5 K,	ΔH=14110 J·mol^{-1}
		ΔS=46.99 J·mol^{-1}·K^{-1}

Molecular Weight 138.2090
Wiswesser Line Notation T66 A AVTJ
Evaluation A

$C_9H_{14}O_4$ (liq) 85KAR/ABD2
Carbisopropoxy methyl methacrylate
Phase Changes
c/liq 276.5 K, ΔH=19867 J·mol^{-1}
Molecular Weight 186.2072
Wiswesser Line Notation 1Y1&OV1OVY1&U1
Evaluation A

$C_9H_{14}O_6$ (liq) 79FUC
Triacetin; Glyceryl triacetate
Heat Capacity 298.15 K, C_p=402 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 218.2060
Wiswesser Line Notation 1VOY1OV1&1OV1
Evaluation B

$C_9H_{14}O_6$ (liq) 83RAB/KHL
Triacetin; Glyceryl triacetate
Heat Capacity 300 K, C_p=384.7 J·mol^{-1}·K^{-1}
Temperature range 9 to 320 K.
Entropy 300 K, S=458.3 J·mol^{-1}·K^{-1}
Phase Changes

c/liq	275.25 K,	ΔH=25800 J·mol^{-1}
		ΔS=93.8 J·mol^{-1}·K^{-1}

Molecular Weight 218.2060
Wiswesser Line Notation 1VOY1OV1&1OV1
Evaluation A
Data also given for vitreous and supercooled liquid states from 10 to 260 K. T(glass)=198 K.

$C_9H_{14}O_6$ (liq) 86NIL/WAD
Triacetin; Glyceryl triacetate
Heat Capacity 298.15 K, C_p=389.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 218.2060
Wiswesser Line Notation 1VOY1OV1&1OV1
Evaluation A

$C_9H_{14}S$ (c) 61LAC/GOO
Thiaadamantane
Heat Capacity 298.15 K, C_p=213 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 154.2696
Wiswesser Line Notation
Evaluation B

$C_9H_{15}N_3O$ (c) 89KHO/ISK
2-Methyl-3-amino-4-methoxymethyl-5-aminomethylpyridine
Heat Capacity 298.15 K, C_p=307.10 J·mol^{-1}·K^{-1}
One temperature.
Entropy 298.15 K, S=370.25 J·mol^{-1}·K^{-1}
Molecular Weight 181.2370
Wiswesser Line Notation T6NJ B1 CZ D1O1 E1Z
Evaluation B

C_9H_{16} (liq) 70CHA/MCC
cis-Bicyclo[6.1.0]nonane
Heat Capacity 315 K, C_p=235.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 124.2254
Wiswesser Line Notation L38TJ -C
Evaluation B

C_9H_{16} (liq) 62GOL/BEL
Hexahydroindan
Heat Capacity 311 K, C_p=219.7 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 124.2254
Wiswesser Line Notation L56TJ
Evaluation C

C_9H_{16} (liq) 63GUD/CAM
Hexahydroindan
Heat Capacity 313 K, C_p=217.1 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K.
Molecular Weight 124.2254
Wiswesser Line Notation L56TJ
Evaluation C

C_9H_{16} (liq) 72FIN/MCC
cis-Hexahydroindan
Heat Capacity 298.15 K, C_p=214.18 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=265.47 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 182.28 K, ΔH=8262.6 J·mol^{-1}
ΔS=45.33 J·mol^{-1}·K^{-1}
c,II/c,I 184.9 K, ΔH=395.0 J·mol^{-1}
ΔS=2.14 J·mol^{-1}·K^{-1}
c,I/liq 236.48 K, ΔH=1397.0 J·mol^{-1}
ΔS=5.91 J·mol^{-1}·K^{-1}
Molecular Weight 124.2254
Wiswesser Line Notation L56TJ -C
Evaluation A

C_9H_{16} (liq) 72FIN/MC(
trans-Hexahydroindan
Heat Capacity 298.15 K, C_p=209.70 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=258.86 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 213.86 K, ΔH=10905.2 J·mol^{-1}
ΔS=50.99 J·mol^{-1}·K^{-1}
Molecular Weight 124.2254
Wiswesser Line Notation L56TJ -T
Evaluation A

C_9H_{16} (liq) 79FUC/PE
Allylcyclohexane
Heat Capacity 298.15 K, C_p=233.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 124.2254
Wiswesser Line Notation L6TJ A2U1
Evaluation B

$C_9H_{16}O_2$ (liq) 79FU(
Ethyl cyclohexanecarboxylate
Heat Capacity 298.15 K, C_p=271.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 156.2242
Wiswesser Line Notation L6TJ AVO2
Evaluation B

$C_9H_{16}O_4$ (c) 74CIN/BE
Azelaic acid
Phase Changes
c/liq 380.0 K, ΔH=32677 J·mol^{-1}
ΔS=85.98 J·mol^{-1}·K^{-1}
Molecular Weight 188.2230
Wiswesser Line Notation QV7VQ
Evaluation B

$(C_9H_{17}N_3O_2 \cdot HBr)_n$ (c) 91RO
Poly-L-lysine hydrobromide· alanine copolymer
Heat Capacity 300 K, C_p=297.5 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 280.1641
Wiswesser Line Notation /*VY4Z &EH &MVYM*&1/ -L
Evaluation B

$(C_9H_{17}N_3O_2 \cdot HBr)_n$ (c) 93ROL/WU
Poly-L-lysine hydrobromide· alanine copolymer
Heat Capacity 300 K, C_p=297.5 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 280.1641
Wiswesser Line Notation /*VY4Z &EH &MVYM*&1/ -L
Evaluation B

$C_9H_{17}N_3O_4$ (c) 75DAU/DE
Tri-L-alanine
Heat Capacity
Temperature range 1 to 300 K. C_p data given graphically only.
Entropy 273 K, S=356.1 J·mol^{-1}·K^{-1}
Molecular Weight 231.2510
Wiswesser Line Notation ZY1&VMY1&VMY1&VQ
Evaluation B

$C_9H_{17}O_2Tl$ (c) 76MEI/SEY
Thallium nonanoate
Phase Changes

c,IV/c,III	300 K,	$\Delta H=1674$ J·mol^{-1}
		$\Delta S=5.44$ J·mol^{-1}·K^{-1}
c,III/c,II	315 K,	$\Delta H=2636$ J·mol^{-1}
		$\Delta S=8.37$ J·mol^{-1}·K^{-1}
c,II/c,I	330 K,	$\Delta H=7531$ J·mol^{-1}
		$\Delta S=22.2$ J·mol^{-1}·K^{-1}
liq/liq	490 K,	$\Delta H=2552$ J·mol^{-1}
		$\Delta S=5.02$ J·mol^{-1}·K^{-1}

Mesophase-isotropic.

c,I/liq	410 K,	$\Delta H=5021$ J·mol^{-1}
		$\Delta S=12.1$ J·mol^{-1}·K^{-1}

Solid-mesophase.
Molecular Weight 361.6021
Wiswesser Line Notation OV8 .TL
Evaluation B
Mesophase-isotropic liquid transtion, 490.0 K, $\Delta H=2760$ J/mol, $\Delta S=5.65$ J/mol·K.

$C_9H_{17}O_2Tl$ (c) 89ROU/TUR
Thallium nonanoate

Heat Capacity	310 K,	$C_p=393$ J·mol^{-1}·K^{-1}

Temperature range 310 to 485 K.
Phase Changes

c,V/c,IV	259.3 K,	$\Delta H=1039$ J·mol^{-1}
		$\Delta S=3.99$ J·mol^{-1}·K^{-1}
c,IV/c,III	299.8 K,	$\Delta H=1563$ J·mol^{-1}
		$\Delta S=5.24$ J·mol^{-1}·K^{-1}
c,III/c,II	315.7 K,	$\Delta H=2860$ J·mol^{-1}
		$\Delta S=9.06$ J·mol^{-1}·K^{-1}
c,II/c,I	332.2 K,	$\Delta H=6934$ J·mol^{-1}
		$\Delta S=20.87$ J·mol^{-1}·K^{-1}
c,I/liq	410.9 K,	$\Delta H=6053$ J·mol^{-1}
		$\Delta S=14.72$ J·mol^{-1}·K^{-1}

Solid-mesophase.
Molecular Weight 361.6021
Wiswesser Line Notation OV8 .TL
Evaluation A

C_9H_{18} (liq) 90MES/TOD
1-Nonene

Heat Capacity	298.15 K,	$C_p=270.36$ J·mol^{-1}·K^{-1}

Temperature range 10 to 330 K.

Entropy	298.15 K,	$S=392.54$ J·mol^{-1}·K^{-1}

Phase Changes

c,II/liq	191.604 K,	$\Delta H=19969.79$ J·mol^{-1}
		$\Delta S=104.22$ J·mol^{-1}·K^{-1}
c,I/liq	191.912 K,	$\Delta H=19358.67$ J·mol^{-1}
		$\Delta S=100.87$ J·mol^{-1}·K^{-1}

Molecular Weight 126.2412
Wiswesser Line Notation 8U1
Evaluation A

C_9H_{18} (liq) 65MES/TOD2
n-Butylcyclopentane

Heat Capacity	298.15 K,	$C_p=245.35$ J·mol^{-1}·K^{-1}

Temperature range 12 to 370 K.

Entropy	298.15 K,	$S=343.84$ J·mol^{-1}·K^{-1}

Phase Changes

c/liq	165.18 K,	$\Delta H=11314$ J·mol^{-1}
		$\Delta S=68.49$ J·mol^{-1}·K^{-1}

Molecular Weight 126.2412
Wiswesser Line Notation L5TJ A4
Evaluation A

C_9H_{18} (liq) 65FIN/MES
n-Propylcyclohexane

Heat Capacity	298.15 K,	$C_p=242.04$ J·mol^{-1}·K^{-1}

Temperature range 10 to 380 K.

Entropy	298.15 K,	$S=311.88$ J·mol^{-1}·K^{-1}

Phase Changes

c/liq	178.25 K,	$\Delta H=13072$ J·mol^{-1}
		$\Delta S=58.19$ J·mol^{-1}·K^{-1}

Molecular Weight 126.2412
Wiswesser Line Notation L6TJ A3
Evaluation A

$C_9H_{18}N_2O_2$ (c) 91ABA/DEL
N-Acetylleucine-N′-methylamide(DL); 2-(Acetylamino)-N,4-dimethylpentanamide(DL)

Heat Capacity	298 K,	$C_p=274.38$ J·mol^{-1}·K^{-1}

Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 186.2534
Wiswesser Line Notation 1VMY1Y1&1&VM1 -DL
Evaluation C

$C_9H_{18}N_2O_2$ (c) 91ABA/DEL
N-Acetylleucine-N′-methylamide(L); 2-(Acetylamino)-N,4-dimethylpentanamide(L)

Heat Capacity	298 K,	$C_p=281.49$ J·mol^{-1}·K^{-1}

Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 186.2534
Wiswesser Line Notation 1VMY1Y1&1&VM1 -L
Evaluation C

$C_9H_{18}N_2O_2$ (c) 91ABA/DEL
N-Acetylisoleucine-N′-methylamide(DL); 2-(Acetylamino)-N,3-dimethylpentanamide(DL)

Heat Capacity	298 K,	$C_p=269.32$ J·mol^{-1}·K^{-1}

Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 186.2534
Wiswesser Line Notation 1VMY2&1&VM1 -DL
Evaluation C

$C_9H_{18}N_2O_2$ (c) 91ABA/DEL
N-Acetylisoleucine-N′-methylamide(L); 2-(Acetylamino)-N,3-dimethylpentanamide(L)

Heat Capacity	298 K,	$C_p=272.27$ J·mol^{-1}·K^{-1}

Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 186.2534
Wiswesser Line Notation 1VMY2&1&VM1 -L
Evaluation C

$C_9H_{18}N_2O_2$ (c) 91ABA/DEL
N-Acetylnorleucine-N′-methylamide(DL); 2-(Acetylamino)-N-methylhexanamide(DL)

Heat Capacity	298 K,	$C_p=287.74$ J·mol^{-1}·K^{-1}

Data extrapolation to 298 K from values obtained at higher temperatures.
Molecular Weight 186.2534
Wiswesser Line Notation 1VMY4&VM1 -DL
Evaluation C

$C_9H_{18}N_2O_3$ (c) 89KUL/KOZ
α-Alanylnorleucine(DL)
Heat Capacity 298 K, C_p=275.7 J·mol^{-1}·K^{-1}
Temperature range 298 to 348 K.
Molecular Weight 202.2528
Wiswesser Line Notation ZY1&VMY4&VQ
Evaluation C

$C_9H_{18}N_2O_3$ (c) 90BAD/KUL
Alanylnorleucine(DL)
Heat Capacity 298 K, C_p=276 J·mol^{-1}·K^{-1}
Temperature range 298, 313, 333, 348 K.
Molecular Weight 202.1738
Wiswesser Line Notation ZY1&VMY4&VQ -DL
Evaluation D

$C_9H_{18}O$ (liq) 89VES/BAR
2,6-Dimethyl-4-heptanone; Diisobutylketone
Heat Capacity 298.15 K, C_p=297.3 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K.
Molecular Weight 142.2406
Wiswesser Line Notation 1Y1&1V1Y1&1
Evaluation A

$C_9H_{18}O$ (liq) 92SVO/KUB
2,6-Dimethyl-4-heptanone; Diisobutylketone
Phase Changes
liq/g 379.3 K, ΔH=38600 J·mol^{-1}
Value corrected to 298.15 K, obtained by extrapolation.
Molecular Weight 142.2406
Wiswesser Line Notation 1Y1&1V1Y1&1
Evaluation A

$C_9H_{18}O$ (liq) 70AND/COU
5-Nonanone; Di-n-butyl ketone
Heat Capacity 298.15 K, C_p=303.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=401.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 110 K, ΔH=373 J·mol^{-1}
ΔS=3.39 J·mol^{-1}·K^{-1}
c,I/liq 269.31 K, ΔH=24930 J·mol^{-1}
ΔS=92.56 J·mol^{-1}·K^{-1}
Molecular Weight 142.2406
Wiswesser Line Notation 4V4
Evaluation A

$C_9H_{18}O$ (liq) 70HAR/HEA
5-Nonanone; Di-n-butyl ketone
Heat Capacity 298.15 K, C_p=303.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2406
Wiswesser Line Notation 4V4
Evaluation B

$C_9H_{18}O$ (liq) 79SAL/PEA
5-Nonanone; Di-n-butyl ketone
Heat Capacity 298.15 K, C_p=306.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2406
Wiswesser Line Notation 4V4
Evaluation B

$C_9H_{18}O$ (liq) 82DYA/VA
Nonanal; Pelargonaldehyde
Entropy 298.15 K, S=397.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq ΔH=30510 J·mol^{-1}
Molecular Weight 142.2406
Wiswesser Line Notation VH8
Evaluation B

$C_9H_{18}O$ (liq) 84VAS/PE
Nonanal; Pelargonaldehyde
Heat Capacity 298.15 K, C_p=290.26 J·mol^{-1}·K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S=396.97 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 253.83 K
Molecular Weight 142.2406
Wiswesser Line Notation VH8
Evaluation A

$C_9H_{18}O_2$ (liq) 84VAS/PE
Butyl pentanoate; Butyl ester of pentanoic acid
Heat Capacity 300 K, C_p=311.0 J·mol^{-1}·K^{-1}
Temperature range 190 to 370 K.
Phase Changes
c/liq 189.37 K, ΔH=17600 J·mol^{-1}
ΔS=92.94 J·mol^{-1}·K^{-1}
Molecular Weight 158.2400
Wiswesser Line Notation 4OV4
Evaluation A

$C_9H_{18}O_2$ (liq) 84VAS/PI
Amyl butanoate; Pentyl butanoate
Heat Capacity 300 K, C_p=311.6 J·mol^{-1}·K^{-1}
Temperature range 200 to 370 K.
Phase Changes
c/liq 200.48 K, ΔH=20010 J·mol^{-1}
ΔS=99.81 J·mol^{-1}·K^{-1}
Molecular Weight 158.2400
Wiswesser Line Notation 50V3
Evaluation A

$C_9H_{18}O_2$ (liq) 88PIN/BI
Methyl octanoate
Heat Capacity 298.15 K, C_p=314.23 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 158.2400
Wiswesser Line Notation 7VO1
Evaluation B

$C_9H_{18}O_2$ (liq) 24GAR/R
Nonanoic acid; Pelargonic acid
Heat Capacity 304 K, C_p=333.9 J·mol^{-1}·K^{-1}
Temperature range −9 to 44 °C. Mean value 18 to 44 °C.
Phase Changes
c,II/c,I 268 K, ΔH=5560 J·mol^{-1}
ΔS=20.7 J·mol^{-1}·K^{-1}
c,I/liq 285.5 K, ΔH=20290 J·mol^{-1}
ΔS=71.1 J·mol^{-1}·K^{-1}
Molecular Weight 158.2400
Wiswesser Line Notation QV8
Evaluation B

$C_9H_{18}O_2$ (liq) 82SCH/MIL

Nonanoic acid; Pelargonic acid

Heat Capacity 298.15 K, C_p=362.37 J·mol^{-1}·K^{-1}

Temperature range 80 to 310 K.

Phase Changes

c,II/c,I 263.0 K, ΔH=8150 J·mol^{-1}

ΔS=28.07 J·mol^{-1}·K^{-1}

c,I/liq 285.53 K, ΔH=19823 J·mol^{-1}

ΔS=69.42 J·mol^{-1}·K^{-1}

Molecular Weight 158.2400

Wiswesser Line Notation QV8

Evaluation B

$C_9H_{18}O_4$ (liq) 82BIR/SIK

2-(2′-Hydroxyethoxy)ethyl pivalate

Heat Capacity 298.15 K, C_p=311.6 J·mol^{-1}·K^{-1}

Temperature range 270 to 370 K. Equation only. C_p=63.18+0.2288 T+0.002671 T^2 J·mol^{-1}·K^{-1}, (adjusted).

Molecular Weight 190.2388

Wiswesser Line Notation Q2O2OVX1&1&1

Evaluation C

C_9H_{20} (liq) 76FIN/MES

2,2,4,4-Tetramethylpentane

Heat Capacity 298.15 K, C_p=266.3 J·mol^{-1}·K^{-1}

Temperature range 10 to 400 K.

Entropy 298.15 K, S=331.8 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 206.61 K, ΔH=9744.1 J·mol^{-1}

ΔS=47.16 J·mol^{-1}·K^{-1}

Molecular Weight 128.2570

Wiswesser Line Notation 1X1&1&1X1&1&1

Evaluation A

C_9H_{20} (liq) 76FIN/MES

2,2,3,3-Tetramethylpentane

Heat Capacity 298.15 K, C_p=271.5 J·mol^{-1}·K^{-1}

Temperature range 10 to 400 K.

Entropy 298.15 K, S=334.8 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 174.45 K, ΔH=7325.45 J·mol^{-1}

ΔS=41.99 J·mol^{-1}·K^{-1}

c,I/liq 263.40 K, ΔH=2332.6 J·mol^{-1}

ΔS=8.86 J·mol^{-1}·K^{-1}

Molecular Weight 128.2570

Wiswesser Line Notation 2X1&1&X1&1&1

Evaluation A

C_9H_{20} (liq) 54STA/WAR

3,3-Diethylpentane: Tetraethylmethane

Heat Capacity 260 K, C_p=260.9 J·mol^{-1}·K^{-1}

Temperature range 90 to 260 K.

Phase Changes

c,II/c,I 210.1 K, ΔH=1272 J·mol^{-1}

Combined heats of transition for multiple phases.

c,I/liq 240.13 K, ΔH=10033 J·mol^{-1}

ΔS=47.82 J·mol^{-1}·K^{-1}

Combined entropies of fusion and transition.

Molecular Weight 128.2570

Wiswesser Line Notation 2X2&2&2

Evaluation B

C_9H_{20} (liq) 76FIN/MES

3,3-Diethylpentane; Tetraethylmethane

Heat Capacity 298.15 K, C_p=278.8 J·mol^{-1}·K^{-1}

Temperature range 10 to 400 K.

Entropy 298.15 K, S=333.4 J·mol^{-1}·K^{-1}

Phase Changes

c,III/c,II 208.25 K, ΔH=483.7 J·mol^{-1}

ΔS=2.32 J·mol^{-1}·K^{-1}

c,II/c,I 210.4 K, ΔH=810.4 J·mol^{-1}

ΔS=3.85 J·mol^{-1}·K^{-1}

c,I/liq 240.10 K, ΔH=10089.7 J·mol^{-1}

ΔS=42.02 J·mol^{-1}·K^{-1}

Molecular Weight 128.2570

Wiswesser Line Notation 2X2&2&2

Evaluation A

C_9H_{20} (liq) 79FUC/PEA

3,3-Diethylpentane; Tetraethylmethane

Heat Capacity 298.15 K, C_p=278.2 J·mol^{-1}·K^{-1}

One temperature.

Molecular Weight 128.2570

Wiswesser Line Notation 2X2&2&2

Evaluation B

C_9H_{20} (liq) 30PAR/HUF

n-Nonane

Heat Capacity 299.1 K, C_p=281.2 J·mol^{-1}·K^{-1}

Temperature range 224 to 299 K. Value is unsmoothed experimental datum.

Molecular Weight 128.2570

Wiswesser Line Notation 9H

Evaluation B

C_9H_{20} (liq) 31HUF/PAR

n-Nonane

Heat Capacity 297.9 K, C_p=280.7 J·mol^{-1}·K^{-1}

Temperature range 93 to 298 K. Value is unsmoothed experimental datum.

Entropy 298.1 K, S=392.9 J·mol^{-1}·K^{-1}

Extrapolation below 90 K, 83.09 J·mol^{-1}·K^{-1}.

Phase Changes

c,I/liq 219.2 K, ΔH=22121 J·mol^{-1}

ΔS=100.9 J·mol^{-1}·K^{-1}

Included heat effect due to transition just below melting point.

Molecular Weight 128.2570

Wiswesser Line Notation 9H

Evaluation B(C_p),C(S)

C_9H_{20} (liq) 47OSB/GIN

n-Nonane

Heat Capacity 298.15 K, C_p=284.01 J·mol^{-1}·K^{-1}

Temperature range 278 to 318 K.

Molecular Weight 128.2570

Wiswesser Line Notation 9H

Evaluation A

C_9H_{20} (liq) 54FIN/GRO2
n-Nonane
Heat Capacity 298.15 K, C_p=284.39 J·mol^{-1}·K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=393.67 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 217.2 K, ΔH=6280 J·mol^{-1}
ΔS=28.91 J·mol^{-1}·K^{-1}
c,I/liq 219.66 K, ΔH=15468 J·mol^{-1}
ΔS=70.42 J·mol^{-1}·K^{-1}
Molecular Weight 128.2570
Wiswesser Line Notation 9H
Evaluation A

C_9H_{20} (liq) 58SWI/ZIE
n-Nonane
Heat Capacity 350 K, C_p=322.2 J·mol^{-1}·K^{-1}
Mean value over the temperature range 22 to 129 °C.
Molecular Weight 128.2570
Wiswesser Line Notation 9H
Evaluation C

C_9H_{20} (liq) 77MIS
n-Nonane
Heat Capacity
Data in document deposited at VINITI, No. 880-77, March 10, 1977.
Molecular Weight 128.2570
Wiswesser Line Notation 9H
Evaluation B (for deposited data)

C_9H_{20} (liq) 79GRO/HAM
n-Nonane
Heat Capacity 298.15 K, C_p=284.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 128.2570
Wiswesser Line Notation 9H
Evaluation B

C_9H_{20} (liq) 82WIL/ING
n-Nonane
Heat Capacity 298.15 K, C_p=283.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 128.2570
Wiswesser Line Notation 9H
Evaluation A

C_9H_{20} (liq) 82ZAR
n-Nonane
Heat Capacity 323 K, C_p=293.2 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 128.2570
Wiswesser Line Notation 9H
Evaluation B

C_9H_{20} (liq) 88AND/PAT
n-Nonane
Heat Capacity 298.15 K, C_p=284.76 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 128.2570
Wiswesser Line Notation 9H
Evaluation B

C_9H_{20} (liq) 91BAN/GA
n-Nonane
Heat Capacity 318.15 K, C_p=292.18 J·mol^{-1}·K^{-1}
Temperature range 318 to 373 K. p=0.1 MPa.
Molecular Weight 128.2570
Wiswesser Line Notation 9H
Evaluation B

C_9H_{20} (liq) 91TRE/CC
n-Nonane
Heat Capacity 298.15 K, C_p=284.34 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 128.2570
Wiswesser Line Notation 9H
Evaluation B

$C_9H_{20}N_2O$ (liq) 90KOZ/SI
Tetraethylurea; Tetraethylcarbamide
Heat Capacity 298.15 K, C_p=355.6 J·mol^{-1}·K^{-1}
Temperature range 160 to 370 K. C_p(c)=77.10+0.7804 T (160 to 2 K); C_p(liq)=235.75+0.4019 T (290 to 370 K) J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 253 K, ΔH=20550 J·mol^{-1}
Molecular Weight 172.2698
Wiswesser Line Notation 2N2&VN2&2
Evaluation B

$C_9H_{20}N_2O$ (c) 87DEL/FI
1,3-Dibutylurea
Heat Capacity
Temperature range 298, 323, 363 K.
Phase Changes
c,II/c,I 311.5 K, ΔH=11100 J·mol^{-1}
ΔS=35.6 J·mol^{-1}·K^{-1}
c/liq 346.9 K, ΔH=14870 J·mol^{-1}
ΔS=42.8 J·mol^{-1}·K^{-1}
Molecular Weight 172.2698
Wiswesser Line Notation 4MVM4
Evaluation A

$C_9H_{20}O$ (c) 90BAT/JA
2,2,4,4-Tetramethylpentan-3-ol
Phase Changes
c,II/c,I 263 K, ΔH=1900 J·mol^{-1}
ΔS=7.03 J·mol^{-1}·K^{-1}
c,I/liq 322 K, ΔH=7300 J·mol^{-1}
ΔS=22.8 J·mol^{-1}·K^{-1}
Molecular Weight 144.2564
Wiswesser Line Notation 1X1&1&YQX1&1&1
Evaluation B

$C_9H_{20}O$ (liq) 79GRI/Y.
1-Nonanol; n-Nonyl alcohol
Heat Capacity 304.17 K. C_p=342.9 J·mol^{-1}·K^{-1}
Temperature range 304 to 464 K. p=0.98 bar.
Molecular Weight 144.2564
Wiswesser Line Notation Q9
Evaluation B

$C_9H_{20}O$ (liq) 86NAZ/BAS2
1-Nonanol; n-Nonyl alcohol
Heat Capacity 303.1 K, C_p=356.3 J·mol^{-1}·K^{-1}
Temperature range 303 to 474 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.470 kJ/kg·K.
Molecular Weight 144.2564
Wiswesser Line Notation Q9
Evaluation B

$C_9H_{20}O_4$ (liq) 82ZAR
Tripropylene glycol
Heat Capacity 298 K, C_p=440.6 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 192.2546
Wiswesser Line Notation QYOYOYQ
Evaluation B

$C_9H_{21}Al$ (liq) 84SHE/NIS
Tripropylaluminum
Heat Capacity 298.15 K, C_p=340.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=370.1 J·mol^{-1}·K^{-1}
Molecular Weight 156.2464
Wiswesser Line Notation 3-AL-3&3
Evaluation A
T(glass)=149.0 K.

$C_9H_{21}Al$ (liq) 91SHE/RAB
Tripropylaluminum
Heat Capacity 298.15 K, C_p=340.5 J·mol^{-1}·K^{-1}
Temperature range 14 to 327 K.
Entropy 298.15 K, S=370.1 J·mol^{-1}·K^{-1}
Molecular Weight 156.2464
Wiswesser Line Notation 3-AL-3&3
Evaluation A
T(glass)=149 K.

$C_9H_{21}CaCl_2N_3O_6$ (c,I) 79MAT/MAN
Tris(sarcosine) calcium chloride
Heat Capacity 298.15 K, C_p=425.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=534.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 130.8 K, ΔH=446 J·mol^{-1}
ΔS=4.3 J·mol^{-1}·K^{-1}
Second order ferroelectric transition. ΔS is not equal to the isothermal $\Delta H/T$.
Molecular Weight 378.2674
Wiswesser Line Notation OV1M1 3 &.CA.G2
Evaluation A

$C_9H_{21}CaCl_2N_3O_6$ (c) 80LOP/TEL
Tris(sarcosine) calcium chloride
Heat Capacity 300 K, C_p=424 J·mol^{-1}·K^{-1}
Temperature range 50 to 330 K. Data given graphically. Value is an estimate from graph.
Phase Changes
c,II/c,I 130.27 K
Molecular Weight 378.2674
Wiswesser Line Notation OV1M1 3 &.CA.G2
Evaluation C

$C_9H_{21}CaCl_2N_3O_6$ (c,I) 81LOP/TEL
Tris(sarcosine) calcium chloride
Heat Capacity
Temperature range 50 to 330 K. Data given graphically.
Phase Changes
c,II/c,I 130.27 K, ΔH=165.3 J·mol^{-1}
ΔS=1.34 J·mol^{-1}·K^{-1}
Second order ferroelectric transition.
Molecular Weight 378.2674
Wiswesser Line Notation OV1M1 3 &.CA.G2
Evaluation A

$C_9H_{24}N_6S_3$ (c,I) 2COP/GAN
Thiourea-cyclohexane adduct; Cyclohexane-thiourea adduct
Heat Capacity 298.15 K, C_p=139.1 J·mol^{-1}·K^{-1}
Temperature range 14 to 297 K. Values for one mole of thiourea.
Entropy 298.15 K, S=173.0 J·mol^{-1}·K^{-1}
Does not include possible zero-point entropy.
Phase Changes
c,VI/c,V 128.8 K, ΔH=3540 J·mol^{-1}
ΔS=27.50 J·mol^{-1}·K^{-1}
c,V/c,IV 130–150 K, ΔH=1026 J·mol^{-1}
ΔS=7.25 J·mol^{-1}·K^{-1}.
c,IV/c,III 153–161 K, ΔH=112 J·mol^{-1}
ΔS=0.78 J·mol^{-1}·K^{-1}.
c,III/c,II 170.8 K, ΔH=440 J·mol^{-1}
ΔS=2.60 J·mol^{-1}·K^{-1}
c,II/c,I 210–240 K, ΔH=260 J·mol^{-1}
ΔS=1.18 J·mol^{-1}·K^{-1}.
Molecular Weight 312.5088
Wiswesser Line Notation ZYZUS 3 &L6TJ
Evaluation A

$C_9H_{24}Si_2$ (c) 75GUS/KAR
1,3-Bis(trimethylsilyl)propane
Heat Capacity 298.15 K, C_p=394.34 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K. Data given graphically.
Entropy 298.15 K, S=517.14 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 223.73 K, ΔH=16058 J·mol^{-1}
ΔS=71.76 J·mol^{-1}·K^{-1}
liq/g 444.52 K, ΔH=43095 J·mol^{-1}
ΔS=96.99 J·mol^{-1}·K^{-1}
Molecular Weight 188.4596
Wiswesser Line Notation 1-SI-1&1&3-SI-1&1&1
Evaluation B

$C_9H_{24}Si_3$ (c) 75GUS/KAR
1,1,3,3,5,5-Hexamethyl-1,3,5-trisilacyclohexane
Heat Capacity 298.15 K, C_p=400.95 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K. Data given graphically.
Entropy 298.15 K, S=477.39 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.28 K, ΔH=16498 J·mol^{-1}
ΔS=61.42 J·mol^{-1}·K^{-1}
liq/g 476.55 K, ΔH=45522 J·mol^{-1}
ΔS=95.52 J·mol^{-1}·K^{-1}
Molecular Weight 216.5451
Wiswesser Line Notation T6-SI- C-SI- E-SI-TJ A1 A1 C1 C1 E1 E1
Evaluation B

$C_{10}D_{10}Fe$ (c) 83SHI/SOR

Ferrocene-d_{10}

Heat Capacity

Temperature range 13 to 300 K. Data graphically only.

Phase Changes

c,III/c,II	164.1 K,	$\Delta H = 878\ J \cdot mol^{-1}$
		$\Delta S = 5.27\ J \cdot mol^{-1} \cdot K^{-1}$

Lambda type transition in the metastable state.

c,II/c,I	251 K,	$\Delta H = 4230\ J \cdot mol^{-1}$
		$\Delta S = 16.83\ J \cdot mol^{-1} \cdot K^{-1}$

Phase transition between stable LT and stable HT phases.

Molecular Weight 196.1150

Wiswesser Line Notation L5ϕJ &1A-E/H-2 5ϕ-FE- ϕL5ϕJ &1A-E/H-2 5

Evaluation A

$C_{10}D_{10}Fe$ (c) 84SOR/SHI

Ferrocene-d_{10}

Heat Capacity	298.15 K,	$C_p = 221.94\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 13 to 300 K.

Entropy	298.15 K,	$S = 233.18\ J \cdot mol^{-1} \cdot K^{-1}$

Phase Changes

c,III/c,II	164.1 K,	$\Delta H = 878\ J \cdot mol^{-1}$
		$\Delta S = 5.27\ J \cdot mol^{-1} \cdot K^{-1}$

Lambda transition. Secondary C_p maximum at 172 K.

c,II/c,I	251 K,	$\Delta H = 4230\ J \cdot mol^{-1}$
		$\Delta S = 16.83\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 196.1150

Wiswesser Line Notation L5ϕJ &1A-E/H-2 5ϕ-FE- ϕL5ϕJ &1A-E/H-2 5

Evaluation A

Data also given for the metastable phases over temperature range 10 to 250 K.

$C_{10}F_{16}$ (liq) 81ZHO/KOS

Perfluorobicyclo[4.4.0]dec-1,6-diene

Heat Capacity	298.15 K,	$C_p = 428.4\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 6 to 300 K. 0.41 mole % impurity of sample

Entropy	298.15 K,	$S = 491.2\ J \cdot mol^{-1} \cdot K^{-1}$

Phase Changes

c,III/c,II	200.0 K,	$\Delta H = 794\ J \cdot mol^{-1}$
		$\Delta S = 3.77\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I	233.4 K,	$\Delta H = 1113\ J \cdot mol^{-1}$
		$\Delta S = 4.77\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq	264.09 K,	$\Delta H = 10473\ J \cdot mol^{-1}$
		$\Delta S = 39.66\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 424.0844

Wiswesser Line Notation L66 AU FUTJ BF BF CF CF DF DF EF EF GF GF HF HF IF IF JF JF

Evaluation A

$C_{10}F_{18}$ (liq) 81ZHO/KOS2

cis-Perfluorodecalin

Heat Capacity	298.15 K,	$C_p = 449.8\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 6 to 310 K.

Entropy	298.15 K,	$S = 514.6\ J \cdot mol^{-1} \cdot K^{-1}$

Phase Changes

c,II/c,I	232.5 K,	$\Delta H = 4243\ J \cdot mol^{-1}$
		$\Delta S = 18.24\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq	266.70 K,	$\Delta H = 10305\ J \cdot mol^{-1}$
		$\Delta S = 38.62\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 462.0812

Wiswesser Line Notation L66TTJ AF BF BF CF CF DF DF EF EF FF GF GF HF HF IF IF JF JF -C

Evaluation B

$C_{10}F_{18}$ (liq) 81ZHO/KOS2

trans-Perfluorodecalin

Heat Capacity	298.15 K,	$C_p = 446.8\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 6 to 310 K.

Entropy	298.15 K,	$S = 517.1\ J \cdot mol^{-1} \cdot K^{-1}$

Phase Changes

c/liq	294.61 K,	$\Delta H = 17962\ J \cdot mol^{-1}$
		$\Delta S = 61.09\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 462.0812

Wiswesser Line Notation L66TTJ AF BF BF CF CF DF DF EF EF FF GF GF HF HF IF IF JF JF -T

Evaluation B

$C_{10}H_2N_4$ (c) 76CLA/WOF

1,2,4,5-Tetracyanobenzene

Heat Capacity	298.15 K,	$C_p = 222.3\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 5 to 300 K.

Entropy	298.15 K,	$S = 252.7\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 178.1526

Wiswesser Line Notation NCR BCN DCN ECN

Evaluation A

$C_{10}H_2O_6$ (c) 73KAR/MOC

Pyromellitic dianhydride

Heat Capacity	300 K,	$C_p = 219.9\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 20 to 300 K.

Entropy	300 K,	$S = 236.5\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 218.1222

Wiswesser Line Notation T C565 DVOV JVOVJ

Evaluation A

$C_{10}H_2O_6$ (c) 77KAR/BAZ

Pyromellitic dianhydride

Heat Capacity	300 K,	$C_p = 219.9\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 60 to 400 K.

Entropy	300 K,	$S = 242.1\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 218.1222

Wiswesser Line Notation T C565 DVOV JVOVJ

Evaluation B

$C_{10}H_2O_6$ (c) 78DUN/RAH

Pyromellitic dianhydride

Heat Capacity	298.15 K,	$C_p = 215.7\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 5 to 300 K.

Entropy	298.15 K,	$S = 237.1\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 218.1222

Wiswesser Line Notation T C565 DVOV JVOVJ

Evaluation A

$C_{10}H_2O_6$ (c) 78MAR/CIO

Pyromellitic dianhydride

Heat Capacity	298.15 K,	$C_p = 231.4\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 298 to 580 K.

Phase Changes

c/liq	557.15 K,	$\Delta H = 15828\ J \cdot mol^{-1}$
		$\Delta S = 28.4\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 218.1222

Wiswesser Line Notation T C565 DVOV JVOVJ

Evaluation D

$C_{10}H_5Cu$ (c) 82BYK/LEB
Copper phenylethynylacetylenide
Heat Capacity 298.15 K, C_p=184.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=202.7 J·mol^{-1}·K^{-1}
Molecular Weight 188.6955
Wiswesser Line Notation -CU-1UU2UU1R
Evaluation A

$C_{10}H_6N_2O_4$ (c) 41SAT/SOG4
1,5-Dinitronaphthalene
Heat Capacity 323 K, C_p=259.4 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 218.1684
Wiswesser Line Notation L66J BNW GNW
Evaluation C
Same data in 40SAT/SOG5.

$C_{10}H_6N_2O_4$ (c) 41SAT/SOG4
1,8-Dinitronaphthalene
Heat Capacity 323 K, C_p=254.4 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 218.1684
Wiswesser Line Notation L66J BNW JNW
Evaluation C
Same data in 40SAT/SOG5.

$C_{10}H_6OS_2$ (c) 75CUC
Naphthalene-1,8-disulfide-S-oxide
Heat Capacity 298 K, C_p=518.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 473 K.
Phase Changes
c/liq 363 K, ΔH=13390 J·mol^{-1}
ΔS=36.9 J·mol^{-1}·K^{-1}
Molecular Weight 206.2768
Wiswesser Line Notation T566 1A L CSSJ CO
Evaluation B

$C_{10}H_7Br$ (c) 81CHA/HAG
2-Bromonaphthalene
Phase Changes
c,III/c,I 319 K, ΔH=5770 J·mol^{-1}
ΔS=18.09 J·mol^{-1}·K^{-1}
c,I/liq 329 K, ΔH=14400 J·mol^{-1}
ΔS=43.77 J·mol^{-1}·K^{-1}
A second order transition occurs between crystalline phases c.I and c.II over the temperature range 275 to 319 K.
Molecular Weight 207.0693
Wiswesser Line Notation L66J CE
Evaluation A

$C_{10}H_7Cl$ (liq) 81GRO/ING
1-Chloronaphthalene
Heat Capacity 298.15 K, C_p=211.37 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 162.6183
Wiswesser Line Notation L66J BG
Evaluation B

$C_{10}H_7Cl$ (liq) 86WIL/LAI
1-Chloronaphthalene
Heat Capacity 298.15 K, C_p=211.28 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 162.6183
Wiswesser Line Notation L66J BG
Evaluation B

$C_{10}H_7Cl$ (liq) 88COS/HUU
1-Chloronaphthalene
Heat Capacity 298.15 K, C_p=212.60 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 162.6183
Wiswesser Line Notation L66J BG
Evaluation B

$C_{10}H_7Cl$ (c) 78LOY/REY
2-Chloronaphthalene
Heat Capacity 250 K, C_p=150 J·mol^{-1}·K^{-1}
Temperature range 4.2 to 300 K. Data given graphically and estimated from graph. Transition at 308 K makes heat capacity at 298 K anomalous.
Phase Changes
c,III/c,II 12 K
Anomalous transition.
c,II/c,I 308 K
Anomalous transition.
Molecular Weight 162.6183
Wiswesser Line Notation L66J CG
Evaluation D(C_p); C(Phase changes)

$C_{10}H_7Cl$ (c) 91VAN/VER
2-Chloronaphthalene
Heat Capacity 298.15 K, C_p=235.64 J·mol^{-1}·K^{-1}
Temperature range 5 to 370 K. There is an extended solid-to-solid transition between 260 and 309 K, of two regions, between 260–290 and 290–309 K.
Entropy 298.15 K, S=202.13 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 309 K
c,I/liq 331.17 K, ΔH=14004 J·mol^{-1}
ΔS=42.29 J·mol^{-1}·K^{-1}
Molecular Weight 162.6183
Wiswesser Line Notation L66J CG
Evaluation A
C_p(liq)=100.208+0.37864(T/K) J·mol^{-1}·K^{-1} (333 to 368 K).
C_p(c)=58.978+0.46312(T/K) J·mol^{-1}·K^{-1} (315 to 325 K).

$C_{10}H_7F$ (c) 78LOY/REY
2-Fluoronaphthalene
Heat Capacity 250 K, C_p=190 J·mol^{-1}·K^{-1}
Temperature range 4.2 to 300 K. Data given graphically and estimated from graph. Transition at 277 K makes heat capacity at 298 K anomalous.
Phase Changes
c,IV/c,II 161 K
Anomalous transition: sharp peak.
c,III/c,II 240 K
Anomalous transition.
c,II/c,I 277 K
Anomalous transition.
c,I/liq 331 K
Molecular Weight 146.1637
Wiswesser Line Notation L66J CF
Evaluation D(C_p): C(Phase changes)

$C_{10}H_8$ (c) 04BOG
Naphthalene
Heat Capacity 298 K, C_p=172 J·mol^{-1}·K^{-1}
Temperature range 283 to 343 K.
Phase Changes
c/liq 352.3 K
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation D

$C_{10}H_8$ (c) 26AND/LYN
Naphthalene
Heat Capacity 298 K, C_p=159.4 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 °C.
Phase Changes
c/liq 353.1 K, ΔH=19000 J·mol^{-1}
ΔS=53.8 J·mol^{-1}·K^{-1}
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation C

$C_{10}H_8$ (c) 30HUF/PAR
Naphthalene
Heat Capacity 295.1 K, C_p=163.6 J·mol^{-1}·K^{-1}
Temperature range 91 to 295 K.
Entropy 298.1 K, S=166.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 53.09 J·mol^{-1}·K^{-1}.
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation B(C_p),C(S)

$C_{10}H_8$ (c) 32SPA/THO
Naphthalene
Heat Capacity 303 K, C_p=169.0 J·mol^{-1}·K^{-1}
Temperature range 30 to 190 °C.
Phase Changes
c/liq 353.0 K, ΔH=19200 J·mol^{-1}
ΔS=54.4 J·mol^{-1}·K^{-1}
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation B

$C_{10}H_8$ (c) 33SOU/BRI
Naphthalene
Heat Capacity 294.68 K, C_p=165.48 J·mol^{-1}·K^{-1}
Temperature range 15 to 295 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=162.84 J·mol^{-1}·K^{-1}
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation A

$C_{10}H_8$ (c) 34PEA/TAN
Naphthalene
Heat Capacity 297.6 K, C_p=168.07 J·mol^{-1}·K^{-1}
Temperature range 94 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=166.86 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 58.32 J·mol^{-1}·K^{-1}.
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation B(C_p),C(S)

$C_{10}H_8$ (c) 38HIC
Naphthalene
Heat Capacity 301.58 K, C_p=168.11 J·mol^{-1}·K^{-1}
Temperature range 58 to 304 K. Value is unsmoothed experimental datum.
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation A

$C_{10}H_8$ (c) 41SCH
Naphthalene
Heat Capacity 298.1 K, C_p=161.5 J·mol^{-1}·K^{-1}
Temperature range 22 to 200 °C, equations only, in t °C. C_p(c) =0.2595+0.001672t cal·g^{-1}·C^{-1} (22 to 80 °C); C_p(liq)=0.3360 +0.0008180t cal·g^{-1}·C^{-1} (80 to 200 °C).
Phase Changes
c/liq 353.4 K, ΔH=19040 J·mol^{-1}
ΔS=53.9 J·mol^{-1}·K^{-1}
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation C

$C_{10}H_8$ (c) 44EIB
Naphthalene
Heat Capacity 298.1 K, C_p=195.8 J·mol^{-1}·K^{-1}
Temperature range 30 to 200 °C, equations only in t °C. C_p(c)=0.365 cal·g^{-1}·C^{-1} (30 to 80 °C); C_p(liq)=0.329+0.000824t cal·g^{-1}·C^{-1} (80 to 200 °C).
Phase Changes
c/liq 353.4 K, ΔH=18790 J·mol^{-1}
ΔS=53.2 J·mol^{-1}·K^{-1}
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation C

$C_{10}H_8$ (c) 50UEB/ORT
Naphthalene
Heat Capacity 298.15 K, C_p=156.1 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Phase Changes
c/liq 353 K, ΔH=18785 J·mol^{-1}
ΔS=53.2 J·mol^{-1}·K^{-1}
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation C

$C_{10}H_8$ (c) 57MAS
Naphthalene
Phase Changes
c/liq 353.44 K, ΔH=18811 J·mol^{-1}
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation A

$C_{10}H_8$ (c) 57MCC/FIN
Naphthalene
Heat Capacity 298.15 K, C_p=165.69 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=167.40 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 353.43 K, ΔH=18226 J·mol^{-1}
ΔS=51.57 J·mol^{-1}·K^{-1}
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation A

$C_{10}H_8$ (c) 64DAV
Naphthalene
Heat Capacity 330 K, $C_p = 213\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 298 to 353 K. Mean value. Temperature range uncertain.
Phase Changes
c/liq 353 K, $\Delta H = 19250\ J \cdot mol^{-1}$
$\Delta S = 55\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature not measured.
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation D

$C_{10}H_8$ (c) 64RAS/BAS
Naphthalene
Heat Capacity 342 K, $C_p = 188.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 342, 384 K.
Phase Changes
c/liq 353.5 K, $\Delta H = 19100\ J \cdot mol^{-1}$
$\Delta S = 54.0\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation C

$C_{10}H_8$ (c) 80AND/CON
Naphthalene
Phase Changes
c,I/liq 353.376 K, $\Delta H = 19046\ J \cdot mol^{-1}$
$\Delta S = 53.90\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation A

$C_{10}H_8$ (c) 80RAD/RAD
Naphthalene
Phase Changes
c,I/liq 353.8 K, $\Delta H = 19000\ J \cdot mol^{-1}$
$\Delta S = 53.70\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation A

$C_{10}H_8$ (c) 84SYU/TUM
Naphthalene
Phase Changes
c/liq 354.1 K, $\Delta H = 19020\ J \cdot mol^{-1}$
$\Delta S = 53.7\ J \cdot mol^{-1} \cdot K^{-1}$
Relative error in determination ± 5%.
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation C

$C_{10}H_8$ (c) 88TOR/BAR
Naphthalene
Phase Changes
liq/g 323 K, $\Delta H = 70850\ J \cdot mol^{-1}$
$\Delta S = 219.3\ J \cdot mol^{-1} \cdot K^{-1}$
c/g 298.15 K, $\Delta H = 72320\ J \cdot mol^{-1}$
$\Delta S = 242.6\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation A

$C_{10}H_8$ (liq) 93CHI/KNI
Naphthalene
Heat Capacity 298.15 K, $C_p = 196.06\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 260 to 700 K.
Entropy 298.15 K, $S = 217.59\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation A
Values at 298.15 K were calculated with graphically extrapolated heat capacities.

$C_{10}H_8O$ (c) 26AND/LYN
α-Naphthol; 1-Hydroxynaphthalene
Heat Capacity 298 K, $C_p = 166.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 22 to 180 °C.
Phase Changes
c/liq 368.2 K, $\Delta H = 23470\ J \cdot mol^{-1}$
$\Delta S = 63.6\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 144.1726
Wiswesser Line Notation L66J BQ
Evaluation C

$C_{10}H_8O$ (c) 67PAC
α-Naphthol; 1-Hydroxynaphthalene
Heat Capacity 393 K, $C_p = 285\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Phase Changes
c/liq 369 K, $\Delta H = 23220\ J \cdot mol^{-1}$
$\Delta S = 62.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 144.1726
Wiswesser Line Notation L66J BQ
Evaluation C

$C_{10}H_8O$ (c) 26AND/LYN
β-Naphthol; 2-Hydroxynaphthalene
Heat Capacity 298 K, $C_p = 172.8\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 22 to 205 °C.
Phase Changes
c/liq 393.6 K, $\Delta H = 18790\ J \cdot mol^{-1}$
$\Delta S = 55.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 144.1726
Wiswesser Line Notation L66J CQ
Evaluation C

$C_{10}H_8O$ (c) 74DAN/DAN
β-Naphthol: 2-Hydroxynapthalene
Heat Capacity
Temperature range 60 to 310 K. Deposited in VINITI, No. 844-74, 8 April 1974.
Entropy 298.15 K, $S = 179.0\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 144.1726
Wiswesser Line Notation L66J CQ
Evaluation A

$C_{10}H_8O_2$ (c) 74DAN/DAN
2,3-Naphthalenediol; 2,3-Hydroxynaphthalene
Heat Capacity
Temperature range 60 to 310 K. Deposited in VINITI, No. 844-74, 8 April, 1974.
Entropy 298.15 K, $S = 192.0\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 160.1720
Wiswesser Line Notation L66J CQ DQ
Evaluation A

$C_{10}H_8O_3$ (c) 89ZHA/HUA
4-Methyl-7-hydroxycoumarin
Phase Changes
c/liq 460.7 K, $\Delta H = 29139\ J\cdot mol^{-1}$
$\Delta S = 63.42\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 176.1714
Wiswesser Line Notation T66 BOVJ E1 IQ
Evaluation B

$C_{10}H_9N$ (c) 40CAM/CAM
β-Naphthylamine; 2-Aminonaphthalene
Heat Capacity 293 K, $C_p = 125.9\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 143.1878
Wiswesser Line Notation L66J CZ
Evaluation C

$C_{10}H_9NO_2$ (c) 89ZHA/HUA
4-Methyl-7-aminocoumarin
Phase Changes
c/liq 499.9 K, $\Delta H = 32091\ J\cdot mol^{-1}$
$\Delta S = 64.82\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 175.1866
Wiswesser Line Notation T66 BOVJ E1 IZ
Evaluation B

$C_{10}H_{10}$ (c) 80FAL
Bullvalene; Tricyclo[3.3.2.0^{4,6}]deca-2,7,9-triene
Heat Capacity 298.15 K, $C_p = 190.38\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 5 to 450 K.
Entropy 298.15 K, $S = 174.66\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 366.5 K, $\Delta H = 15250\ J\cdot mol^{-1}$
$\Delta S = 41.61\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 130.1890
Wiswesser Line Notation L737 B C 1A J BU EU IUTJ
Evaluation A

$C_{10}H_{10}Br_2CuN_2$ (c) 90DEY/SOM
Bis(pyridine)copper bromide
Heat Capacity 300 K, $C_p = 1330\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 260 to 300 K. C_p value is a graphical estimate.
Phase Changes
c,II/c,I 278 K, $\Delta H = 2510\ J\cdot mol^{-1}$
$\Delta S = 9.08\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 381.5564
Wiswesser Line Notation T6NJ 2 .CU E2
Evaluation B

$C_{10}H_{10}Cl_2CuN_2$ (c) 90DEY/SOM
Bis(pyridine)copper chloride
Heat Capacity 300 K, $C_p = 540\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 270 to 310 K. C_p value is a graphical estimate.
Phase Changes
c,II/c,I 289 K, $\Delta H = 1067\ J\cdot mol^{-1}$
$\Delta S = 3.31\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 335.5470
Wiswesser Line Notation T6NJ 2 .CU G2
Evaluation B

$C_{10}H_{10}Cl_4N_2Si$ (c) 91KON/SE
Bis-(pyridine)silicon tetrachloride
Phase Changes
c/liq 438.65 K, $\Delta H = 128000\ J\cdot mol^{-1}$
Molecular Weight 328.0999
Wiswesser Line Notation
Evaluation A

$C_{10}H_{10}Co$ (c) 75RAB/NI
Cobaltocene
Heat Capacity 298.15 K, $C_p = 197.3\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 5 to 298.15 K.
Entropy 298.15 K, $S = 236.1\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c,II/c,I 92 K, $\Delta H = 238\ J\cdot mol^{-1}$
$\Delta S = 2.73\ J\cdot mol^{-1}\cdot K^{-1}$
Lambda transition between 70 to 140 K with a maximum at 92 K.
Molecular Weight 189.1222
Wiswesser Line Notation L5ϕJ ϕ-CO- ϕL5ϕJ
Evaluation A
See also 78RAB/NIS.

$C_{10}H_{10}Co$ (c) 76POM/AZ
Cobaltocene
Heat Capacity
Temperature range 118 to 298 K. Data given graphicall $C_p = 62.92 - 0.460T + 6.07\times10^{-3}T^2 - 9.53\times10^{-6}T^3$ (118 to 298 K). C value calculated from equation.
Molecular Weight 189.1222
Wiswesser Line Notation L5ϕJ ϕ-CO- ϕL5ϕJ
Evaluation C

$C_{10}H_{10}Co$ (c) 78RAB/NI
Cobaltocene
Heat Capacity 298.15 K, $C_p = 197.5\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 5 to 300 K.
Entropy 298.15 K, $S = 236.0\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c,II/c,I 93.5 K, $\Delta H = 238\ J\cdot mol^{-1}$
$\Delta S = 2.72\ J\cdot mol^{-1}\cdot K^{-1}$
Lambda transition between 70 to 120 K with a maximum at 93.5 K.
Molecular Weight 189.1222
Wiswesser Line Notation L5ϕJ ϕ-CO- ϕL5ϕJ
Evaluation A

$C_{10}H_{10}Cr$ (c) 75RAB/NI
Chromocene
Heat Capacity 298.15 K, $C_p = 199.1\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 5 to 298.15 K.
Entropy 298.15 K, $S = 236.0\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c,II/c,I 99.5 K, $\Delta H = 265\ J\cdot mol^{-1}$
$\Delta S = 2.57\ J\cdot mol^{-1}\cdot K^{-1}$
Lambda transition between 75 to 140 K with a maximum at 99.7 K an another flat peak at 118 K.
Molecular Weight 182.1850
Wiswesser Line Notation L5ϕJ ϕ-CR- ϕL5ϕJ
Evaluation A
See also 78RAB/NIS.

$C_{10}H_{10}Cr$ (c) 76POM/AZO
Chromocene
Heat Capacity
Temperature range 121 to 298 K. Data given graphically. $C_p = -253.6 + 0.632T + 33.52\times10^3 T^{-1}$ J·mol^{-1}·K^{-1}. (213 to 298 K).
Phase Changes
c,II/c,I 160–230 K, $\Delta S = 1.5$ J·mol^{-1}·K^{-1}
Lambda type transition.
Molecular Weight 182.1850
Wiswesser Line Notation L5ϕJ ϕ-CR- ϕL5ϕJ
Evaluation C(C_p), A(Phase changes)

$C_{10}H_{10}Cr$ (c) 78RAB/NIS
Chromocene
Heat Capacity 298.15 K, $C_p = 199.2$ J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, $S = 236.0$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 99.7 K, $\Delta H = 265$ J·mol^{-1}
$\Delta S = 2.55$ J·mol^{-1}·K^{-1}
Lambda transition between 75 to 140 K with a maximum at 99.7 K and another flat peak at 118 K.
Molecular Weight 182.1850
Wiswesser Line Notation L5ϕJ ϕ-CR- ϕL5ϕJ
Evaluation A

$C_{10}H_{10}Cr$ (c) 84CHH/POM
Chromocene
Heat Capacity 298 K, $C_p = 198.5$ J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K. Unsmoothed experimental datum.
Molecular Weight 182.1850
Wiswesser Line Notation L5ϕJ ϕ-CR- ϕL5ϕJ
Evaluation B
Lambda anomaly at 100 K.

$C_{10}H_{10}F_6FeP$ (c) 86SOR/SHI
Ferrocenium hexafluorophosphate
Heat Capacity
Temperature range 12 to 393 K. Data given graphically.
Phase Changes
c,IV/c III 210.95 K
c,III/c,II 213.05 K, $\Delta H = 1950$ J·mol^{-1}
$\Delta S = 9.54$ J·mol^{-1}·K^{-1}
$\Delta\Delta H$ and $\Delta\Delta S$ are total of c,IV/c,III and c,III/c,II transitions.
c,II/c,I 346.94 K, $\Delta H = 4840$ J·mol^{-1}
$\Delta S = 13.99$ J·mol^{-1}·K^{-1}
Molecular Weight 331.0002
Wiswesser Line Notation L5ϕJ ϕ-FE- ϕL5ϕJ &PFFFFFF
Evaluation A

$C_{10}H_{10}Fe$ (c) 60EDW/KIN
Ferrocene
Heat Capacity
Temperature range 195 to 200 K. Heat capacity measured and given graphically in region of transition.
Phase Changes
c,II/c,I 169 K, $\Delta H = 854$ J·mol^{-1}
$\Delta S = 5.31$ J·mol^{-1}·K^{-1}
Lambda transtion at 163.9 K with a secondary transition at 169 K. Data given for overall transition.
Molecular Weight 186.0360
Wiswesser Line Notation L5ϕJ ϕ-FE- ϕL5ϕJ
Evaluation A

$C_{10}H_{10}Fe$ (c) 62EDW/KIN
Ferrocene
Heat Capacity 298.16 K, $C_p = 195.9$ J·mol^{-1}·K^{-1}
Temperature range 0 to 300 K. Debye function used to evaluate heat capacity between 0 and 17 K.
Entropy 298.15 K, $S = 216.2$ J·mol^{-1}·K^{-1}
Phase Changes
Maximum transition between 163 and 165 K (163.9 K); secondary transition 171 K (graphical estimate).
Molecular Weight 186.0360
Wiswesser Line Notation L5ϕJ ϕ-FE- ϕL5ϕJ
Evaluation A

$C_{10}H_{10}Fe$ (c) 76AZO/CAL
Ferrocene
Heat Capacity 200 K, $C_p = 131$ J·mol^{-1}·K^{-1}
Temperature range 120 to 200 K.
Phase Changes
Maximum peak at 164 K; secondary peak at 169 K; c,III/c,II triclinic/monoclinic transition.
Molecular Weight 186.0360
Wiswesser Line Notation L5ϕJ ϕ-FE- ϕL5ϕJ
Evaluation B

$C_{10}H_{10}Fe$ (c) 76POM/AZO
Ferrocene
Heat Capacity
Temperature range 120 to 200 K. Data given graphically.
Phase Changes
c,II/c,I 164 K, $\Delta H = 853$ J·mol^{-1}
$\Delta S = 5.31$ J·mol^{-1}·K^{-1}
Molecular Weight 186.0360
Wiswesser Line Notation L5ϕJ ϕ-FE- ϕL5ϕJ
Evaluation A

$C_{10}H_{10}Fe$ (c) 81OGA/SOR
Ferrocene
Heat Capacity 298.15 K, $C_p = 189.56$ J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, $S = 211.85$ J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 163.9 K, $\Delta H = 900$ J·mol^{-1}
$\Delta S = 5.5$ J·mol^{-1}·K^{-1}
Lambda transition with a subsidiary C_p maximum at 169 K between metastable LT and undercooled HT phases.
c,II/c,I 242 K, $\Delta H = 4145$ J·mol^{-1}
$\Delta S = 17.13$ J·mol^{-1}·K^{-1}
Phase transition between stable LT and stable HT phases.
Molecular Weight 186.0360
Wiswesser Line Notation L5ϕJ ϕ-FE- ϕL5ϕJ
Evaluation A

$C_{10}H_{10}Fe$ (c) 81TOM/CUR
Ferrocene
Heat Capacity 298 K, $C_p = 192.5$ J·mol^{-1}·K^{-1}
Temperature range 293 to 393 K. Equation given.
Phase Changes
c/liq 447.0 K
Molecular Weight 186.0360
Wiswesser Line Notation L5ϕJ ϕ-FE- ϕL5ϕJ
Evaluation B

$C_{10}H_{10}Mn$ (c) 75RAB/NIS
Manganocene
Heat Capacity 298.15 K, C_p=208.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 298.15 K.
Entropy 298.15 K, S=251.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 55–75 K, ΔH=41 J·mol^{-1}
ΔS=0.63 J·mol^{-1}·K^{-1}
Lambda transition.
Molecular Weight 185.1270
Wiswesser Line Notation L5ϕJ ϕ-MN– ϕL5ϕJ
Evaluation A
See also 78RAB/NIS.

$C_{10}H_{10}Mn$ (c) 78RAB/NIS
Manganocene
Heat Capacity 298.15 K, C_p=208.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=251.5 J·mol^{-1}·K^{-1}
Molecular Weight 185.1270
Wiswesser Line Notation L5ϕJ ϕ-MN– ϕL5ϕJ
Evaluation A

$C_{10}H_{10}N_2O_2$ (c) 82CUE/SOL
N-Ethanol isatoxime
Phase Changes
c/liq 505 K, ΔH=28900 J·mol^{-1}
ΔS=57.2 J·mol^{-1}·K^{-1}
Molecular Weight 190.2012
Wiswesser Line Notation T56 BMVHJ DUNO2
Evaluation D

$C_{10}H_{10}Ni$ (c) 75RAB/NIS
Nickelocene
Heat Capacity 298.15 K, C_p=205.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 298.15 K.
Entropy 298.15 K, S=253.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 100–190 K, ΔH=182 J·mol^{-1}
ΔS=1.32 J·mol^{-1}·K^{-1}
Lambda transition.
Molecular Weight 188.8890
Wiswesser Line Notation L5ϕJ ϕ-NI– ϕL5ϕJ
Evaluation A
See also 78RAB/NIS.

$C_{10}H_{10}Ni$ (c) 76AZO/CAL
Nickelocene
Heat Capacity 298 K, C_p=171 J·mol^{-1}·K^{-1}
Temperature range 130 to 300 K.
Phase Changes
c,II/c,I 170–240 K, ΔS=5.3 J·mol^{-1}·K^{-1}
No peak is observed on heat capacity curve, but a deviation from normal variation occurs between 170 to 240 K.
Molecular Weight 188.8890
Wiswesser Line Notation L5ϕJ ϕ-NI– ϕL5ϕJ
Evaluation C

$C_{10}H_{10}Ni$ (c) 76POM/AZO
Nickelocene
Heat Capacity
Temperature range 127 to 303 K. Data given graphically. C_p=87.705−0.649T+5.86×10^{-3}T^2−9.29×10^{-6}T^3 J·mol^{-1}·K^{-1} (127 to 170 K: 240 to 303 K). C_p value calculated from equation.
Phase Changes
c,II/c,I 170–240 K, ΔS=5.2 J·mol^{-1}·K^{-1}
Molecular Weight 188.8890
Wiswesser Line Notation L5ϕJ ϕ-NI– ϕL5ϕJ
Evaluation C(C_p), A(Phase changes)

$C_{10}H_{10}Ni$ (c) 78RAB/NIS
Nickelocene
Heat Capacity 298.15 K, C_p=205.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=253.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 100–190 K, ΔH=182 J·mol^{-1}
ΔS=1.34 J·mol^{-1}·K^{-1}
Lambda transition over the temperature range 100 to 190 K.
Molecular Weight 188.8890
Wiswesser Line Notation L5ϕJ ϕ-NI– ϕL5ϕJ
Evaluation A

$C_{10}H_{10}O_2$ (c) 83SME/STE
9-Oxatetracyclo[5.4.0.0^{3,10}.0^{4,8}]undec-5-en-2-one
Heat Capacity 298.15 K, C_p=214.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 162.1878
Wiswesser Line Notation
Evaluation C

$C_{10}H_{10}O_2$ (c) 83SME/STE
anti-^{9,10}-10-endo-Hydroxytricylco[4.2.1.1^{2,5}]-deca-3,7-dien-9-one
Heat Capacity 298.15 K, C_p=230.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 162.1878
Wiswesser Line Notation
Evaluation C

$C_{10}H_{10}O_2$ (c) 84BEC/RUE
Homocubane-4-carboxylic acid;
4-Carboxypentacyclo [4.3.0.0^{2,5}.0^{3,8}.0^{4,7}] nonane
Heat Capacity 298 K, C_p=207 J·mol^{-1}·K^{-1}
C_p given as 0.305 cal·K^{-1}·g^{-1}.
Phase Changes
liq/g ΔH=82006 J·mol^{-1}
$\Delta\Delta H$ from 80DUC/GRU.
Molecular Weight 162.1878
Wiswesser Line Notation L444 B4 D5 4ABCD ITJ AVQ
Evaluation B

$C_{10}H_{10}O_4$ (liq) 69RAB/MAR
Dimethyl o-phthalate
Heat Capacity 300 K, C_p=303.76 J·mol^{-1}·K^{-1}
Temperature range 80 to 360 K.
Entropy 300 K, S=365.47 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 274.18 K, ΔH=16945 J·mol^{-1}
ΔS=61.8 J·mol^{-1}·K^{-1}
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR BVO1
Evaluation C
T(glass)=192 K; ΔH=527 J·mol^{-1}, ΔS=2.63 J·mol^{-1}·K^{-1}.

$C_{10}H_{10}O_4$ (liq) 70MAR/RAB
Dimethyl o-phthalate
Heat Capacity 300 K, C_p=303.8 J·mol^{-1}·K^{-1}
Temperature range 60 to 360 K.
Entropy 300 K, S=365.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 274.18 K, ΔH=16945 J·mol^{-1}
ΔS=61.8 J·mol^{-1}·K^{-1}
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR BVO1
Evaluation B
See also 69RAB/MAR. T(glass)=192.0 °C.

$C_{10}H_{10}O_4$ (liq) 78MIL
Dimethyl o-phthalate
Heat Capacity 298.15 K, C_p=309.3 J·mol^{-1}·K^{-1}
Temperature range 250 to 370 K. Data graphically and by equation only.
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR BVO1
Evaluation B

$C_{10}H_{10}O_4$ (liq) 84VAS/PET
Dimethyl o-phthalate
Heat Capacity 300 K, C_p=303.8 J·mol^{-1}·K^{-1}
Temperature range 25 to 360 K.
Entropy 300 K, S=365.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 274.18 K
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR BVO1
Evaluation A

$C_{10}H_{10}O_4$ (liq) 86RAB/NOV
Dimethyl o-phthalate
Heat Capacity 298.15 K, C_p=303.1 J·mol^{-1}·K^{-1}
Temperature range 6 to 120 K.
Entropy 298.15 K, S=353.9 J·mol^{-1}·K^{-1}
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR BVO1
Evaluation A
Low temperature study of vitreous and crystalline forms. Thermodynamic functions calculated for temperature range 0 to 360 K.

$C_{10}H_{10}O_4$ (c) 56SMI/DOL
Dimethyl terephthalate; Dimethyl p-phthalate
Heat Capacity 353 K, C_p=276.1 J·mol^{-1}·K^{-1}
Temperature range 80 to 190 °C. Equation only.
Phase Changes
c/liq 413.8 K, ΔH=32100 J·mol^{-1}
ΔS=77.6 J·mol^{-1}·K^{-1}
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR DVO1
Evaluation B

$C_{10}H_{10}O_4$ (c) 68ELL/CHR
Dimethyl terephthalate; Dimethyl p-phthalate
Heat Capacity 298.15 K, C_p=261.1 J·mol^{-1}·K^{-1}
Temperature range 30 to 200 °C.
Phase Changes
c/liq 413.79 K, ΔH=31631 J·mol^{-1}
ΔS=76.44 J·mol^{-1}·K^{-1}
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR DVO1
Evaluation B

$C_{10}H_{10}O_4$ (c) 82KAR/SHV2
Dimethyl terephthalate; Dimethyl p-phthalate
Phase Changes
c/liq 415.4 K, ΔH=32000 J·mol^{-1}
ΔS=77.0 J·mol^{-1}·K^{-1}
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR DVO1
Evaluation B

$C_{10}H_{10}Ru$ (c) 76POM/AZO
Ruthenocene
Heat Capacity
Temperature range 100 to 300 K. Data given graphically. C_p=74.33+2.59T−1.50×10^{-3}T^2+2.31×10^{-5}T^3−4.35×10^{-8}T^4 J·mol^{-1}·K^{-1} (100 to 300 K).
Molecular Weight 231.2590
Wiswesser Line Notation L5ϕJ ϕ-RU- ϕL5ϕJ
Evaluation C

$C_{10}H_{10}V$ (c) 75RAB/NIS
Vanadocene
Heat Capacity 298.15 K, C_p=204.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 298.15 K.
Entropy 298.15 K, S=240.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 130–200 K, ΔH=196 J·mol^{-1}
ΔS=1.21 J·mol^{-1}·K^{-1}
Lambda transition.
Molecular Weight 181.1305
Wiswesser Line Notation L5ϕJ ϕ-VA- ϕL5ϕJ
Evaluation A
Author reported S=304.2 J·mol^{-1}·K^{-1}.

$C_{10}H_{10}V$ (c) 78RAB/NIS
Vanadocene
Heat Capacity 298.15 K, C_p=204.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=240.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 150–200 K, ΔH=196 J·mol^{-1}
ΔS=1.21 J·mol^{-1}·K^{-1}
Lambda transition between 120 to 200 K.
Molecular Weight 181.1305
Wiswesser Line Notation L5ϕJ ϕ-VA- ϕL5ϕJ
Evaluation A

$C_{10}H_{10}V$ (c) 80CAL/BER
Vanadocene
Heat Capacity 298 K, C_p=203.3 J·mol^{-1}·K^{-1}
Temperature range 100 to 300 K. C_p between 235 to 300 K given by equation.
Phase Changes
c,II/c,I 120–235 K, ΔH=820 J·mol^{-1}
ΔS=4.64 J·mol^{-1}·K^{-1}
Lambda transition between 120 to 235 K.
Molecular Weight 181.1305
Wiswesser Line Notation L5ϕJ ϕ-VA- ϕL5ϕJ
Evaluation B

$C_{10}H_{11}N$ (c) 87MEI/DOG
2,4,6-Trimethylphenyl isocyanide
Heat Capacity 298.15 K, C_p=241.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 145.2036
Wiswesser Line Notation CNR B1 D1 F1
Evaluation C

$C_{10}H_{11}N$ (c) 87MEI/DOG
2,4,6-Trimethylbenzonitrile
Heat Capacity 298.15 K, C_p=220.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 145.2036
Wiswesser Line Notation NCR B1 D1 F1
Evaluation C

$C_{10}H_{11}NO$ (c) 93ACR/SEV
2,4,6-Trimethylbenzonitrile N-oxide
Heat Capacity 298.15 K, C_p=236.10 J·mol^{-1}·K^{-1}
Temperature range 6 to 319 K.
Entropy 298.15 K, S=265.08 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 224.3 K, ΔH=80 J·mol^{-1}
ΔS=0.35 J·mol^{-1}·K^{-1}
c,I/g 298.15 K, ΔH=87800 J·mol^{-1}
ΔS=265.08 J·mol^{-1}·K^{-1}
p=0.109 Pa.
Molecular Weight 161.2030
Wiswesser Line Notation
Evaluation A

$C_{10}H_{11}NO_3$ (c) 91WU/XIO
N-Salicylidene-β-alanine
Phase Changes
c/liq 408 K, ΔH=28500 J·mol^{-1}
ΔS=69.86 J·mol^{-1}·K^{-1}
Molecular Weight 193.2018
Wiswesser Line Notation OV2NU1R DQ
Evaluation A

$C_{10}H_{12}$ (liq) 57MCC/FIN
1,2,3,4-Tetrahydronaphthalene
Heat Capacity 298.15 K, C_p=217.44 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S=251.46 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 237.36 K, ΔH=12447 J·mol^{-1}
ΔS=52.44 J·mol^{-1}·K^{-1}
Molecular Weight 132.2048
Wiswesser Line Notation L66&TJ
Evaluation A

$C_{10}H_{12}$ (c) 77LEB/LIT4
endo-Dicyclopentadiene
Heat Capacity 298.15 K, C_p=188.7 J·mol^{-1}·K^{-1}
Temperature range 14 to 330 K.
Entropy 298.15 K, S=230.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 216 K, ΔH=9660 J·mol^{-1}
ΔS=40.0 J·mol^{-1}·K^{-1}
c,I/liq 304.8 K, ΔH=2220 J·mol^{-1}
ΔS=6.1 J·mol^{-1}·K^{-1}
Molecular Weight 132.2048
Wiswesser Line Notation L C555 A EU IUTJ -C
Evaluation A

$C_{10}H_{12}N_2O_3$ (c) 82CUE/SOL
2-Ethoxyisonitrosoacetanilide
Phase Changes
c/liq 405 K, ΔH=23000 J·mol^{-1}
ΔS=56.8 J·mol^{-1}·K^{-1}
Molecular Weight 208.2164
Wiswesser Line Notation QNU1VMR BO2
Evaluation D

$C_{10}H_{12}N_2O_3$ (c) 82CUE/SOL
4-Ethoxyisonitrosoacetanilide
Phase Changes
c/liq 490 K, ΔH=7600 J·mol^{-1}
ΔS=15.5 J·mol^{-1}·K^{-1}
Molecular Weight 208.2164
Wiswesser Line Notation QVU1MR DO2
Evaluation D

$C_{10}H_{12}N_2S$ (c) 28SHI
N-Allyl-N′-phenylthiourea
Heat Capacity 323 K, C_p=59.0 J·mol^{-1}·K^{-1}
Temperature range: C_p measured at 50 °, 70 °C, 99.8 °C.
Phase Changes
c/liq 375 K, ΔH=27614 J·mol^{-1}
ΔS=73.6 J·mol^{-1}·K^{-1}
Molecular Weight 192.2782
Wiswesser Line Notation 1U2MYMUS&R
Evaluation B

$C_{10}H_{12}O_2$ (liq) 83KAR/ABD
Eugenol; 5-Allylguaiacol
Heat Capacity 293 K, C_p=343.2 J·mol^{-1}·K^{-1}
Temperature range 243 to 293 K. C_p given as 2090 J·kg^{-1}·K^{-1}.
Molecular Weight 164.2036
Wiswesser Line Notation QR B01 D2U1
Evaluation B

$C_{10}H_{12}O_4$ (c) 65SIL/DAU
2-Monobenzoylglycerol
Heat Capacity 298 K, C_p=236.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 196.2024
Wiswesser Line Notation Q1Y1QOVR
Evaluation B

$C_{10}H_{12}O_4$ (c) 65SIL/DAU
1-Monobenzoylglycerol
Heat Capacity 298 K, C_p=238.9 J·mol^{-1}·K^{-1}
One temperature. β_L form.
Molecular Weight 196.2024
Wiswesser Line Notation Q1YQ1OVR
Evaluation B

$C_{10}H_{13}NO_2$ (c) 71PRI
Propyl N-phenylcarbamate
Heat Capacity 298 K, C_p=263.6 J·mol^{-1}·K^{-1}
Temperature range 200 to 390 K. Complete data deposited VINITI, No. 2713-71, 25 March 1971.
Phase Changes
c/liq 331 K, ΔH=21079 J·mol^{-1}
ΔS=63.7 J·mol^{-1}·K^{-1}
Molecular Weight 179.2182
Wiswesser Line Notation 3OVMR
Evaluation B

$C_{10}H_{14}$ (liq) 31HUF/PAR
1,2,3,4-Tetramethylbenzene; Prehnitene
Heat Capacity 291.9 K, C_p=236.0 J·mol^{-1}·K^{-1}
Temperature range 91 to 292 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=290.8 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 76.32 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 265.4 K, ΔH=11230 J·mol^{-1}
ΔS=42.3 J·mol^{-1}·K^{-1}
Molecular Weight 134.2206
Wiswesser Line Notation 1R B1 C1 D1
Evaluation B(C_p),C(S)

$C_{10}H_{14}$ (liq) 47KUR
1,2,3,4-Tetramethylbenzene; Prehnitene
Heat Capacity 298 K, C_p=244.3 J·mol^{-1}·K^{-1}
Temperature range 12 to 198 °C, mean C_p, four temperatures.
Molecular Weight 134.2206
Wiswesser Line Notation 1R B1 C1 D1
Evaluation D

$C_{10}H_{14}$ (liq) 31HUF/PAR
1,2,3,5-Tetramethylbenzene; Isodurene
Heat Capacity 297.1 K, C_p=240.2 J·mol^{-1}·K^{-1}
Temperature range 92 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=310.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 80.54 J·mol^{-1}·K^{-1}.
Phase Changes
c,I/liq 248.6 K, ΔH=12937 J·mol^{-1}
ΔS=52.0 J·mol^{-1}·K^{-1}
Value includes heat effect for solid transition below melting point.
Molecular Weight 134.2206
Wiswesser Line Notation 1R B1 C1 E1
Evaluation B(C_p),C(S)

$C_{10}H_{14}$ (liq) 31HUF/PAR
1,2,4,5-Tetramethylbenzene; Durene
Heat Capacity 297.1 K, C_p=215.1 J·mol^{-1}·K^{-1}
Temperature range 92 to 297.1 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=245.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 76.69 J·mol^{-1}·K^{-1}.
Molecular Weight 134.2206
Wiswesser Line Notation 1R B1 D1 E1
Evaluation B(C_p),C(S)

$C_{10}H_{14}$ (c) 33FER/THO
1,2,4,5-Tetramethylbenzene; Durene
Heat Capacity 303.15 K, C_p=215.6 J·mol^{-1}·K^{-1}
Temperature range 303 to 393 K.
Phase Changes
c/liq 352.05 K, ΔH=21340 J·mol^{-1}
Molecular Weight 134.2206
Wiswesser Line Notation 1R B1 D1 E1
Evaluation C

$C_{10}H_{14}$ (liq) 44EIB
1,2,4,5-Tetramethylbenzene; Durene
Heat Capacity 298.1 K, C_p=220.1 J·mol^{-1}·K^{-1}
Temperature range 25 to 200 °C, equations only in t °C. C_p(c) =0.3662+0.001033t cal·g^{-1}·C^{-1} (25 to 45 °C); C_p(liq)=0.424 +0.000589t cal·g^{-1}·C^{-1} (79 to 200 °C).
Phase Changes
c/liq 352.4 K, ΔH=20880 J·mol^{-1}
ΔS=59.3 J·mol^{-1}·K^{-1}
Molecular Weight 134.2206
Wiswesser Line Notation 1R B1 D1 E1
Evaluation C

$C_{10}H_{14}$ (liq) 47KUR
1,2,4,5-Tetramethylbenzene; Durene
Heat Capacity 353 K, C_p=275.7 J·mol^{-1}·K^{-1}
Temperature range 80 to 193 °C, mean C_p, three temperatures.
Molecular Weight 134.2206
Wiswesser Line Notation 1R B1 D1 E1
Evaluation D

$C_{10}H_{14}$ (c) 89COL/JIM
1,2,4,5-Tetramethylbenzene; Durene
Heat Capacity 298.15 K, C_p=204.02 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 134.2206
Wiswesser Line Notation 1R B1 D1 E1
Evaluation C

$C_{10}H_{14}$ (liq) 30HUF/PAR
tert-Butylbenzene
Heat Capacity 294.3 K, C_p=238.11 J·mol^{-1}·K^{-1}
Temperature range 92 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=278.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 67.70 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 215.0 K, ΔH=8397 J·mol^{-1}
ΔS=39.06 J·mol^{-1}·K^{-1}
Molecular Weight 134.2206
Wiswesser Line Notation 1X1&1&R
Evaluation B(C_p),C(S)

$C_{10}H_{14}$ (liq) 31HUF/PAR
p-Cymene; 1-Isopropyl-4-methylbenzene
Heat Capacity 297.1 K, C_p=236.4 J·mol^{-1}·K^{-1}
Temperature range 92 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=306.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 80.00 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 204.2 K, ΔH=9661 J·mol^{-1}
ΔS=47.3 J·mol^{-1}·K^{-1}
Molecular Weight 134.2206
Wiswesser Line Notation 1Y1&R D1
Evaluation B(C_p),C(S)

$C_{10}H_{14}$ (liq) 47KUR
p-Cymene; 1-Isopropyl-4-methylbenzene
Heat Capacity 298 K, C_p=242.3 J·mol^{-1}·K^{-1}
Temperature range 10 to 166 °C, mean C_p, four temperatures.
Molecular Weight 134.2206
Wiswesser Line Notation 1Y1&R D1
Evaluation D

$C_{10}H_{14}$ (liq) 79AND/GRI
sec-Butylbenzene
Heat Capacity 293.74 K, C_p=241.7 J·mol^{-1}·K^{-1}
Temperature range 294 to 430 K. Unsmoothed experimental datum given as 1.801 kJ/kg·K.
Molecular Weight 134.2206
Wiswesser Line Notation 2Y1&R
Evaluation B

$C_{10}H_{14}$ (liq) 31HUF/PAR
n-Butylbenzene
Heat Capacity 298.2 K, C_p=240.2 J·mol^{-1}·K^{-1}
Temperature range 94 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=321.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 78.95 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 184.6 K, ΔH=10979 J·mol^{-1}
ΔS=59.5 J·mol^{-1}·K^{-1}
Molecular Weight 134.2206
Wiswesser Line Notation 4R
Evaluation B(C_p),C(S)

$C_{10}H_{14}$ (liq) 48TSC
n-Butylbenzene
Heat Capacity 293 K, C_p=203 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 134.2206
Wiswesser Line Notation 4R
Evaluation C

$C_{10}H_{14}$ (liq) 65MES/TOD
n-Butylbenzene
Heat Capacity 298.15 K, C_p=243.34 J·mol^{-1}·K^{-1}
Temperature range 10 to 380 K.
Entropy 298.15 K, S=321.21 J·mol^{-1}·K^{-1}
Phase Changes
c,II/liq 185.14 K, ΔH=11259 J·mol^{-1}
ΔS=60.81 J·mol^{-1}·K^{-1}
Metastable crystals.
c,I/liq 185.30 K, ΔH=11221 J·mol^{-1}
ΔS=60.56 J·mol^{-1}·K^{-1}
Molecular Weight 134.2206
Wiswesser Line Notation 4R
Evaluation A

$C_{10}H_{14}$ (liq) 73GOO2
n-Butylbenzene
Heat Capacity 298.15 K, C_p=241 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 134.2206
Wiswesser Line Notation 4R
Evaluation B

$C_{10}H_{14}CuO_4$ (c) 81TEG/FER
Copper acetylacetonate
Heat Capacity 298 K, C_p=213.4 J·mol^{-1}·K^{-1}
Temperature range 4.2 to 450 K.
Entropy 298 K, S=372.8 J·mol^{-1}·K^{-1}
Molecular Weight 261.7642
Wiswesser Line Notation D6O-CU-O ADJ D1 F1 B-& BD6O-CU-O ADJ D1 F1
Evaluation B

$C_{10}H_{14}O_4Zn$ (c) 86GRI/LAZ
Zinc acetylacetonate
Phase Changes
c/liq 400.5 K, ΔH=18200 J·mol^{-1}
ΔS=45.5 J·mol^{-1}·K^{-1}
Molecular Weight 263.5982
Wiswesser Line Notation D60-ZN-O ADJ D1 F1 B-& BD6O-ZN-O AD. D1 F1
Evaluation A

$C_{10}H_{14}Si$ (liq) 78LEB/RAB
1-Phenyl-1-methyl-1-silacyclobutane
Heat Capacity 298.15 K, C_p=273.2 J·mol^{-1}·K^{-1}
Temperature range 60 to 330 K.
Entropy 298.15 K, S=332.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 210.10 K, ΔH=12280 J·mol^{-1}
ΔS=58.5 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation T4-SI-TJ A1 AR
Evaluation A
T(glass)=140 K.

$C_{10}H_{14}Si$ (liq) 74LEB/ARC
Vinyldimethylphenylsilane
Heat Capacity 300 K, C_p=285.6 J·mol^{-1}·K^{-1}
Temperature range 50 to 300 K.
Entropy 300 K, S=376.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 190.70 K, ΔH=12259 J·mol^{-1}
ΔS=64.3 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation 1U1-SI-1&1&R
Evaluation A
T(glass)=129.0 K. Data given for glassy state from 50 to 190 K.

$C_{10}H_{14}Si$ (liq) 77LEB/RAB
Vinyldimethylphenylsilane
Heat Capacity 298.15 K, C_p=284.8 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 298.15 K, S=374.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 190.70 K, ΔH=12259 J·mol^{-1}
ΔS=64.4 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation 1U1-SI-1&1&R
Evaluation A
T(glass)=129.5 K.

$C_{10}H_{14}Si$ (liq) 81LEB/LEI
Vinyldimethylphenylsilane
Heat Capacity 298.15 K, C_p=284.8 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=374.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 190.70 K, ΔH=12300 J·mol^{-1}
ΔS=64.4 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation 1U1-SI-1&1&R
Evaluation A
T(glass)=129 K.

$(C_{10}H_{14}Si)_n$ (c) 75LEB/ARO
Polyvinyldimethylphenylsilane
Heat Capacity 298.15 K, C_p=231.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 298.15 K, S=247.2 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation /*1Y*-SI-1&1&R/
Evaluation B

$(C_{10}H_{14}Si)_n$ (c) 81LEB/LEB
Polyvinyldimethylphenylsilane
Heat Capacity 298.15 K, C_p=231.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=247.2 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation /*1Y*-SI-1&1&R/
Evaluation A

$(C_{10}H_{14}Si)_n$ (gls) 77LEB/RAB2
Polyvinyldimethylphenylsilane
Heat Capacity 298.15 K. C_p=231.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 298.15 K, S=247.2 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation /*1Y*-SI-1&1&R/
Evaluation A

$(C_{10}H_{14}Si)_n$ (gls) 78LEB/RAB3
Poly-1-phenyl-1-methyl-1-silatrimethylene
Heat Capacity 298.15 K, C_p=279.5 J·mol^{-1}·K^{-1}
Temperature range 60 to 330 K. Rubber like elastic state.
Entropy 298.15 K, S=275.1 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation /*-SI-1&R&3*/
Evaluation A
T(glass)=242 K.

$C_{10}H_{15}Cl$ (c) 88PAR/KAW
2-Chloroadamantane
Phase Changes
c,III/c,II 227 K, ΔH=470 J·mol^{-1}
ΔS=2.3 J·mol^{-1}·K^{-1}
c,II/c,I 242 K, ΔH=8300 J·mol^{-1}
ΔS=35 J·mol^{-1}·K^{-1}
Molecular Weight 170.6815
Wiswesser Line Notation L66 B6/B-H/DI A B- C 1B ITJ AG
Evaluation A

$C_{10}H_{15}F$ (c) 91KAW/GIL
1-Fluoroadamantane
Phase Changes
c,II/c,I 231 K, ΔH=1600 J·mol^{-1}
ΔS=6.9 J·mol^{-1}·K^{-1}
On heating.
Molecular Weight 154.2269
Wiswesser Line Notation L66 B6/B-H/DI A B- C 1B ITJ FF
Evaluation A

$C_{10}H_{15}N$ (liq) 34KOL/UDO
N,N-Diethylaniline
Heat Capacity 302.0 K, C_p=274.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 149.2352
Wiswesser Line Notation 2N2&R
Evaluation C

$C_{10}H_{15}N$ (liq) 34KOL/UDO2
N,N-Diethylaniline
Heat Capacity 302.3 K, C_p=274.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 149.2352
Wiswesser Line Notation 2N2&R
Evaluation C

$C_{10}H_{15}NO$ (c) 77MEI/BLO
Carvoxime(L)
Heat Capacity 298.15 K, C_p=255.7 J·mol^{-1}·K^{-1}
Temperature range 160 to 385 K.
Phase Changes
c/liq 346.5 K, ΔH=22700 J·mol^{-1}
ΔS=65.5 J·mol^{-1}·K^{-1}
Molecular Weight 165.2346
Wiswesser Line Notation L6Y BUTJ AUNQ B1 EY1&U1 -L
Evaluation B

$C_{10}H_{15}NO$ (c) 77MEI/BLO
Carvoxime(DL)
Heat Capacity 298.15 K, C_p=255.2 J·mol^{-1}·K^{-1}
Temperature range 160 to 385 K.
Phase Changes
c/liq 365.1 K, ΔH=17020 J·mol^{-1}
ΔS=46.6 J·mol^{-1}·K^{-1}
Molecular Weight 165.2346
Wiswesser Line Notation L6Y BUTJ AUNQ B1 EY1&U1
Evaluation B

$C_{10}H_{16}$ (liq) 78GOO/SCO
exo-Tetrahydrodicyclopentadiene
Heat Capacity 298.15 K, C_p=236.50 J·mol^{-1}·K^{-1}
Temperature range 275 to 365 K. Equation only. C_p calculated from equation. Cs=0.046061+0.0012371 T cal·g^{-1}·K^{-1} (275 to 365 K).
Molecular Weight 136.2364
Wiswesser Line Notation L C555 ATJ -T
Evaluation B

$C_{10}H_{16}$ (liq) 79SMI/GOO
exo-Tetrahydrodicyclopentadiene
Heat Capacity 298.15 K, C_p=236.6 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.415 cal·K^{-1}·g^{-1}.
Molecular Weight 136.2364
Wiswesser Line Notation L C555 ATJ -T
Evaluation B

$C_{10}H_{16}$ (liq) 80GOO/THO
exo-Tetrahydrodicyclopentadiene
Heat Capacity 298.15 K, C_p=213.87 J·mol^{-1}·K^{-1}
Temperature range 260 to 465 K. Equation only. C_p calculated from equation C_p (cal·K^{-1}·g^{-1})=0.10423+0.76872×10^{-3}T+0.46992 × 10^{-6}T^2 (260 to 465 K).
Molecular Weight 136.2364
Wiswesser Line Notation L C555 ATJ -T
Evaluation B

$C_{10}H_{16}$ (liq) 34KOL/UDO
Sabinene
Heat Capacity 297.0 K, C_p=252.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 136.2364
Wiswesser Line Notation L35 DYTJ AY1&1 DU1
Evaluation C

$C_{10}H_{16}$ (liq) 34KOL/UDO2
Sabinene
Heat Capacity 288.3 K, C_p=252.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 136.2364
Wiswesser Line Notation L35 DYTJ AY1&1 DU1
Evaluation C

$C_{10}H_{16}$ (c) 71BOY/SAN
Tricyclo[5.2.1.0^{2,6}]decane
Heat Capacity 329 K, C_p=241.4 J·mol^{-1}·K^{-1}
Temperature range 329 to 390 K. Four temperatures.
Phase Changes
c/liq 352 K, ΔH=2950 J·mol^{-1}
ΔS=8.4 J·mol^{-1}·K^{-1}
Molecular Weight 136.2364
Wiswesser Line Notation L556/FH 2AF JTJ
Evaluation C

$C_{10}H_{16}$ (c,I) 60CHA/WES
Adamantane; Tricyclo[3.3.1.1^{3,7}]decane
Heat Capacity 298.15 K, C_p=189.74 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=195.83 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 208.62 K, ΔH=3376 J·mol^{-1}
ΔS=16.18 J·mol^{-1}·K^{-1}
Molecular Weight 136.2364
Wiswesser Line Notation L66 B6/B-H/DI A B- C 1B ITJ
Evaluation A

$C_{10}H_{16}$ (c,I) 61WES
Adamantane; Tricyclo[3.3.1.1^{3,7}]decane
Heat Capacity 298.15 K, C_p=189.74 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K. Only values at 298.15 K given.
Entropy 298.15 K, S=195.83 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 208.62 K, ΔH=3376 J·mol^{-1}
ΔS=161.8 J·mol^{-1}·K^{-1}
Molecular Weight 136.2364
Wiswesser Line Notation L66 B6/B-H/DI A B- C 1B ITJ
Evaluation A
Details reported in other papers.

$C_{10}H_{16}$ (liq) 33KOL/UDO
Limonene
Heat Capacity 293.4 K, C_p=249.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 136.2364
Wiswesser Line Notation L6UTJ A1 DY1&U1
Evaluation C

$C_{10}H_{16}$ (liq) 34KOL/UDO2
Limonene
Heat Capacity 293.3 K, C_p=249.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 136.2364
Wiswesser Line Notation L6UTJ A1 DY1&U1
Evaluation C

$C_{10}H_{16}BrN$ (c) 89VAN/WHI
4-Phenylbutylammonium bromide
Phase Changes
c,III/c,II 353 K, ΔH=9600 J·mol^{-1}
ΔS=3.25 J·mol^{-1}·K^{-1}
c,II/c,I 393 K, ΔH=1400 J·mol^{-1}
ΔS=0.43 J·mol^{-1}·K^{-1}
Molecular Weight 230.1471
Wiswesser Line Notation Z4R &EH
Evaluation A

$C_{10}H_{16}ClN$ (c) 89VAN/WHI
4-Phenylbutylammonium chloride
Phase Changes
c,IV/c,III 243 K, ΔH=4030 J·mol^{-1}
ΔS=2.00 J·mol^{-1}·K^{-1}
c,III/c,II 274 K, ΔH=650 J·mol^{-1}
ΔS=0.29 J·mol^{-1}·K^{-1}
c,II/c,I 295 K, ΔH=270 J·mol^{-1}
ΔS=0.19 J·mol^{-1}·K^{-1}
Molecular Weight 185.6961
Wiswesser Line Notation Z4R &GH
Evaluation A

$C_{10}H_{16}N_2ClO_4$ (c) 65CHI/NAK
Wurster's Blue perchlorate; N,N,N′,N′-Tetramethyl-p-phenylene-diamine perchlorate
Heat Capacity 200 K, C_p=264 J·mol^{-1}·K^{-1}
Temperature range 80 to 200 K. Data graphically only and estimated from graph.
Phase Changes
c,II/c,I 189.9 K, ΔH=1709.6 J·mol^{-1}
ΔS=9.16 J·mol^{-1}·K^{-1}
Transition is probably first-order.
Molecular Weight 263.7004
Wiswesser Line Notation 1N1&R DN1&1 &GWW
Evaluation A

$C_{10}H_{16}N_2O_3$ (c) 89VAN/WHI
4-Phenylbutylammonium nitrate
Phase Changes
c,II/c,I 336 K, ΔH=19100 J·mol^{-1}
ΔS=6.83 J·mol^{-1}·K^{-1}
Molecular Weight 212.2480
Wiswesser Line Notation Z4R &WNQ
Evaluation A

$C_{10}H_{16}O$ (liq) 88BAG/GUR
3,7-Dimethyl-6-octen-1-yn-3-ol
Heat Capacity 313.55 K, C_p=385.2 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 152.2358
Wiswesser Line Notation 1YU3XQ1UU1
Evaluation B

$C_{10}H_{16}O$ (c) 31FRA
Camphor
Heat Capacity 298.1 K, C_p=271.2 J·mol^{-1}·K^{-1}
Temperature range 307 to 483 K.
Phase Changes
c/liq 451.5 K, ΔH=6820 J·mol^{-1}
ΔS=15.10 J·mol^{-1}·K^{-1}
Molecular Weight 152.2358
Wiswesser Line Notation L55 A CVTJ A1 A1 B1
Evaluation C
Synthetic camphor.

$C_{10}H_{16}O$ (c,I) 35WHI/MOR
Camphor(D)
Heat Capacity 259 K, C_p=243 J·mol^{-1}·K^{-1}
Temperature range 213 to 259 K.
Phase Changes
c,II/c,I 243 K, ΔH=7780 J·mol^{-1}
ΔS=32.0 J·mol^{-1}·K^{-1}
Molecular Weight 152.2358
Wiswesser Line Notation L55 A CVTJ A1 A1 B1 -D
Evaluation C

$C_{10}H_{16}O$ (c,I) 53SCH
Camphor(D)
Heat Capacity
Temperature range 238 to 247 K. C_p data given graphically only.
Phase Changes
c,II/c,I 243.9 K, ΔH=6990 J·mol^{-1}
ΔS=28.7 J·mol^{-1}·K^{-1}
Molecular Weight 152.2358
Wiswesser Line Notation L55 A CVTJ A1 A1 B1 -D
Evaluation C

$C_{10}H_{16}O$ (c,I) 89NAG/MAT
Camphor(D)
Heat Capacity 300.13 K, C_p=247.3 J·mol^{-1}·K^{-1}
Temperature range 14 to 375 K. Unsmoothed experimental datum.
Entropy 298.15 K, S=289.76 J·mol^{-1}·K^{-1}
Annealed sample.
Phase Changes
c,II/c,I 244.19 K
Molecular Weight 152.2358
Wiswesser Line Notation L55 A CVTJ A1 A1 B1 -D
Evaluation A

$C_{10}H_{16}O$ (c,I) 53SCH
Camphor(DL)
Heat Capacity
C_p data given graphically only. Temperature range −180 to 180 °C.
Phase Changes
c,II/c,I 210 K, ΔH=840 J·mol^{-1}
ΔS=4.0 J·mol^{-1}·K^{-1}
Molecular Weight 152.2358
Wiswesser Line Notation L55 A CVTJ A1 A1 B1
Evaluation C

$C_{10}H_{16}O$ (c,I) 89NAG/MAT
Camphor(DL)
Heat Capacity 251.22 K, C_p=238.7 J·mol^{-1}·K^{-1}
Temperature range 36 to 252 K. Unsmoothed experimental datum.
Annealed sample.
Entropy 298.15 K, S=290.15 J·mol^{-1}·K^{-1}
Annealed sample.
Phase Changes
c,II/c,I 218.2 K
Molecular Weight 152.2358
Wiswesser Line Notation L55 A CVTJ A1 A1 B1
Evaluation A

$C_{10}H_{16}O$ (c,I) 89NAG/MAT
Camphor(DL)
Heat Capacity 301.55 K, C_p=251.2 J·mol^{-1}·K^{-1}
Temperature range 14 to 375 K. Unsmoothed experimental datum.
Quenched sample.
Entropy 298.15 K, S=291.76 J·mol^{-1}·K^{-1}
Quenched sample.
Phase Changes
c,II/c,I 209.1 K
Molecular Weight 152.2358
Wiswesser Line Notation L55 A CVTJ A1 A1 B1
Evaluation A

$C_{10}H_{16}O$ (c) 88SAL/ABA
1-Hydroxyadamantane
Phase Changes
c,III/c,II 369.16 K, ΔH=2500 J·mol^{-1}
ΔS=6.77 J·mol^{-1}·K^{-1}
c,II/c,I 529.16 K, ΔH=7130 J·mol^{-1}
ΔS=13.25 J·mol^{-1}·K^{-1}
Molecular Weight 152.2358
Wiswesser Line Notation L66 B6 /B-H/ A B- C 1B ITJ FQ
Evaluation A

$C_{10}H_{16}O$ (c) 88SAL/ABA
2-Hydroxyadamantane
Phase Changes
c,IV/c,III 325.16 K, ΔH=300 J·mol^{-1}
ΔS=0.92 J·mol^{-1}·K^{-1}
c,III/c,II 391.16 K, ΔH=3740 J·mol^{-1}
ΔS=9.56 J·mol^{-1}·K^{-1}
c,II/c,I 516.16 K, ΔH=7750 J·mol^{-1}
ΔS=15.02 J·mol^{-1}·K^{-1}
Molecular Weight 152.2358
Wiswesser Line Notation L66 B6 /B-H/ A B- C 1B ITJ AQ
Evaluation A

$C_{10}H_{16}O$ (c) 89SAL/ABA
2-Hydroxyadamantane
Phase Changes
c,IV/c,III 325.16 K, ΔH=300 J·mol^{-1}
ΔS=0.92 J·mol^{-1}·K^{-1}
c,III/c,II 391.16 K, ΔH=3740 J·mol^{-1}
ΔS=9.56 J·mol^{-1}·K^{-1}
c,II/c,I 516.16 K, ΔH=7750 J·mol^{-1}
ΔS=15.02 J·mol^{-1}·K^{-1}
Molecular Weight 152.2358
Wiswesser Line Notation L66 B6 /B-H/ A B- C 1B ITJ AQ
Evaluation A

$C_{10}H_{16}O$ (c) 89SAL/ABA
1-Hydroxyadamantane
Phase Changes
c,III/c,II 369.16 K, ΔH=2500 J·mol^{-1}
ΔS=6.77 J·mol^{-1}·K^{-1}
c,II/c,I 529.16 K, ΔH=7130 J·mol^{-1}
ΔS=13.25 J·mol^{-1}·K^{-1}
Molecular Weight 152.2358
Wiswesser Line Notation L66 B6 /B-H/ A B- C 1B ITJ FQ
Evaluation A

$C_{10}H_{16}O$ (liq) 33KOL/UDO
Pulegone
Heat Capacity 293.3 K, C_p=274.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 152.2358
Wiswesser Line Notation L6VYTJ BUY1&1 E1
Evaluation C

$C_{10}H_{16}O$ (liq) 34KOL/UDO2
Pulegone
Heat Capacity 293.3 K, C_p=274.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 152.2358
Wiswesser Line Notation L6VYTJ BUY1&1 E1
Evaluation C

$C_{10}H_{16}O$ (liq) 82KAR/IGA
Citral; Geranial
Heat Capacity 293 K, C_p=304.5 J·mol^{-1}·K^{-1}
Temperature range 233 to 293 K. C_p given as 2000 J·kg^{-1}·K^{-1}.
Molecular Weight 152.2358
Wiswesser Line Notation VHOYUY1&3UY1&1
Evaluation B

$(C_{10}H_{16}O_4)_n$ (c) 84RAB/NIS
Polybutylene glycol adipate
Heat Capacity 298.15 K, C_p=316.7 J·mol^{-1}·K^{-1}
Temperature range 80 to 470 K. 100% crystallinity. C_p(298.15 K)=393.6 J·mol^{-1}·K^{-1} for the highly elastic state.
Entropy 298.15 K, S=334.9 J·mol^{-1}·K^{-1}
100% crystallinity. S °(298.15 K)−S °(O)=379.9 J·mol^{-1}·K^{-1} for the highly elastic state.
Phase Changes
c/liq 328.8 K, ΔH=24800 J·mol^{-1}
Molecular Weight 200.2340
Wiswesser Line Notation /*OV4VO4*/
Evaluation B
T(glass)=199 K.

$C_{10}H_{16}O_6$ (liq) 92VER/BEC
Methanetricarboxylic acid triethyl ester
Heat Capacity 298.15 K, C_p=419.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 232.2328
Wiswesser Line Notation 2OVYVO2&VO2
Evaluation B

$C_{10}H_{16}S_4$ (c) 62CHA/WES
1,3,5,7-Tetramethyl-2,4,6,8-tetrathiaadamantane
Heat Capacity 298.15 K, C_p=295.85 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=300.83 J·mol^{-1}·K^{-1}
Molecular Weight 264.4764
Wiswesser Line Notation T66 B6/B-H/DI A B- C 1B I AS B-S CS ESTJ B1 D1 F1 H1
Evaluation A

$C_{10}H_{18}$ (liq) 62GOL/BEL
Pinane
Heat Capacity 311 K, C_p=231.4 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 138.2522
Wiswesser Line Notation L46 ATJ A1 A1 E1
Evaluation C

$C_{10}H_{18}$ (liq) 63GUD/CAM
Pinane
Heat Capacity 313 K, C_p=231.8 J·mol^{-1}·K^{-1}
Temperature range 313 to 523 K.
Molecular Weight 138.2522
Wiswesser Line Notation L46 ATJ A1 A1 E1
Evaluation C

$C_{10}H_{18}$ (liq) 63GUD/CAM
Methylhydroindan
Heat Capacity 313 K, C_p=260.7 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K.
Molecular Weight 138.2522
Wiswesser Line Notation L56TJ X1
Evaluation C

$C_{10}H_{18}$ (liq) 70CHA/MCC
cis-Bicyclo[5.3.0]decane
Heat Capacity 377 K, C_p=311.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L57TJ -C
Evaluation B

$C_{10}H_{18}$ (liq) 62GOL/BEL
Bicyclopentyl
Heat Capacity 311 K, C_p=229.7 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 138.2522
Wiswesser Line Notation L5TJ A- AL5TJ
Evaluation C

$C_{10}H_{18}$ (liq) 76GOO/LEE
Bicyclopentyl
Heat Capacity 298.15 K, C_p=238.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L5TJ A- AL5TJ
Evaluation B

$C_{10}H_{18}$ (liq) 62GOL/BEL
Decahydronaphthalene; Decalin
Heat Capacity 311 K, C_p=219.2 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ
Evaluation D

$C_{10}H_{18}$ (liq) 49PAR/HAT
cis-Decahydronaphthalene; cis-Decalin
Heat Capacity 298.15 K, C_p=220.06 J·mol^{-1}·K^{-1}
Temperature range 80 to 298.15 K.
Phase Changes
c/liq 230.1 K, ΔH=2209 J·mol^{-1}
ΔS=9.6 J·mol^{-1}·K^{-1}
Molecular Weight 138.2522
Wiswesser Line Notation L66TTJ -C
Evaluation B

$C_{10}H_{18}$ (liq) 53SEY
cis-Decahydronaphthalene; cis-Decalin
Heat Capacity 298 K, C_p=233.51 J·mol^{-1}·K^{-1}
Temperature range 293 to 343 K.
Phase Changes
Lambda type transition in liquid state at 323 K.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -C
Evaluation B

$C_{10}H_{18}$ (liq) 57MCC/FIN
cis-Decahydronaphthalene; cis-Decalin
Heat Capacity 298.15 K, C_p=232.00 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S=265.01 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 242.78 K, ΔH=14414 J·mol^{-1}
ΔS=59.37 J·mol^{-1}·K^{-1}
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -C
Evaluation A

$C_{10}H_{18}$ (liq) 63GUD/CAM
cis-Decahydronaphthalene; cis-Decalin
Heat Capacity 313 K, C_p=251.0 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -C
Evaluation C

$C_{10}H_{18}$ (liq) 88SHI/OGA
cis-Decahydronaphthalene; cis-Decalin
Heat Capacity 298.15 K, C_p=232.20 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -C
Evaluation A

$C_{10}H_{18}$ (liq) 88SHI/OGA2
cis-Decahydronaphthalene; cis-Decalin
Heat Capacity 298.15 K, C_p=232.20 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -C
Evaluation A

$C_{10}H_{18}$ (liq) 89OHN/FUJ
cis-Decahydronaphthalene; cis-Decalin
Heat Capacity 298.15 K, C_p=232.08 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -C
Evaluation B

$C_{10}H_{18}$ (liq) 49PAR/HAT
trans-Decahydronaphthalene; trans-Decalin
Heat Capacity 298.15 K, C_p=217.72 J·mol^{-1}·K^{-1}
Temperature range 80 to 298.15 K.
Phase Changes
c/liq 242.4 K, ΔH=3244 J·mol^{-1}
ΔS=13.4 J·mol^{-1}·K^{-1}
Molecular Weight 138.2522
Wiswesser Line Notation L66TTJ -T
Evaluation B

$C_{10}H_{18}$ (liq) 53SEY
trans-Decahydronaphthalene; trans-Decalin
Heat Capacity 298 K, C_p=226.86 J·mol^{-1}·K^{-1}
Temperature range 293 to 413 K.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -T
Evaluation B

$C_{10}H_{18}$ (liq) 57MCC/FIN
trans-Decahydronaphthalene; trans-Decalin
Heat Capacity 298.15 K, C_p=228.49 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S=264.93 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 216.1 K, ΔH=2135.5 J·mol^{-1}
ΔS=9.88 J·mol^{-1}·K^{-1}
c,I/liq 230.18 K, ΔH=9489 J·mol^{-1}
ΔS=41.22 J·mol^{-1}·K^{-1}
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -T
Evaluation A

$C_{10}H_{18}$ (liq) 63GUD/CAM
trans-Decahydronaphthalene; trans-Decalin
Heat Capacity 313 K, C_p=250.6 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -T
Evaluation C

$C_{10}H_{18}$ (liq) 88SHI/OGA
trans-Decahydronaphthalene; trans-Decalin
Heat Capacity 298.15 K, C_p=229.17 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -T
Evaluation A

$C_{10}H_{18}$ (liq) 88SHI/OGA2
trans-Decahydronaphthalene; trans-Decalin
Heat Capacity 298.15 K, C_p=229.17 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -T
Evaluation A

$C_{10}H_{18}$ (liq) 89OHN/FUJ
trans-Decahydronaphthalene; trans-Decalin
Heat Capacity 298.15 K, C_p=229.17 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -T
Evaluation B

$C_{10}H_{18}O$ (liq) 33KOL/UDO
2,6-Dimethylocta-2,7-dien-6-ol; Coriandrol; Linalool
Heat Capacity 293.1 K, C_p=372.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 154.2516
Wiswesser Line Notation 1Y1&U3XQ1&1U1
Evaluation C

$C_{10}H_{18}O$ (liq) 34KOL/UDO2
2,6-Dimethylocta-2,7-dien-6-ol; Coriandrol; Linalool
Heat Capacity 293.1 K, C_p=372.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 154.2516
Wiswesser Line Notation 1Y1&U3XQ1&1U1
Evaluation C

$C_{10}H_{18}O_4$ (liq) 86NIL/WAD
Ethyleneglycoldibutanoate
Heat Capacity 298.15 K, C_p=380.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 202.2498
Wiswesser Line Notation 3VO2OV3
Evaluation A

$C_{10}H_{18}O_4$ (c) 74CIN/BER
Sebacic acid
Phase Changes
c/liq 404.0 K, ΔH=40807 J·mol^{-1}
ΔS=101.0 J·mol^{-1}·K^{-1}
Molecular Weight 202.2498
Wiswesser Line Notation QV8VQ
Evaluation B

$C_{10}H_{19}NO_2$ (liq) 85KAR/ABD2
Diethylaminoethyl methacrylate
Phase Changes
c/liq 207.5 K, ΔH=13080 J·mol^{-1}
ΔS=63.04 J·mol^{-1}·K^{-1}
Molecular Weight 185.2656
Wiswesser Line Notation 1UY1&VO2N2&2
Evaluation A

$C_{10}H_{19}O_2Tl$ (c) 88LOP/CHE
Thallium (I) n-decanoate
Heat Capacity 300 K, C_p=426.5 J·mol^{-1}·K^{-1}
Temperature range 6 to 480 K.
Entropy 300 K, S=403.3 J·mol^{-1}·K^{-1}
Phase Changes
c,V/c,IV 232.4 K, ΔH=2411 J·mol^{-1}
ΔS=10.39 J·mol^{-1}·K^{-1}
c,IV/c,III 288.6 K, ΔH=599 J·mol^{-1}
ΔS=2.08 J·mol^{-1}·K^{-1}
c,III/c,II 306.8 K, ΔH=4240 J·mol^{-1}
ΔS=13.89 J·mol^{-1}·K^{-1}
c,II/c,I 405.0 K, ΔH=3974 J·mol^{-1}
ΔS=12.14 J·mol^{-1}·K^{-1}.
c,I/liq 405.0 K, ΔH=5670 J·mol^{-1}
ΔS=13.97 J·mol^{-1}·K^{-1}
Solid-mesophase.
liq/liq 484.0 K, ΔH=2552 J·mol^{-1}
ΔS=5.24 J·mol^{-1}·K^{-1}
Mesophase-isotropic liquid.
Molecular Weight 375.6289
Wiswesser Line Notation OV9 .TL
Evaluation A

$C_{10}H_{20}$ (c) 80BY
2,2,5,5-Tetramethylhex-3-ene
Phase Changes
c,III/c,II 235.7 K, ΔH=1210 J·mol^{-1}
ΔS=5.13 J·mol^{-1}·K^{-1}
c,II/c,I 243.5 K, ΔH=4330 J·mol^{-1}
ΔS=17.8 J·mol^{-1}·K^{-1}
c,I/liq 268.8 K, ΔH=10250 J·mol^{-1}
ΔS=38.1 J·mol^{-1}·K^{-1}
Molecular Weight 140.2688
Wiswesser Line Notation 1X1&1&1U1X1&1&1
Evaluation A

$C_{10}H_{20}$ (liq) 57MCC/FIN
1-Decene
Heat Capacity 298.15 K, C_p=300.83 J·mol^{-1}·K^{-1}
Temperature range 11 to 360 K.
Entropy 298.15 K, S=425.01 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 198.3 K, ΔH=7950 J·mol^{-1}
ΔS=40.09 J·mol^{-1}·K^{-1}
c,I/liq 206.89 K, ΔH=13807 J·mol^{-1}
ΔS=66.74 J·mol^{-1}·K^{-1}
Molecular Weight 140.2680
Wiswesser Line Notation 9U1
Evaluation A

$C_{10}H_{20}$ (liq) 63GUD/CAN
1,4-Diethylcyclohexane
Heat Capacity 313 K, C_p=261.1 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K. 70% cis, 30% trans.
Molecular Weight 140.2680
Wiswesser Line Notation L6TJ A2 D2
Evaluation C

$C_{10}H_{20}$ (liq) 63GUD/CAN
Diethylcyclohexane
Heat Capacity 313 K, C_p=261.9 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K.
Molecular Weight 140.2680
Wiswesser Line Notation L6TJ A2 X2
Evaluation C

$C_{10}H_{20}$ (liq) 65FIN/ME
n-Butylcyclohexane
Heat Capacity 298.15 K, C_p=271.04 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=344.97 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 198.42 K, ΔH=14159 J·mol^{-1}
ΔS=71.36 J·mol^{-1}·K^{-1}
Molecular Weight 140.2680
Wiswesser Line Notation L6TJ A4
Evaluation A

$C_{10}H_{20}$ (liq) 63GUD/CAN
tert-Butylcyclohexane
Heat Capacity 313 K, C_p=264.8 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K.
Molecular Weight 140.2680
Wiswesser Line Notation L6TJ AX1&1&1
Evaluation C

$C_{10}H_{20}BrFeN_2S_4$ (c) 83YOS/SOR
Bromo bis(N,N-diethyldithiocarbamate) iron (III)
Heat Capacity 298.095 K, C_p=434.5 J·mol^{-1}·K^{-1}
Temperature range 0.4 to 393 K. Unsmoothed experimental datum.
Phase Changes
c,IV/c,III 1.347 K
Lambda type ferromagnetic transition.
c,III/c,II 9 K, ΔH=97.0 J·mol^{-1}
ΔS=11.05 J·mol^{-1}·K^{-1}
Schottky type anomaly. $\Delta\Delta H$ and $\Delta\Delta S$ values are the total of both transitions.
c,II/c,I 265.7 K, ΔH=1960 J·mol^{-1}
ΔS=7.51 J·mol^{-1}·K^{-1}
Non-magnetic phase transition.
Molecular Weight 432.2724
Wiswesser Line Notation SUYS&N2&2 2 .FE E
Evaluation A(Phase changes), C(C_p)
Values given for sample A. (see text)

$C_{10}H_{20}FeIN_2S_4$ (c) 80YOS/SOR
Iodo bis(N,N-diethyldithiocarbamato) iron (III)
Heat Capacity 296.531 K, C_p=435.6 J·mol^{-1}·K^{-1}
Temperature range 0.4 to 300 K. Data given from 0.4 to 19.8 K via ^{3}He calorimeter, and from 14 to 300 K via an adiabatic calorimeter; unsmoothed experimental datum.
Phase Changes
c,III/c,II 1.93 K, ΔH=13.2 J·mol^{-1}
ΔS=5.57 J·mol^{-1}·K^{-1}
Total entropy and enthalpy given for an antiferromagnetic to para-magnetic phase transition with a maximum at 1.937 K and a Schottky-type anomalies around 12 K are 11.36 J·mol^{-1}·K^{-1} and 134.5 J·mol^{-1}, respectively, for the temperature range 0.4 to 40 K.
Molecular Weight 553.9950
Wiswesser Line Notation SUYS&N2&2 2 .FE I
Evaluation A

$C_{10}H_{20}O$ (liq) 80DYA/VAS
Decanal; Capric aldehyde; Capraldehyde
Heat Capacity
Temperature range 50 to 350 K.
Phase Changes
c/liq 269.47 K, ΔH=30600 J·mol^{-1}
ΔS=113.6 J·mol^{-1}·K^{-1}
97.10 mol% purity.
Molecular Weight 156.2674
Wiswesser Line Notation VH9
Evaluation B
Manuscript deposited in Cent. Sci. Res. Inst. Tech. Eng. Petrochemicals, July 27, 1979.

$C_{10}H_{20}O$ (liq) 82DYA/VAS
Decanal; Capric aldehyde; Capraldehyde
Entropy 298.15 K, S=429.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq ΔH=34500 J·mol^{-1}
Molecular Weight 156.2674
Wiswesser Line Notation VH9
Evaluation B

$C_{10}H_{20}O$ (liq) 84VAS/PET
Decanal; Capric aldehyde; Capraldehyde
Heat Capacity 298.15 K, C_p=319.67 J·mol^{-1}·K^{-1}
Temperature range 10 to 337.5 K.
Entropy 298.15 K, S=429.46 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.25 K
Molecular Weight 156.2674
Wiswesser Line Notation VH9
Evaluation A

$C_{10}H_{20}O_2$ (c) 1889EYK
Decanoic acid; Capric acid
Phase Changes
c/liq 300.1 K, ΔH=29217 J·mol^{-1}
ΔS=97.4 J·mol^{-1}·K^{-1}
Molecular Weight 172.2668
Wiswesser Line Notation QV9
Evaluation C

$C_{10}H_{20}O_2$ (c) 24GAR/RAN
Decanoic acid; Capric acid
Heat Capacity 285 K, C_p=361.1 J·mol^{-1}·K^{-1}
Temperature range 0 to 65 °C. Mean value 0 to 24 °C.
Phase Changes
c/liq 304.4 K, ΔH=27990 J·mol^{-1}
ΔS=92.0 J·mol^{-1}·K^{-1}
Molecular Weight 172.2668
Wiswesser Line Notation QV9
Evaluation B

$C_{10}H_{20}O_2$ (c) 82SCH/MIL2
Decanoic acid; Capric acid
Heat Capacity 298.15 K, C_p=475.59 J·mol^{-1}·K^{-1}
Temperature range 80 to 345 K.
Phase Changes
c,I/liq 304.55 K, ΔH=27798 J·mol^{-1}
ΔS=91.28 J·mol^{-1}·K^{-1}
Molecular Weight 172.2668
Wiswesser Line Notation QV9
Evaluation B

$C_{10}H_{22}$ (liq) 30PAR/HUF
n-Decane
Heat Capacity 295.5 K, C_p=309.6 J·mol^{-1}·K^{-1}
Temperature range 242 to 296 K. Value is unsmoothed experimental datum.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 31HUF/PAR
n-Decane
Heat Capacity 297.7 K, C_p=311.3 J·mol^{-1}·K^{-1}
Temperature range 91 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=428.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 92.05 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 243.1 K, ΔH=28778 J·mol^{-1}
ΔS=118.4 J·mol^{-1}·K^{-1}
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B(C_p),C(S)

$C_{10}H_{22}$ (liq) 47OSB/GIN
n-Decane
Heat Capacity 298.15 K, $C_p = 313.97\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 278 to 318 K.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation A

$C_{10}H_{22}$ (liq) 52SCH/SAG
n-Decane
Heat Capacity 299.8 K, $C_p = 312.29\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 80 to 200 °F.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 54FIN/GRO2
n-Decane
Heat Capacity 298.15 K, $C_p = 314.47\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 12 to 300 K.
Entropy 298.15 K, $S = 425.89\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 243.51 K, $\Delta H = 28715\ J \cdot mol^{-1}$
$\Delta S = 117.92\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation A

$C_{10}H_{22}$ (liq) 75GRI/RAS
n-Decane
Heat Capacity 298 K, $C_p = 311.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 300 to 463 K.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 79GRO/HAM
n-Decane
Heat Capacity 298.15 K, $C_p = 313.3\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 82WIL/ING
n-Decane
Heat Capacity 298.15 K, $C_p = 312.5\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation A

$C_{10}H_{22}$ (liq) 82ZAR
n-Decane
Heat Capacity 298 K, $C_p = 312.8\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 298, 323, 363 K.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 83SID/SVI
n-Decane
Heat Capacity 293.15 K, $C_p = 310.26\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 84GRO/IN(
n-Decane
Heat Capacity 298.15 K, $C_p = 313.93\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 84ROU/GR(
n-Decane
Heat Capacity 298.15 K, $C_p = 314.21\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 85BAL/BR.
n-Decane
Heat Capacity 298.15 K, $C_p = 313.24\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 85COS/PA
n-Decane
Heat Capacity 298.15 K, $C_p = 314.82\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 85LAI/ROI
n-Decane
Heat Capacity 298.15 K, $C_p = 312.99\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 85LAI/ROI
n-Decane
Heat Capacity 298.15 K, $C_p = 313.09\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 85LAI/WI
n-Decane
Heat Capacity 298.15 K, $C_p = 313.09\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation A

$C_{10}H_{22}$ (liq) 86GAT/WOO
n-Decane
Heat Capacity 298.15 K, C_p=313.56 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 368.15 K.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation C

$C_{10}H_{22}$ (liq) 86TAR/AIC
n-Decane
Heat Capacity 298.15 K, C_p=315.46 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 87WIL/ING
n-Decane
Heat Capacity 298.15 K, C_p=315.46 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 88AND/PAT
n-Decane
Heat Capacity 298.15 K, C_p=315.46 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 88COS/HUU
n-Decane
Heat Capacity 298.15 K, C_p=315.32 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 88KUZ/KHA
n-Decane
Heat Capacity 298.23 K, C_p=315.0 J·mol^{-1}·K^{-1}
Temperature range 293 to 420 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.214 kJ/kg·K.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 88PER/AIC
n-Decane
Heat Capacity 298.15 K, C_p=313.46 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation A

$C_{10}H_{22}$ (liq) 88PIN/BRA
n-Decane
Heat Capacity 298.15 K, C_p=313.13 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 91BAN/GAR
n-Decane
Heat Capacity 318.15 K, C_p=323.87 J·mol^{-1}·K^{-1}
Temperature range 313 to 373 K. p=0.1 MPa.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 91TRE/COS
n-Decane
Heat Capacity 298.15 K, C_p=315.46 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 93CZA2
n-Decane
Heat Capacity 298.9 K, C_p=314.45 J·mol^{-1}·K^{-1}
One temperature. p=0.1 MPa.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 30PAR/HUF
2,7-Dimethyloctane
Heat Capacity 295.0 K, C_p=301.7 J·mol^{-1}·K^{-1}
Temperature range 223 to 295 K. Value is unsmoothed experimental datum.
Molecular Weight 142.2838
Wiswesser Line Notation 1Y1&4Y1&1
Evaluation B

$C_{10}H_{22}$ (liq) 41PAR/WES
5-Methylnonane
Heat Capacity 298.1 K, C_p=314.43 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.1 K, S=423.8 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 81.09 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 186.7 K, ΔH=16640 J·mol^{-1}
ΔS=89.13 J·mol^{-1}·K^{-1}
Molecular Weight 142.2838
Wiswesser Line Notation 4Y4&1
Evaluation B(C_p),C(S)

$C_{10}H_{22}$ (liq) 41PAR/WES
4-Methylnonane(DL)
Heat Capacity 298.1 K, C_p=317.36 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.1 K, S=425.5 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 78.99 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 174.7 K, ΔH=15188 J·mol^{-1}
ΔS=86.94 J·mol^{-1}·K^{-1}
Molecular Weight 142.2838
Wiswesser Line Notation 5Y3&1 -DL
Evaluation B(C_p),C(S)

$C_{10}H_{22}$ (liq) 41PAR/WES
3-Methylnonane(DL)
Heat Capacity 298.1 K, C_p=308.99 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.1 K, S=427.2 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 77.70 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 188.5 K, ΔH=18698 J·mol^{-1}
ΔS=99.20 J·mol^{-1}·K^{-1}
Molecular Weight 142.2838
Wiswesser Line Notation 6Y2&1 -DL
Evaluation B(C_p),C(S)

$C_{10}H_{22}$ (liq) 41PAR/WES
2-Methylnonane
Heat Capacity 298.1 K, C_p=313.30 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.1 K, S=420.1 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 81.42 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 198.8 K, ΔH=17489 J·mol^{-1}
ΔS=87.97 J·mol^{-1}·K^{-1}
Molecular Weight 142.2838
Wiswesser Line Notation 7Y1&1
Evaluation B(C_p),C(S)

$C_{10}H_{22}N_2O_{10}$ (c,I) 77CLA/CLE
Urea-trioxane inclusion compound
Heat Capacity 298.15 K, C_p=400.0 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Phase Changes
c,IV/c,III 189.91 K, ΔH=715.1 J·mol^{-1}
ΔS=3.77 J·mol^{-1}·K^{-1}
ΔS given in article does not agree with ΔH and T.
c,III/c,II 200.8 K, ΔH=633.5 J·mol^{-1}
ΔS=3.15 J·mol^{-1}·K^{-1}
ΔS given in article does not agree with ΔH and T.
c,II/c,I 242.51 K, ΔH=1878 J·mol^{-1}
ΔS=7.74 J·mol^{-1}·K^{-1}
ΔS given in article does not agree with ΔH and T.
Molecular Weight 330.2912
Wiswesser Line Notation T6O CO EOTJ 3 &ZVZ
Evaluation A

$C_{10}H_{22}N_4$ (liq) 88BOB/KAM
Dipiperazinylethane
Heat Capacity 413 K, C_p=540 J·mol^{-1}·K^{-1}
Temperature range 413 to 473 K.
Molecular Weight 174.2886
Wiswesser Line Notation T6M DNTJ D2- DT6M DNTJ
Evaluation D

$C_{10}H_{22}O$ (liq) 75WOY/KAI
1-Decanol; n-Decyl alcohol
Heat Capacity 303.15 K, C_p=377.30 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 158.2832
Wiswesser Line Notation Q10
Evaluation B

$C_{10}H_{22}O$ (liq) 79GRI/YAN
1-Decanol; n-Decyl alcohol
Heat Capacity 305.79 K, C_p=377.8 J·mol^{-1}·K^{-1}
Temperature range 305 to 463 K. p=0.98 bar.
Molecular Weight 158.2832
Wiswesser Line Notation Q10
Evaluation B

$C_{10}H_{22}O$ (liq) 79SVE
1-Decanol; n-Decyl alcohol
Heat Capacity 301 K, C_p=377 J·mol^{-1}·K^{-1}
Temperature range 301 to 461 K.
Phase Changes
liq/g 323.15 K, ΔH=78180 J·mol^{-1}
ΔS=241.93 J·mol^{-1}·K^{-1}
No pressure measurement.
Molecular Weight 158.2832
Wiswesser Line Notation Q10
Evaluation B

$C_{10}H_{22}O$ (liq) 85COS/PAT
1-Decanol; n-Decyl alcohol
Heat Capacity 298.15 K, C_p=369.96 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 158.2832
Wiswesser Line Notation Q10
Evaluation B

$C_{10}H_{22}O$ (liq) 88AND/PAT
1-Decanol; n-Decyl alcohol
Heat Capacity 298.15 K, C_p=372.98 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 158.2832
Wiswesser Line Notation Q10
Evaluation B

$C_{10}H_{22}O$ (liq) 88NAZ/BAS
1-Decanol; n-Decyl alcohol
Heat Capacity 304.05 K, C_p=387.8 J·mol^{-1}·K^{-1}
Temperature range 304 to 497 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.45 kJ/kg·K. C_p data given at pressures from 0.1 to 50 MPa.
Molecular Weight 158.2832
Wiswesser Line Notation Q10
Evaluation B

$C_{10}H_{22}O$ (liq) 88CAC/COS
3,7-Dimethyl-1-octanol
Heat Capacity 298.15 K, C_p=367.21 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 158.2832
Wiswesser Line Notation Q2Y1&3Y1&1
Evaluation B

$C_{10}H_{22}O$ (liq) 88CAC/COS
4-Propyl-4-heptanol
Heat Capacity 298.15 K, C_p=446.60 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 158.2832
Wiswesser Line Notation QX3&3&3
Evaluation B

$C_{10}H_{22}O$ (liq) 88CAC/COS
5-Decanol
Heat Capacity 298.15 K, C_p=405.77 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 158.2832
Wiswesser Line Notation QY5&4
Evaluation B

$C_{10}H_{22}O_2$ (liq) 47CON/ELV
6-Methyl-5,7-dioxaundecane; Acetaldehyde dibutyl acetal
Heat Capacity 298 K, C_p=352.20 J·mol^{-1}·K^{-1}
Temperature range 298 to 353 K.
Molecular Weight 174.2826
Wiswesser Line Notation 4OY1&O4
Evaluation B

$C_{10}H_{22}O_5$ (liq) 91TRE/COS
2,5,8,11,14-Pentaoxapentadecane
Heat Capacity 298.15 K, C_p=457.10 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 222.2808
Wiswesser Line Notation 1O2O2O2O2O1
Evaluation B

$C_{10}H_{22}O_6$ (liq) 79STE/TAM
1,14-Dihydroxy-3,6,9,12-tetraoxatetradecane; Pentaethylene glycol
Heat Capacity 298 K, C_p=515.5 J·mol^{-1}·K^{-1}
Temperature range 273 to 513 K.
Molecular Weight 238.2802
Wiswesser Line Notation Q2O2O2O2O2Q
Evaluation B

$C_{10}H_{22}S$ (liq) 66GOO/DEP
1-Decanethiol; n-Decyl mercaptan
Heat Capacity 298.15 K, C_p=349.63 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 174.3438
Wiswesser Line Notation SH10
Evaluation A

$C_{10}H_{22}S$ (liq) 70FIN/MCC
1-Decanethiol; n-Decyl mercaptan
Heat Capacity 298.15 K, C_p=350.41 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=476.13 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 247.86 K, ΔH=33317 J·mol^{-1}
ΔS=134.42 J·mol^{-1}·K^{-1}
Molecular Weight 174.3438
Wiswesser Line Notation SH10
Evaluation A

$C_{10}H_{22}S$ (liq) 82TUT/GAB
1-Decanethiol; n-Decyl mercaptan
Heat Capacity 300 K, C_p=365.44 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K. C_p=346.70+3.600×10^{-2}T +8.824×10^{-5}T^2.
Molecular Weight 174.3438
Wiswesser Line Notation SH10
Evaluation B

$C_{10}H_{24}ClN$ (c) 88VAN/WHI
Di-n-pentylammonium chloride
Heat Capacity 296.32 K, C_p=353.9 J·mol^{-1}·K^{-1}
Temperature range 25 to 350 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 243.84 K, ΔH=1312.5 J·mol^{-1}
ΔS=5.38 J·mol^{-1}·K^{-1}
Molecular Weight 193.7593
Wiswesser Line Notation 5M5 &GH
Evaluation A

$C_{10}H_{24}N_4$ (c) 80CLA/STE
Cyclam; 1,4,8,11-Tetraazacyclotetradecane
Heat Capacity 298.15 K, C_p=374.61 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.87 J·g^{-1}·K^{-1}.
Molecular Weight 200.3264
Wiswesser Line Notation T14M DM HM KMTJ
Evaluation B

$C_{10}H_{24}N_4{\cdot}Cu(NO_3)_2$ (c) 80CLA/STE
Bis(nitrato)(1,4,8,11-tetraazacyclotetradecane) copper (II); 1,4,8,11-Tetraazacyclotetradecane copper (II) nitrate
Heat Capacity 298.15 K, C_p=915.40 J·mol^{-1}·K^{-1}
One temperature. C_p given as 2.36 J·g^{-1}·K^{-1}.
Molecular Weight 387.8822
Wiswesser Line Notation T14M DM HM KMTJ &.CU..N-O3*2
Evaluation B

$C_{10}H_{25}N_5$ (liq) 88BOB/KAM
N-(2-Aminoethyl-N′-[(2-aminoethyl)2-aminoethyl] piperazine
Heat Capacity 333 K, C_p=529 J·mol^{-1}·K^{-1}
Temperature range 333 to 473 K.
Molecular Weight 191.3190
Wiswesser Line Notation T6N DNTJ A2M2Z D2Z
Evaluation D

$C_{10}H_{26}N_6S_3$ (c,I) 72COP/GAN
Cycloheptane-thiourea adduct; Thiourea-cycloheptane adduct
Heat Capacity 298.15 K, C_p=148.3 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Values for one mole of thiourea.
Entropy 298.15 K, S=179.0 J·mol^{-1}·K^{-1}
Does not include possible zero-point entropy.
Phase Changes
c,V/c,IV 162.4 K, ΔH=368 J·mol^{-1}
ΔS=2.24 J·mol^{-1}·K^{-1}
c,IV/c,III 241 K, ΔH=568 J·mol^{-1}
ΔS=2.36 J·mol^{-1}·K^{-1}
c,III/c,II 262 K, ΔH=93 J·mol^{-1}
ΔS=0.36 J·mol^{-1}·K^{-1}
Shallow hump at 270 to 290 K, ΔH=4802 J·mol^{-1} (thiourea), ΔS=34.50 J·mol^{-1}·K^{-1}.
Molecular Weight 326.5356
Wiswesser Line Notation ZYZUS 3 &L7TJ
Evaluation A

$C_{10}H_{26}O_3Si_3$ (liq) 87DZH/KUL3
1,1,3,3-Tetraethyl-5,5-dimethylcyclotrisiloxane
Heat Capacity 298.15 K, C_p=502.8 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=616.9 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 195–210 K, ΔH=131 J·mol^{-1}
ΔS=0.946 J·mol^{-1}·K^{-1}
c,I/liq 260.03 K, ΔH=9522 J·mol^{-1}
ΔS=36.75 J·mol^{-1}·K^{-1}
Molecular Weight 278.5701
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E1 E1
Evaluation A

$C_{10}H_{25}O_5U$ (liq) 65FER/SCO
Uranium pentaethylate
Heat Capacity 298.15 K, C_p=392.4 J·mol^{-1}·K^{-1}
Temperature range 20 to 400 K.
Entropy 298.15 K, S=561.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 223.8 K, ΔH=14034 J·mol^{-1}
c,I/liq 257.5 K, ΔH=2375 J·mol^{-1}
Molecular Weight 403.2785
Wiswesser Line Notation 2O-U-O2&O2&O2&O2
Evaluation A

$C_{10}H_{28}Cl_4MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(pentylammonium) manganese II
Phase Changes
c.IV/c.III 203 K, ΔH=53.2 J·mol^{-1}
ΔS=0.26 J·mol^{-1}·K^{-1}
c,III/c,II 208 K, ΔH=506.8 J·mol^{-1}
ΔS=2.43 J·mol^{-1}·K^{-1}
c,II/c,I 364 K, ΔH=3.6 J·mol^{-1}
ΔS=0.009 J·mol^{-1}·K^{-1}
Molecular Weight 373.0946
Wiswesser Line Notation 5ZH 2 .MN G4
Evaluation A

$C_{10}H_{28}Cl_4N_2Zn$ (c) 84CUE/TEL
Bis-pentylammonium tetrachloro zincate
Heat Capacity 300 K, C_p=518.27 J·mol^{-1}·K^{-1}
Temperature range 55 to 355 K.
Entropy 300 K, S=525.82 J·mol^{-1}·K^{-1}
Phase Changes
c,V/c,IV 141.5 K, ΔH=441 J·mol^{-1}
ΔS=3.08 J·mol^{-1}·K^{-1}
c,IV/c,III 147.95 K, ΔH=499 J·mol^{-1}
ΔS=3.33 J·mol^{-1}·K^{-1}
c,III/c,II 249.95 K, ΔH=3584 J·mol^{-1}
ΔS=14.38 J·mol^{-1}·K^{-1}
c,II/c,I 349.05 K, ΔH=8672 J·mol^{-1}
ΔS=24.36 J·mol^{-1}·K^{-1}
c,I/liq 437 K, ΔH=6800 J·mol^{-1}
Solid-isotropic liquid.
Molecular Weight 383.5366
Wiswesser Line Notation 5ZH 2 .ZN G4
Evaluation B

$C_{11}H_{10}$ (liq) 57MCC/FIN
1-Methylnaphthalene
Heat Capacity 298.15 K, C_p=224.39 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S=254.81 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 240.70 K, ΔH=4979 J·mol^{-1}
ΔS=20.68 J·mol^{-1}·K^{-1}
c,I/liq 242.70 K, ΔH=6945 J·mol^{-1}
ΔS=28.62 J·mol^{-1}·K^{-1}
Molecular Weight 142.2000
Wiswesser Line Notation L66J B1
Evaluation A

$C_{11}H_{10}$ (liq) 31HUF/PAF
2-Methylnaphthalene
Heat Capacity 310.4 K, C_p=228.0 J·mol^{-1}·K^{-1}
Temperature range 94 to 310 K. Value is unsmoothed experimenta
datum.
Entropy 298.1 K, S=203.8 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 65.86 J·mol^{-1}·K^{-1}. Value is for crystal. Di
not observe transition at 288 K with ΔS=19.2 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 307.2 K, ΔH=11966 J·mol^{-1}
ΔS=39.0 J·mol^{-1}·K^{-1}
Molecular Weight 142.2000
Wiswesser Line Notation L66J C1
Evaluation B(C_p),C(S)

$C_{11}H_{10}$ (liq) 57MCC/FI
2-Methylnaphthalene
Heat Capacity 298.15 K, C_p=195.98 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=219.99 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 288.5 K, ΔH=5606 J·mol^{-1}
ΔS=19.43 J·mol^{-1}·K^{-1}
c,I/liq 307.73 K, ΔH=12125 J·mol^{-1}
ΔS=39.40 J·mol^{-1}·K^{-1}
Molecular Weight 142.2000
Wiswesser Line Notation L66J C1
Evaluation A

$(C_{11}H_{10}N_2O)_n$ (c) 91RO
Poly-L-tryptophane
Heat Capacity 300 K, C_p=190.6 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 186.2128
Wiswesser Line Notation /*VY1- DT56 BMJ &M*/ -L
Evaluation B

$(C_{11}H_{10}N_2O)_n$ (c) 93ROL/XE
Poly-L-tryptophane
Heat Capacity 300 K, C_p=190.6 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 186.2128
Wiswesser Line Notation /*VY1- DT56 BMJ &M*/ -L
Evaluation B

$C_{11}H_{10}O_4$ (c) 84LEB/LE
p-Methacryloyloxybenzoic acid
Heat Capacity 298.15 K, C_p=257.9 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S=284.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 455 K, ΔH=34000 J·mol^{-1}
ΔS=75 J·mol^{-1}·K^{-1}
Molecular Weight 206.1976
Wiswesser Line Notation QVR DOVY1&U1
Evaluation A

$(C_{11}H_{10}O_4)_n$ (gls) 84LEB/LE
Poly-p-methyacryloyloxybenzoic acid
Heat Capacity 298.15 K, C_p=258.9 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S=261.5 J·mol^{-1}·K^{-1}
Molecular Weight 206.1976
Wiswesser Line Notation /*X1*&1&VOR DVQ/
Evaluation A
T(glass)=316 K.

$C_{11}H_{11}F_6FeP$ (c) 86SOR/SHI
(Cyclohexatriene)(cyclopentadienyl) iron(II) hexafluorophosphate
Heat Capacity
Temperature range 12 to 393 K. Data given graphically.
Phase Changes

c,V/c,IV	158.3 K,	$\Delta H = 1190\ J\cdot mol^{-1}$
		$\Delta S = 8.01\ J\cdot mol^{-1}\cdot K^{-1}$
c,IV/c,III	265.9 K	
c,III/c,II	280.2 K	
c,II/c,I	321.5 K,	$\Delta H = 4540\ J\cdot mol^{-1}$
		$\Delta S = 14.55\ J\cdot mol^{-1}\cdot K^{-1}$

$\Delta\Delta H$ and $\Delta\Delta S$ are total of c,IV/c,III; c,III/c,II; and c,II/c,I transitions.
Molecular Weight 344.0191
Wiswesser Line Notation L6ϕJ ϕ-FE- ϕL5ϕJ &PFFFFFF
Evaluation A

$C_{11}H_{12}N_2O$ (c) 41SAT/SOG2
Antipyrene
Heat Capacity 323 K, $C_p = 268.2\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 188.2286
Wiswesser Line Notation T5NNVJ A1 BR& E1
Evaluation C
Same data as 40SAT/SOG3.

$C_{11}H_{12}N_2O_2$ (c) 63COL/HUT
Tryptophane(L)
Heat Capacity 298.15 K, $C_p = 238.15\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 11 to 305 K.
Entropy 298.15 K, $S = 251.04\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 204.2280
Wiswesser Line Notation T56 BMJ D1YZVQ -L
Evaluation A

$C_{11}H_{12}N_2O_4$ (c) 41HUF
Hippurylglycine
Heat Capacity 296.7 K, $C_p = 277.52\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 85 to 297 K.
Entropy 298.1 K, $S = 314.6\ J\cdot mol^{-1}\cdot K^{-1}$
Extrapolation below 90 K, $101.01\ J\cdot mol^{-1}\cdot K^{-1}$.
Molecular Weight 236.2268
Wiswesser Line Notation QV1MV1MVR
Evaluation A(C_p),C(S)

$C_{11}H_{12}O_2$ (liq) 58DVO
Benzyl methacrylate
Heat Capacity 296.6 K, $C_p = 269.9\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Molecular Weight 176.2146
Wiswesser Line Notation 1UY1&VO1R
Evaluation C

$C_{11}H_{12}O_2$ (liq) 1881REI
trans-Ethyl cinnamate
Heat Capacity 298 K, $C_p = 274.1\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 289 to 465 K.
Molecular Weight 176.2146
Wiswesser Line Notation 2OV1U1R -T
Evaluation D

$C_{11}H_{12}O_2$ (liq) 84BEC/RUE
4-Carbomethoxyhomocubane
Heat Capacity 298 K, $C_p = 288\ J\cdot mol^{-1}\cdot K^{-1}$
C_p given as $0.391\ cal\cdot K^{-1}\cdot g^{-1}$.
Phase Changes
liq/g 303–343 K, $\Delta H = 79956\ J\cdot mol^{-1}$
Derived from vapor pressure measurements.
Molecular Weight 176.2146
Wiswesser Line Notation L444 B4 D5 4ABCD ITJ AVO1
Evaluation B

$C_{11}H_{13}N_3O$ (c) 41SAT/SOG2
Aminoantipyrene
Heat Capacity 323 K, $C_p = 294.6\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 203.2432
Wiswesser Line Notation T5NNVJ A1 BR& DZ E1
Evaluation C
Same data as 40SAT/SOG3.

$C_{11}H_{14}$ (liq) 81LEE/FIN
1,1-Dimethylindan
Heat Capacity 298.15 K, $C_p = 249.4\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 10 to 400 K.
Entropy 298.15 K, $S = 288.1\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 227.35 K, $\Delta H = 11993\ J\cdot mol^{-1}$
Molecular Weight 146.2316
Wiswesser Line Notation L56 T&J B1 B1
Evaluation A

$C_{11}H_{14}$ (liq) 81LEE/FIN
4,6-Dimethylindan
Heat Capacity 298.15 K, $C_p = 240.9\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 10 to 400 K.
Entropy 298.15 K, $S = 295.4\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 256.45 K, $\Delta H = 12881\ J\cdot mol^{-1}$
Molecular Weight 146.2316
Wiswesser Line Notation L56 T&J F1 H1
Evaluation A

$C_{11}H_{14}$ (liq) 81LEE/FIN
4,7-Dimethylindan
Heat Capacity 298.15 K, $C_p = 241.5\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 10 to 400 K.
Entropy 298.15 K, $S = 293.2\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 272.635 K, $\Delta H = 13517\ J\cdot mol^{-1}$
Molecular Weight 146.2316
Wiswesser Line Notation L56 T&J F1 I1
Evaluation A

$C_{11}H_{14}N_2$ (c) 81LEB/RYA
Gramine; 3-Dimethylaminomethyl indole
Heat Capacity $C_p = 283.5\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 298 to 393 K. Data given over temperature range.
Molecular Weight 174.2450
Wiswesser Line Notation T56 BMJ D1N1&1
Evaluation B

$C_{11}H_{14}O_2$ (liq) 1881REI
Ethyl hydrocinnamate
Heat Capacity 298 K, C_p=286.6 J·mol^{-1}·K^{-1}
Temperature range 289 to 457 K.
Molecular Weight 178.2304
Wiswesser Line Notation 2OV2R
Evaluation D

$C_{11}H_{14}O_2$ (c) 88COL/JIM
2,3,4,5-Tetramethylbenzoic acid
Heat Capacity 298.15 K, C_p=249.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 178.2304
Wiswesser Line Notation QVR B1 C1 D1 E1
Evaluation B

$C_{11}H_{14}O_2$ (c) 88COL/JIM
2,3,4,6-Tetramethylbenzoic acid
Heat Capacity 298.15 K, C_p=267.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 178.2304
Wiswesser Line Notation QVR B1 C1 D1 F1
Evaluation B

$C_{11}H_{14}O_2$ (c) 88COL/JIM
2,3,5,6-Tetramethylbenzoic acid
Heat Capacity 298.15 K, C_p=231.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 178.2304
Wiswesser Line Notation QVR B1 C1 E1 F1
Evaluation B

$C_{11}H_{14}O_3$ (liq) 93GIM/AUD
tert-Butyl peroxybenzoate
Heat Capacity
Temperature range 293 to 353 K. C_p(liq)=1.03+2.13e^{-3}T(K) J/K· g (20 to 80 °C).
Molecular Weight 178.2304
Wiswesser Line Notation 1X1&1&OOVR
Evaluation B

$C_{11}H_{15}Cl$ (c) 82GYO/YOS
Chloropentamethylbenzene
Heat Capacity 300 K, C_p=244.60 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K. C_p for phases II, III, and IV.
Entropy 300 K, S=311.48 J·mol^{-1}·K^{-1}
Temperature range 300 K, S for phases II, III, and IV.
Phase Changes

c,IV/c,III	84.0 K,	ΔH=930 J·mol^{-1}
		ΔS=11.1 J·mol^{-1}·K^{-1}
c,III/c,II	153.5 K,	ΔH=1330 J·mol^{-1}
		ΔS=8.8 J·mol^{-1}·K^{-1}
c,II′/c,II	180.4 K,	ΔH=1330 J·mol^{-1}
		ΔS=7.7 J·mol^{-1}·K^{-1}
c,III′/c,II	187.2 K,	ΔH=1500 J·mol^{-1}
		ΔS=8.5 J·mol^{-1}·K^{-1}

Phase changes c,II′/c,II and c,III′/c,II are monotropic transitions.
Molecular Weight 182.6925
Wiswesser Line Notation GR B1 C1 D1 E1 F1
Evaluation A

$C_{11}H_{15}N$ (c) 87MEI/DO
1-Adamantyl cyanide
Heat Capacity 298.15 K, C_p=218.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 161.2462
Wiswesser Line Notation L66 B6 /B-H/ A B- C 1B ITJ FCN
Evaluation C

$C_{11}H_{15}N$ (c) 92ABB/JIM
1-Adamantyl cyanide
Heat Capacity 298.15 K, C_p=201.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 161.2462
Wiswesser Line Notation L66 B6 /B-H/ A B- C 1B ITJ FCN
Evaluation B

$C_{11}H_{15}N$ (c) 87MEI/DO
1-Adamantyl isonitrile
Heat Capacity 298.15 K, C_p=215.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 161.2462
Wiswesser Line Notation L66 B6 /B-H/ A B- C 1B ITJ FNC
Evaluation C

$C_{11}H_{16}$ (c,I) 31HUF/PA
Pentamethylbenzene
Heat Capacity 283.8 K, C_p=251.0 J·mol^{-1}·K^{-1}
Temperature range 92 to 304 K. Value is unsmoothed experiment datum.
Entropy 298.1 K, S=294.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 102.9 J·mol^{-1}·K^{-1}.
Phase Changes

c,II/c,I	296.8 K,	ΔH=1979 J·mol^{-1}
		ΔS=6.7 J·mol^{-1}·K^{-1}

Molecular Weight 148.2474
Wiswesser Line Notation 1R B1 C1 D1 E1
Evaluation B(C_p),C(S)

$C_{11}H_{16}$ (c) 33FER/TH
Pentamethylbenzene
Heat Capacity 303 K, C_p=267.3 J·mol^{-1}·K^{-1}
Temperature range 303 to 393 K.
Phase Changes

c,II/c,I	296.35 K,	ΔH=1799 J·mol^{-1}
c,I/liq	327.45 K,	ΔH=12343 J·mol^{-1}

Molecular Weight 148.2474
Wiswesser Line Notation 1R B1 C1 D1 E1
Evaluation C

$C_{11}H_{16}$ (c,I) 44E
Pentamethylbenzene
Heat Capacity 298.1 K, C_p=270.3 J·mol^{-1}·K^{-1}
Temperature range 25 to 200 °C, equations only, in t °C
C_p(c)=0.3914+0.001760t cal·g^{-1}· C (25 to 40 °C)
C_p(liq)=0.432+0.000425t cal·g^{-1}·C^{-1} (55 to 200 °C).
Phase Changes

c/liq	328.2 K,	ΔH=10670 J·mol^{-1}
		ΔS=32.5 J·mol^{-1}·K^{-1}

Molecular Weight 148.2474
Wiswesser Line Notation 1R B1 C1 D1 E1
Evaluation C

$C_{11}H_{16}$ (c) 89COL/JIM
Pentamethylbenzene
Heat Capacity 298.15 K, C_p=210.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 148.2474
Wiswesser Line Notation 1R B1 C1 D1 E1
Evaluation C

$C_{11}H_{16}Si$ (liq) 79LEB/LEB2
Vinyldimethylbenzylsilane
Heat Capacity 298.15 K, C_p=312.2 J·mol^{-1}·K^{-1}
Temperature range 9 to 330 K.
Entropy 298.15 K, S=399.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/liq 199.57 K, ΔH=10900 J·mol^{-1}
ΔS=54.6 J·mol^{-1}·K^{-1}
c,I/liq 204.14 K, ΔH=11570 J·mol^{-1}
ΔS=56.7 J·mol^{-1}·K^{-1}
Molecular Weight 176.3329
Wiswesser Line Notation 1U1-SI-1&1&1R
Evaluation A
T(glass)≈145 K.

$C_{11}H_{16}Si$ (liq) 81LEB/LEB
Vinyldimethylbenzylsilane
Heat Capacity 298.15 K, C_p=312.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=399.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 204.14 K, ΔH=11600 J·mol^{-1}
ΔS=56.7 J·mol^{-1}·K^{-1}
Molecular Weight 176.3329
Wiswesser Line Notation 1U1-SI-1&1&1R
Evaluation A
T(glass)=145 K.

$(C_{11}H_{16}Si)_n$ (gls) 81LEB/LEB
Polyvinyldimethylbenzylsilane
Heat Capacity 298.15 K, C_p=310.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K. Highly elastic state.
Entropy 298.15 K, S=294.0 J·mol^{-1}·K^{-1}
Highly elastic state.
Molecular Weight 176.3329
Wiswesser Line Notation /*1Y*-SI-1&1&1R/
Evaluation A
T(glass)~279 K.

$(C_{11}H_{16}Si)_n$ (gls) 79LEB/LEB2
Polyvinyldimethylbenzylsilane
Heat Capacity 298.15 K, C_p≈310.5 J·mol^{-1}·K^{-1}
Temperature range 9 to 330 K.
Entropy 298.15 K, S=294.0 J·mol^{-1}·K^{-1}
Molecular Weight 176.3329
Wiswesser Line Notation /*1Y*-SI-1&1&1R/
Evaluation A
T(glass)=279 K.

$C_{11}H_{17}NO$ (c) 89ABB/JIM
1-Adamantyl carboxamide
Heat Capacity 298.15 K, C_p≈220.5 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.23 J·g^{-1}·K^{-1}.
Phase Changes
c/g 298.15 K, ΔH=108000 J·mol^{-1}
ΔS=362.2 J·mol^{-1}·K^{-1}
Molecular Weight 179.2614
Wiswesser Line Notation L66 B6/B-H/D1 A B- C 1B ITJ BVZ
Evaluation A

$(C_{11}H_{17}N_3O_3)_n$ (c) 91ROL
Poly-L-proline· glycine· proline copolymer
Heat Capacity 300 K, C_p≈300.1 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 251.2846
Wiswesser Line Notation /*V- BT5NTJ AV1MV- BT5NTJ A*/ -L
Evaluation B

$(C_{11}H_{17}N_3O_3)_n$ (c) 93ROL/WUN
Poly-L-proline· glycine· proline copolymer
Heat Capacity 300 K, C_p=300.1 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 251.2846
Wiswesser Line Notation /*V BT5NTJ AV1MV- BT5NTJ A*/ -L
Evaluation B

$C_{11}H_{18}BrN$ (c) 89VAN/WHI
5-Phenylpentylammonium bromide
Phase Changes
c,II/c,I 345 K, ΔH=17600 J·mol^{-1}
ΔS=6.1 J·mol^{-1}·K^{-1}
Molecular Weight 244.1739
Wiswesser Line Notation Z5R &EH
Evaluation A

$C_{11}H_{18}ClN$ (c) 89VAN/WHI
5-Phenylpentylammonim chloride
Phase Changes
c,II/c,I 359 K, ΔH=19500 J·mol^{-1}
ΔS=6.58 J·mol^{-1}·K^{-1}
Molecular Weight 199.7229
Wiswesser Line Notation Z5R &GH
Evaluation A

$C_{11}H_{20}$ (liq) 62GOL/BEL
Ethylhydroindan
Heat Capacity 311 K, C_p≈281.6 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 152.2790
Wiswesser Line Notation L56TJ X2
Evaluation C

$C_{11}H_{20}$ (liq) 63GUD/CAM
Ethylhydroindan
Heat Capacity 313 K, C_p=279.9 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K.
Molecular Weight 152.2790
Wiswesser Line Notation L56TJ X2
Evaluation C

$C_{11}H_{20}$ (liq) 62GOL/BEL
α-Methyldecalin
Heat Capacity 311 K, C_p=269.0 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 152.2790
Wiswesser Line Notation L66TJ B1
Evaluation C

$C_{11}H_{20}$ (liq) 63GUD/CAM
α-Methyldecalin
Heat Capacity 313 K, C_p=266.5 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K.
Molecular Weight 152.2790
Wiswesser Line Notation L66TJ B1
Evaluation C

$C_{11}H_{20}$ (liq) 62GOL/BEL
β-Methyldecalin
Heat Capacity 311 K, C_p=253.1 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 152.2790
Wiswesser Line Notation L66TJ C1
Evaluation C

$C_{11}H_{20}$ (liq) 63GUD/CAM
β-Methyldecalin
Heat Capacity 313 K, C_p=258.6 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K.
Molecular Weight 152.2790
Wiswesser Line Notation L66TJ C1
Evaluation C

$C_{11}H_{20}$ (c) 75PAR/STE
Bicyclo[3.3.3]undecane; Manxane
Heat Capacity 298.15 K, C_p=213.2 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/g 298.15 K, ΔH=6359.7 J·mol^{-1}
ΔS=21.33 J·mol^{-1}·K^{-1}
Molecular Weight 152.2790
Wiswesser Line Notation T88 A B CTJ
Evaluation B(C_p), A(Phase changes)

$C_{11}H_{20}O_2$ (liq) 81LEB/YEV
Undecanolactone
Heat Capacity 298.15 K, C_p=342.7 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 388 K. 0.92 mole % impurity in sample.
Entropy 298.15 K, S=369.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 250.2 K, ΔH=3360 J·mol^{-1}
ΔS=13.4 J·mol^{-1}·K^{-1}
c,I/liq 275.33 K, ΔH=12610 J·mol^{-1}
ΔS=45.8 J·mol^{-1}·K^{-1}
Molecular Weight 184.2778
Wiswesser Line Notation T-12-VOTJ
Evaluation A

$C_{11}H_{20}O_2$ (liq) 81LEB/YEV2
Undecanolactone
Heat Capacity 298.15 K, C_p=342.7 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 388 K. 0.92 mole % impurity in sample.
Entropy 298.15 K, S=369.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 250.2 K, ΔH=3360 J·mol^{-1}
ΔS=13.4 J·mol^{-1}·K^{-1}
c,I/liq 275.33 K, ΔH=12610 J·mol^{-1}
ΔS=45.8 J·mol^{-1}·K^{-1}
Molecular Weight 184.2778
Wiswesser Line Notation T-12-VOTJ
Evaluation A

$C_{11}H_{20}O_4$ (c) 74CIN/BER
Undecanedioic acid
Phase Changes
c/liq 385.0 K, ΔH=39652 J·mol^{-1}
ΔS=103.0 J·mol^{-1}·K^{-1}
Molecular Weight 216.2766
Wiswesser Line Notation QV9VQ
Evaluation B

$C_{11}H_{21}O_2Tl$ (c) 89ROU/TUI
Thallium undecanoate
Heat Capacity
Temperature range 360 to 460 K.
Phase Changes
c,V/c,IV 306.2 K, ΔH=3359 J·mol^{-1}
ΔS=10.98 J·mol^{-1}·K^{-1}
c,IV/c,III 312.4 K, ΔH=2120 J·mol^{-1}
ΔS=6.82 J·mol^{-1}·K^{-1}
c,III/c,II 325.6 K, ΔH=3442 J·mol^{-1}
ΔS=10.56 J·mol^{-1}·K^{-1}
c,II/c,I 351.1 K, ΔH=7051 J·mol^{-1}
ΔS=20.12 J·mol^{-1}·K^{-1}
c,I/liq 404.2 K, ΔH=6103 J·mol^{-1}
ΔS=15.13 J·mol^{-1}·K^{-1}
Solid mesophase.
Molecular Weight 389.6557
Wiswesser Line Notation OV10 .TL
Evaluation A
Mesophase-isotropic liquid transition, 477.1 K, ΔH=2302 J/mol ΔS=4.82 J/mol·K.

$C_{11}H_{22}$ (liq) 57MCC/FIN
1-Undecene
Heat Capacity 298.15 K, C_p=329.95 J·mol^{-1}·K^{-1}
Temperature range 11 to 360 K.
Entropy 298.15 K, S=456.56 J·mol^{-1}·K^{-1}
Does not include S_0.
Phase Changes
c,II/c,I 217.3 K, ΔH=9213 J·mol^{-1}
ΔS=42.40 J·mol^{-1}·K^{-1}
c,I/liq 223.99 K, ΔH=16991 J·mol^{-1}
ΔS=75.86 J·mol^{-1}·K^{-1}
Molecular Weight 154.2948
Wiswesser Line Notation 10U1
Evaluation A

$C_{11}H_{22}O$ (liq) 70HAR/HE
6-Undecanone
Heat Capacity 298.15 K, C_p=362.7 J·mol^{-1}·K^{-1}
One temperature. An estimate.
Molecular Weight 170.2942
Wiswesser Line Notation 5V5
Evaluation B

$C_{11}H_{22}O_2$ (liq) 79FU
Methyldecanoate; Methyl caprate
Heat Capacity 298.15 K, C_p=382.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 186.2936
Wiswesser Line Notation 9VO1
Evaluation B

$C_{11}H_{22}O_2$ (c,I) 24GAR/RAN
Undecanoic acid
Heat Capacity 293 K, C_p=415.1 J·mol^{-1}·K^{-1}
Temperature range 0 to 66 °C. Mean value 14 to 21 °C.
Phase Changes
c,II/c,I 290 K, ΔH=7700 J·mol^{-1}
ΔS=26.6 J·mol^{-1}·K^{-1}
c,I/liq 301.4 K, ΔH=25100 J·mol^{-1}
ΔS=83.3 J·mol^{-1}·K^{-1}
Molecular Weight 186.2936
Wiswesser Line Notation QV10
Evaluation B

$C_{11}H_{22}O_2$ (c) 82SCH/MIL
Undecanoic acid
Heat Capacity 298.15 K, C_p=768.8 J·mol^{-1}·K^{-1}
Temperature range 80 to 330 K.
Phase Changes
c,II/c,I 290.3 K, ΔH=8150 J·mol^{-1}
ΔS=28.07 J·mol^{-1}·K^{-1}
c,I/liq 301.63 K, ΔH=25980 J·mol^{-1}
ΔS=86.13 J·mol^{-1}·K^{-1}
Molecular Weight 186.2936
Wiswesser Line Notation QV10
Evaluation B

$C_{11}H_{24}$ (liq) 31HUF/PAR
n-Undecane
Heat Capacity 298.0 K, C_p=342.7 J·mol^{-1}·K^{-1}
Temperature range 92 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=464.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 100.08 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 236.1 K, ΔH=6339 J·mol^{-1}
ΔS=26.8 J·mol^{-1}·K^{-1}
c,I/liq 247.2 K, ΔH=22313 J·mol^{-1}
ΔS=90.3 J·mol^{-1}·K^{-1}
Molecular Weight 156.3106
Wiswesser Line Notation 11H
Evaluation B(C_p),C(S)

$C_{11}H_{24}$ (liq) 54FIN/GRO2
n-Undecane
Heat Capacity 298.15 K, C_p=345.05 J·mol^{-1}·K^{-1}
Temperature range 12 to 320 K.
Entropy 298.1 K, S=458.15 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 236.6 K, ΔH=6858 J·mol^{-1}
ΔS=23.99 J·mol^{-1}·K^{-1}
c,I/liq 247.59 K, ΔH=22179 J·mol^{-1}
ΔS=89.58 J·mol^{-1}·K^{-1}
Molecular Weight 156.3106
Wiswesser Line Notation 11H
Evaluation A

$C_{11}H_{24}$ (liq) 71MES/FIN
2-Methyldecane
Heat Capacity 298.15 K, C_p=341.21 J·mol^{-1}·K^{-1}
Temperature range 11 to 390 K.
Entropy 298.15 K, S=453.80 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 224.31 K, ΔH=25087 J·mol^{-1}
ΔS=111.84 J·mol^{-1}·K^{-1}
Molecular Weight 156.3106
Wiswesser Line Notation 8Y1&1
Evaluation A

$C_{11}H_{24}$ (liq) 84GRI/AND
n-Undecane
Heat Capacity 292.29 K, C_p=341.1 J·mol^{-1}·K^{-1}
Temperature range 292 to 433 K. Unsmoothed experimental datum given as 2.181 kJ/kg·K.
Molecular Weight 156.3106
Wiswesser Line Notation 11H
Evaluation B

$C_{11}H_{24}O$ (liq) 82VAS/PET
1-Undecanol; n-Undecyl alcohol
Heat Capacity 303 K, C_p=419.8 J·mol^{-1}·K^{-1}
Temperature range 303 to 508 K.
Molecular Weight 172.3100
Wiswesser Line Notation Q11
Evaluation B

$C_{11}H_{24}O$ (liq) 87NAZ/BAL
1-Undecanol; n-Undecyl alcohol
Heat Capacity 303.65 K, C_p=414.8 J·mol^{-1}·K^{-1}
Temperature range 303 to 500 K. p=0.1 MPa. Unsmoothed experimental datum given as 2.407 kJ/kg·K. C_p data given from 303.65 to 523.15 K for the pressure range 2.5 to 50 MPa.
Molecular Weight 172.3100
Wiswesser Line Notation Q11
Evaluation B

$C_{11}H_{24}O$ (liq) 88AND/PAT
1-Undecanol; n-Undecyl alcohol
Heat Capacity 298.15 K, C_p=406.34 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 172.3100
Wiswesser Line Notation Q11
Evaluation B

$C_{11}H_{24}O$ (liq) 89KHA/ZYK
1-Undecanol; n-Undecyl alcohol
Heat Capacity 303.15 K, C_p=406.8 J·mol^{-1}·K^{-1}
Temperature range 293 to 513 K.
Molecular Weight 172.3100
Wiswesser Line Notation Q11
Evaluation B

$C_{11}H_{24}O$ (liq) 75AND/MAR
2-Oxadodecane; Methyl-n-decyl ether
Heat Capacity 298.15 K, C_p=370.8 J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Entropy 298.15 K, S=490.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 243.47 K, ΔH=31720 J·mol^{-1}
ΔS=130.31 J·mol^{-1}·K^{-1}
Molecular Weight 172.3100
Wiswesser Line Notation 10O1
Evaluation A

$C_{11}H_{24}O$ (liq) 75FEN/HAR
2-Oxadodecane; Methyl-n-decyl ether
Heat Capacity 298.15 K, C_p=370.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 172.3100
Wiswesser Line Notation 10O1
Evaluation B

$C_{11}H_{28}N_6S_3$ (c,I) 72COP/GAN

Thiourea-cyclooctane adduct; Cyclooctane-thiourea adduct

Heat Capacity 298.15 K, C_p=164.3 J·mol^{-1}·K^{-1}

Temperature range 12 to 300 K. Values for one mole of thiourea.

Entropy 298.15 K. S=187.1 J·mol^{-1}·K^{-1}

Does not include possible zero-point entropy.

Phase Changes

c,IV/c,III	187.2 K,	ΔH=2110 J·mol^{-1}
		ΔS=11.26 J·mol^{-1}·K^{-1}
c,III/c,II	240 K,	ΔH=21414 J·mol^{-1}
		ΔS=94.41 J·mol^{-1}·K^{-1}
c,II/c,I	265 K,	ΔH=703 J·mol^{-1}
		ΔS=2.65 J·mol^{-1}·K^{-1}

Molecular Weight 410.5149

Wiswesser Line Notation ZYZUS &L8TJ 2.98

Evaluation A

$C_{12}Cl_{10}$ (c) 87SAI/ATA

Decachlorobiphenyl; Perchlorobiphenyl

Heat Capacity 298.15 K, C_p=344.0 J·mol^{-1}·K^{-1}

Temperature range 3 to 300 K.

Entropy 298.15 K, S=455.8 J·mol^{-1}·K^{-1}

Molecular Weight 498.6620

Wiswesser Line Notation GR BG CG DG EG FR BG CG DG EG FG

Evaluation A

$C_{12}D_{10}$ (c) 83ATA/SAI

Biphenyl-d_{10}

Heat Capacity

Temperature range 3 to 300 K. Data given graphically.

Phase Changes

c,III/c,II	20.2 K,	ΔH=0.18 J·mol^{-1}
		ΔS=0.009 J·mol^{-1}·K^{-1}

Anomalous region: 18.5 to 22.5 K.

c,II/c,I	36.8 K,	ΔH=4.61 J·mol^{-1}
		ΔS=0.128 J·mol^{-1}·K^{-1}

Anomalous region: 28 to 44 K.

Molecular Weight 164.2900

Wiswesser Line Notation RR &1A-E/H-2 5 &2A-E/H-2 5

Evaluation A

$C_{12}D_{10}$ (c) 87SAI/ATA2

Biphenyl-d_{10}

Heat Capacity 298.15 K, C_p=228.85 J·mol^{-1}·K^{-1}

Temperature range 3 to 300 K.

Entropy 298.15 K, S=230.88 J·mol^{-1}·K^{-1}

Phase Changes

c,III/c,II	20.2 K,	ΔH=0.18 J·mol^{-1}
		ΔS=0.009 J·mol^{-1}·K^{-1}

Lock-in transition.

c,II/c,I	36.8 K,	ΔH=4.61 J·mol^{-1}
		ΔS=0.128 J·mol^{-1}·K^{-1}

Twist transition.

Molecular Weight 164.2900

Wiswesser Line Notation RR &1A-E/H-2 5 &2A-E/H-2 5

Evaluation A

$C_{12}D_{18}$ (c) 92FUJ/IN

Hexamethylbenzene, deuterated

Heat Capacity 300 K, C_p=290.51 J·mol^{-1}·K^{-1}

Temperature range 4 to 300 K.

Entropy 300 K. S=348.06 J·mol^{-1}·K^{-1}

Phase Changes

c,III/c,II	132.4 K,	ΔH=1730 J·mol^{-1}
		ΔS=13.1 J·mol^{-1}·K^{-1}
c,III/c,I	381 K	
c,I/liq	437 K	

Molecular Weight 180.4164

Wiswesser Line Notation 1R B1 C1 D1 E1 F1 &1/H-2 3 &5/H-2 &8/H-2 3 &11/H-2 3 &14/H-2 3 &17/H-2 3

Evaluation A

$C_{12}F_{10}$ (c) 71PAU/RA

Decafluorobiphenyl; Perfluorobiphenyl

Heat Capacity 300.7 K, C_p=323.4 J·mol^{-1}·K^{-1}

Temperature range 13 to 350 K. Complete article deposited at VINI No. 2536-71, 2 January 1971.

Entropy 298.15 K, S=380.62 J·mol^{-1}·K^{-1}

Phase Changes

Melting point and enthalpy of fusion given only in complete pap

ΔS fusion=63.85 J·mol^{-1}·K^{-1}.

Molecular Weight 334.1160

Wiswesser Line Notation FR BF CF DF EF FR BF CF DF EF FF

Evaluation B

$C_{12}F_{10}$ (c) 87SAI/A

Decafluorobiphenyl; Perfluorobiphenyl

Heat Capacity 298.15 K, C_p=317.4 J·mol^{-1}·K^{-1}

Temperature range 3 to 300 K.

Entropy 298.15 K, S=377.4 J·mol^{-1}·K^{-1}

Molecular Weight 334.1160

Wiswesser Line Notation FR BF CF DF EF FR BF CF DF EF FF

Evaluation A

$C_{12}F_{22}$ (c) 65COX/GU

Docosafluorobicyclohexyl; Perfluorobicyclohexyl

Heat Capacity 298 K, C_p=899 J·mol^{-1}·K^{-1}

One temperature.

Molecular Weight 562.0968

Wiswesser Line Notation L6TJ AF AF BF BF CF CF DF DF EF EF F-FL6TJ AF AF BF BF CF CF DF DF EF EF FF

Evaluation B

$C_{12}F_{26}$ (c) 93LEB/B

n-Perfluorododecane

Heat Capacity 298.15 K C_p=546.8 J·mol^{-1}·K^{-1}

Temperature range 0 to 320 K.

Entropy 298.15 K S=763.3 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I	177.52 K	ΔH=5070 J·mol^{-1}
		ΔS=22.6 J·mol^{-1}·K^{-1}

Molecular Weight 638.0904

Wiswesser Line Notation FXFFXFFXFFXFFXFFXFF-XFFXFFXF FFXFFXFFF

Evaluation A

$C_{12}Fe_3O_{12}$ (c) 89SEL/SHE
Dodecacarbonyl triiron
Heat Capacity 298.15 K, C_p=541.9 J·mol^{-1}·K^{-1}
Temperature range 7 to 300 K.
Entropy 298.15 K, S=635.3 J·mol^{-1}·K^{-1}
Molecular Weight 503.6658
Wiswesser Line Notation CO 12 .FE
Evaluation A

$C_{12}H_6F_6$ (liq) 78RIP/WRI
Benzene:hexafluorobenzene complex
Heat Capacity 305 K, C_p=370 J·mol^{-1}·K^{-1}
Temperature range 60 to 320 K.
Phase Changes
Transitions observed at 199.0, 247.5, 272.0 K; no heat data given.
c,I/liq 297.2 K, ΔH=21870 J·mol^{-1}
ΔS=73.6 J·mol^{-1}·K^{-1}
Molecular Weight 264.1698
Wiswesser Line Notation FR BF CF DF EF FF &R
Evaluation C

$C_{12}H_6N_2O_2$ (c) 62STR/BAR
1,5-Naphthylenediisocyanate; 1,5-Diisocyanatonaphthalene
Heat Capacity 298 K, C_p=223.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 210.1916
Wiswesser Line Notation L66J CNCO GNCO
Evaluation D

$C_{12}H_7Cl_2NO_3$ (c) 81VOR/BOR
2,4-Dichloro-4′-nitrodiphenyl ether
Phase Changes
c/liq 343 K, ΔH=2700 J·mol^{-1}
ΔS=7.87 J·mol^{-1}·K^{-1}
liq/g 643 K, ΔH=115900 J·mol^{-1}
ΔS=180.2 J·mol^{-1}·K^{-1}
Molecular Weight 284.0982
Wiswesser Line Notation WNR DOR BG DG
Evaluation C

$C_{12}H_8$ (c) 69SAD/STE
Acenaphthylene
Heat Capacity 298 K, C_p=166.4 J·mol^{-1}·K^{-1}
Temperature range 20 to 89 °C, equation only; liquid 90 to 150 °C, equation only.
Phase Changes
c/liq 362.6 K, ΔH=6940 J·mol^{-1}
ΔS=19.14 J·mol^{-1}·K^{-1}
Molecular Weight 152.1952
Wiswesser Line Notation L566 1A LJ
Evaluation C

$C_{12}H_8Cl_2O_2S$ (c) 85NOV/TSV
4.4′-Dichlorodiphenyl sulphone
Heat Capacity 298.15 K, C_p=269.3 J·mol^{-1}·K^{-1}
Temperature range 14 to 480 K.
Entropy 298.15 K, S=314.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 422 K, ΔH=24400 J·mol^{-1}
ΔS=57.8 J·mol^{-1}·K^{-1}
Molecular Weight 287.1600
Wiswesser Line Notation GR DSWR DG
Evaluation A

$C_{12}H_8Cl_2O_2S$ (c) 90SAI/KAM
4,4′-Dichlorodiphenyl sulfone
Heat Capacity
Temperature range 100 to 250 K. Data given graphically.
Phase Changes
c,III/c,II 115 K
c,II/c,I 146 K, ΔH=41 J·mol^{-1}
ΔS=0.30 J·mol^{-1}·K^{-1}
Molecular Weight 287.1600
Wiswesser Line Notation GR DSWR DG
Evaluation A

$C_{12}H_8F_2$ (c) 86SAI/ATA
4,4′-Difluorobiphenyl
Heat Capacity 298.15 K, C_p=222.77 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, S=237.59 J·mol^{-1}·K^{-1}
Phase Changes
liq/g 298.15 K, ΔH=91200 J·mol^{-1}
ΔS=305 J·mol^{-1}·K^{-1}
p=0.5092 Pa, data from 64SMI/GOR.
Molecular Weight 190.1920
Wiswesser Line Notation FR DR DF
Evaluation A

$C_{12}H_8N_2$ (c) 91SAB/ELW
Phenazine
Heat Capacity 298.15 K, C_p=234.3 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 447.89 K, ΔH=18880 J·mol^{-1}
Molecular Weight 180.2086
Wiswesser Line Notation T C666 BN INJ
Evaluation B

$C_{12}H_8N_2$ (c) 92SAB/ELW4
Phenazine
Phase Changes
c/liq 447.89 K, ΔH=18880 J·mol^{-1}
c/g 298.15 K, ΔH=96970 J·mol^{-1}
Molecular Weight 180.2086
Wiswesser Line Notation T C666 BN INJ
Evaluation A

$C_{12}H_8N_2$ (c) 77SCH/PET
Benzo[c]cinnoline
Phase Changes
c/liq 429 K, ΔH=20900 J·mol^{-1}
Molecular Weight 180.2086
Wiswesser Line Notation T C666 HNNJ
Evaluation A

$C_{12}H_8N_2O_5$ (c) 78MAR/CIO
4,4′-Dinitrodiphenyl ether; Bis-(4-nitrophenyl) ether
Heat Capacity 298 K, C_p=421.7 J·mol^{-1}·K^{-1}
Temperature range 298 to 491 K. Values for solid seem odd; minimum at 345 K of 276 J·mol^{-1}·K^{-1}, rising to 552 J·mol^{-1} at 410 K.
Phase Changes
c/liq 418.2 K, ΔH=10295 J·mol^{-1}
ΔS=24.6 J·mol^{-1}·K^{-1}
Molecular Weight 260.2056
Wiswesser Line Notation WNR DOR DNW
Evaluation D

$C_{12}H_8O$ (c,l) 90CHI/GAM

Dibenzofuran; Diphenylene oxide

Heat Capacity 298.15 K, C_p=199.01 J·mol^{-1}·K^{-1}.
Temperature range 5 to 720 K. Data graphically extrapolated. C_p (298.15 K, liq)=237.57 J· mol-1·K, graphically extrapolated.

Entropy 298.15 K, S=196.18 J·mol^{-1}·K^{-1}
S (298.15 K, liq)=244.97 J · mol^{-1}·K^{-1}.

Phase Changes

c,II/c,I 292.5 K, ΔH=0.00 J·mol^{-1}

c,I/liq 355.31 K, ΔH=19293.65 J·mol^{-1}
ΔS=54.30 J·mol^{-1}·K^{-1}

Molecular Weight 168.1946

Wiswesser Line Notation T B656 HOJ

Evaluation A

$C_{12}H_8O$ (c) 91SAB

Dibenzofuran; Diphenylene oxide

Phase Changes

c/liq 355.51 K

Molecular Weight 168.1946

Wiswesser Line Notation T B656 HOJ

Evaluation A

$C_{12}H_8OS$ (c) 93STE/CHI

Phenoxathiin

Heat Capacity 298.15 K, C_p=213.77 J·mol^{-1}·K^{-1}
Temperature range 5 to 700 K.

Entropy 298.15 K, S=222.66 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 328.778 K, ΔH=20266.6 J·mol^{-1}

Molecular Weight 200.2546

Wiswesser Line Notation T666 BS IOJ

Evaluation A

$C_{12}H_8OS_2$ (c) 75CUC

Diphenylene-2,2′-disulfide-S-oxide

Heat Capacity 303 K, C_p=745.2 J·mol^{-1}·K^{-1}
Temperature range 303 to 523 K.

Phase Changes

c/liq 407 K, ΔH=17990 J·mol^{-1}
ΔS=44.2 J·mol^{-1}·K^{-1}

Molecular Weight 232.3146

Wiswesser Line Notation T B666 HSSJ HO

Evaluation B

$(C_{12}H_8O_3S)_n$ (c) 92VAR/JIN

Poly(oxy-1,4-phenylene sulphonyl-1,4-phenylene)

Heat Capacity 300 K, C_p=228.9 J·mol^{-1}·K^{-1}
Temperature range 150 to 620 K. C_p(c)=exp[−183.0187 +100.4943(lnT)−18.0408(lnT)^2+1.08967(lnT)^3] (150 to 270 K) and exp[292.7648−147.5393(lnT)+25.10034(lnT)^2−1.4140(lnT)^3 (280 to 490 K); C_p(liq)=356.3796+0.07318T (530 to 620 K).

Molecular Weight 232.2534

Wiswesser Line Notation /*OR DSWR D*/

Evaluation A
T(glass)=497.4 K.

$C_{12}H_8O_4$ (c) 92STE/CHI

Naphthalene-2,6-dicarboxylic acid

Heat Capacity 298.15 K, C_p=230.3 J·mol^{-1}·K^{-1}
Temperature range 305 to 665 K. C/R(c)=0.0763T+4.983 (305 to 665 K), R=8.31451 J/K· mol.

Molecular Weight 216.1928

Wiswesser Line Notation L66J CVQ HVQ

Evaluation A

$C_{12}H_8S$ (c) 83ORO/MR

Dibenzothiophene

Heat Capacity 298.15 K, C_p=194.6 J·mol^{-1}·K^{-1}
Temperature range 220 to 560 K. C_p=0.6709 (T/K)−5.4 (220 to 371 K) J·mol^{-1}·K^{-1}.

Phase Changes

c/liq 371.0 K, ΔH=21580 J·mol^{-1}
ΔS=58.17 J·mol^{-1}·K^{-1}

Molecular Weight 184.2552

Wiswesser Line Notation T B656 HSJ

Evaluation A
C_p(liq)=0.4215 (T/K)+123.8 (370.1 to 560 K) J·mol^{-1}·K^{-1}.

$C_{12}H_8S$ (c) 91CHI/KI

Dibenzothiophene

Heat Capacity 298.15 K, C_p=198.30 J·mol^{-1}·K^{-1}
Temperature range 5 to 800 K.

Entropy 298.15 K, S=204.20 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 371.821 K, ΔH=21708 J·mol^{-1}
ΔS=58.38 J·mol^{-1}·K^{-1}

Molecular Weight 184.2552

Wiswesser Line Notation T B656 HSJ

Evaluation A

$C_{12}H_8S_2$ (c) 89SAB/W

Thianthrene

Heat Capacity 298.15 K, C_p=224.97 J·mol^{-1}·K^{-1}
One temperature.

Molecular Weight 216.3152

Wiswesser Line Notation T666 BS ISJ

Evaluation A

$C_{12}H_8S_2$ (c) 93STE/C

Thianthrene

Heat Capacity 298.15 K, C_p=220.17 J·mol^{-1}·K^{-1}
Temperature range 5 to 700 K.

Entropy 298.15 K, S=230.89 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 429.576 K, ΔH=27555.1 J·mol^{-1}

Molecular Weight 216.3152

Wiswesser Line Notation T666 BS ISJ

Evaluation A

$C_{12}H_9Cl$ (c) 74GEI/DZ

2 Chlorobiphenyl

Heat Capacity 298.15 K, C_p=208.03 J·mol^{-1}·K^{-1}
Temperature range 12 to 330 K.

Entropy 298.15 K, S=303.76 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 304.94 K, ΔH=14518 J·mol^{-1}
ΔS=47.61 J·mol^{-1}·K^{-1}

Molecular Weight 188.6561

Wiswesser Line Notation GR BR

Evaluation A

$C_{12}H_9Cl$ (c) 77GEI/K

2-Chlorobiphenyl

Heat Capacity 298.15 K, C_p=211.92 J·mol^{-1}·K^{-1}
Based on previously published work of authors, not available in det on C_p 12 to 370 K.

Entropy 298.15 K, S=254.30 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 304.94 K, ΔH=14518 J·mol^{-1}
ΔS=47.61 J·mol^{-1}·K^{-1}

Molecular Weight 188.6561

Wiswesser Line Notation GR BR

Evaluation B

$C_{12}H_9Cl$ (c) 75GEI/DZH
4-Chlorobiphenyl
Heat Capacity 298.15 K, C_p=243.8 J·mol^{-1}·K^{-1}
Temperature range 12 to 370 K.
Entropy 298.15 K, S=256.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 348.55 K, ΔH=13318 J·mol^{-1}
ΔS=38.21 J·mol^{-1}·K^{-1}
Molecular Weight 188.6561
Wiswesser Line Notation GR DR
Evaluation A
Debye temperature=91 K.

$C_{12}H_9Cl$ (c) 77GEI/KAR
4-Chlorobiphenyl
Heat Capacity 298.15 K, C_p=243.76 J·mol^{-1}·K^{-1}
Based on previously published work of authors, not available in detail, on C_p 12 to 370 K.
Entropy 298.15 K, S=256.90 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 348.55 K, ΔH=13318 J·mol^{-1}
ΔS=38.21 J·mol^{-1}·K^{-1}
Molecular Weight 188.6561
Wiswesser Line Notation GR DR
Evaluation B

$C_{12}H_9Cl_3Si$ (c) 74GEI/DZH2
o-Trichlorosilylbiphenyl
Heat Capacity
Temperature range 12 to 370 K. Depositied in VINITI No. 7671-73, 21 December 1973.
Entropy 298.15 K S=348.40 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 289.5 ΔH=57.7 J·mol^{-1}
ΔS=0.20 J·mol^{-1}·K^{-1}
trans-cis conformational transition
c,I/liq 339.18 K ΔH=20719 J·mol^{-1}
ΔS=61.09 J·mol^{-1}·K^{-1}
Molecular Weight 287.6476
Wiswesser Line Notation G-SI-GGR BR
Evaluation B
This compound is erroneously named in the English translation of 74GEI/DZH2 as: o,o'-Bistrichloro-silylbiphenyl.

$C_{12}H_9Cl_3Si$ (c) 77GEI/KAR
o-Trichlorosilylbiphenyl
Heat Capacity 298.15 K, C_p=337.86 J·mol^{-1}·K^{-1}
Temperature range 12 to 370 K.
Based on previously published work of authors, not available in detail.
Entropy 298.15 K, S=348.40 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 289.5 K ΔH=57.7 J·mol^{-1}
ΔS=0.20 J·mol^{-1}·K^{-1}
trans-cis conformational transition
c,I/liq 339.18 K, ΔH=20719 J·mol^{-1}
ΔS=61.09 J·mol^{-1}·K^{-1}
Molecular Weight 287.6476
Wiswesser Line Notation G-SI-GGR BR
Evaluation B

$C_{12}H_9Cl_3Si$ (c) 76GEI/DZH
p-Trichlorosilylbiphenyl
Heat Capacity 298.15 K, C_p=291.1 J·mol^{-1}·K^{-1}
Temperature range 12 to 380 K.
Entropy 298.15 K, S=328.8 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I
Anomaly on heat capacity curve from 207 to 221 K.
c/liq 372.90 K, ΔH=18569 J·mol^{-1}
ΔS=49.80 J·mol^{-1}·K^{-1}
Molecular Weight 287.6476
Wiswesser Line Notation G-SI-GGR DR
Evaluation A
See also 77GEI/KAR.

$C_{12}H_9Cl_3Si$ (c) 77GEI/KAR
p-Trichlorosilylbiphenyl
Heat Capacity 298.15 K, C_p=291.08 J·mol^{-1}·K^{-1}
Based on previously published work of authors, not available in detail, on C_p 12 to 370 K.
Entropy 298.15 K, S=328.78 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 372.90 K, ΔH=18569 J·mol^{-1}
ΔS=49.80 J·mol^{-1}·K^{-1}
Molecular Weight 287.6476
Wiswesser Line Notation G-SI-GGR DR
Evaluation B

$C_{12}H_9N$ (c) 80RAD/RAD
Carbazole
Heat Capacity 298.15 K, C_p=190.8 J·mol^{-1}·K^{-1}
Temperature range 180 to 410 K. C_p=54.87+0.2328T+7.477×10^{-4} T^2.
Phase Changes
c/liq 521.1 K, ΔH=27200 J·mol^{-1}
ΔS=52.19 J·mol^{-1}·K^{-1}
Molecular Weight 167.2098
Wiswesser Line Notation T B656 HMJ
Evaluation B

$C_{12}H_9N$ (c) 90JIM/ROU
Carbazole
Heat Capacity 298.15 K, C_p=194.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 167.2098
Wiswesser Line Notation T B656 HMJ
Evaluation A

$C_{12}H_9N$ (c) 92SAB/ELW3
Carbazole
Phase Changes
c/liq 518.33 K, ΔH=27080 J·mol^{-1}
Molecular Weight 167.2098
Wiswesser Line Notation T B656 HMJ
Evaluation A

$C_{12}H_9NS$ (c) 92SAB/ELW
Phenothiazine
Phase Changes
c/liq 458.40 K, ΔH=25660 J·mol^{-1}
Molecular Weight 199.2698
Wiswesser Line Notation T C666 BM ISJ
Evaluation A

$C_{12}H_{10}$ (c) 44EIB
Acenaphthene
Heat Capacity 298.1 K, C_p=210.5 J·mol^{-1}·K^{-1}
Temperature range 25 to 200 °C, equations only in t °C. C_p(c)=0.2756+0.001854t cal·g^{-1}·C^{-1} (25 to 60 °C); C_p(liq)=0.409+0.000598t cal·g^{-1}·C^{-1} (95 to 200 °C).
Phase Changes
c/liq 367.8 K, ΔH=25100 J·mol^{-1}
ΔS=68.2 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation L566 1A LT&&J
Evaluation C

$C_{12}H_{10}$ (c) 69SAD/STE
Acenaphthene
Heat Capacity 298 K, C_p=185.8 J·mol^{-1}·K^{-1}
Temperature range 20 to 93 °C, equation only; liquid, 93 to 200 °C, equation only.
Phase Changes
c/liq 366.4 K, ΔH=20233 J·mol^{-1}
ΔS=55.22 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation L566 1A LT&&J
Evaluation C

$C_{12}H_{10}$ (c) 77FIN/MES
Acenaphthene
Heat Capacity 298.15 K, C_p=190.37 J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, S=188.87 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 366.56 K, ΔH=21462.2 J·mol^{-1}
ΔS=58.55 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation L566 1A LT&&J
Evaluation A

$C_{12}H_{10}$ (c) 1889EYK
Biphenyl; Diphenyl
Phase Changes
c/liq 314.3 K, ΔH=18945 J·mol^{-1}
ΔS=60.3 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation C

$C_{12}H_{10}$ (c) 30HUF/PAR
Biphenyl; Diphenyl
Heat Capacity 294.4 K, C_p=194.1 J·mol^{-1}·K^{-1}
Temperature range 93 to 295 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=205.9 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 65.4 J·mol^{-1}·K^{-1}.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation B(C_p),C(S)

$C_{12}H_{10}$ (liq) 31FOR/BRU
Biphenyl; Diphenyl
Heat Capacity 350.8 K, C_p=263.2 J·mol^{-1}·K^{-1}
Temperature range 350 to 620 K. Value is unsmoothed experimental datum.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation B

$C_{12}H_{10}$ (liq) 31NEW/KAU
Biphenyl; Diphenyl
Heat Capacity 298 K, C_p=259.54 J·mol^{-1}·K^{-1}
Temperature range 100 to 300 °C, equation only, in t °C. C_p(liq)=0.388+0.00057t cal·g^{-1}·C^{-1}.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation C

$C_{12}H_{10}$ (c) 32SPA/THO
Biphenyl; Diphenyl
Heat Capacity 303 K, C_p=197.9 J·mol^{-1}·K^{-1}
Temperature range 30 to 100 °C.
Phase Changes
c/liq 341.5 K, ΔH=18648 J·mol^{-1}
ΔS=54.6 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation B

$C_{12}H_{10}$ (c) 41SCH
Biphenyl; Diphenyl
Heat Capacity 298.1 K, C_p=197.9 J·mol^{-1}·K^{-1}
Temperature range 20 to 200 °C, equations only, in t °C C_p(c)=0.2745+0.001235t cal·g^{-1}·C^{-1} (20 to 69 °C); C_p(liq =0.3917+0.0005206t cal·g^{-1}·C^{-1} (69 to 200 °C).
Phase Changes
c/liq 342 K, ΔH=18594 J·mol^{-1}
ΔS=54.4 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation C

$C_{12}H_{10}$ (liq) 50KUF
Biphenyl; Diphenyl
Heat Capacity 370 K, C_p=300.0 J·mol^{-1}·K^{-1}
Temperature range 98 to 255 °C. Mp 70.8 °C.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation B

$C_{12}H_{10}$ (c) 50UEB/OR
Biphenyl; Diphenyl
Heat Capacity 298.15 K, C_p=190.8 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Phase Changes
c/liq 343 K, ΔH=18575 J·mol^{-1}
ΔS=54.2 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation C

$C_{12}H_{10}$ (liq) 56MC
Biphenyl; Diphenyl
Heat Capacity 422 K, C_p=301.2 J·mol^{-1}·K^{-1}
Temperature range 300 to 600 °C.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation C
Quoted in 58WAL/BRO.

$C_{12}H_{10}$ (liq) 58WAL/BRO
Biphenyl; Diphenyl
Heat Capacity 370 K, C_p=285.3 J·mol^{-1}·K^{-1}
Temperature range 200 to 600 °F.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation B

$C_{12}H_{10}$ (c) 79SMI
Biphenyl; Diphenyl
Phase Changes
c/liq 344.1 K, ΔH=18800 J·mol^{-1}
ΔS=54.6 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation A

$C_{12}H_{10}$ (liq) 80ATA/CHI
Biphenyl; Diphenyl
Heat Capacity
C_p data given graphically. Temperature range 3 to 300 K.
Phase Changes
c,III/c,II 11.0 K, ΔH=0.293 J·mol^{-1}
ΔS=0.025 J·mol^{-1}·K^{-1}
c,III/c,II: anomalous region 7.5 to 14.0 K.
c,II/c,I 40.4 K, ΔH=5.02 J·mol^{-1}
ΔS=0.129 J·mol^{-1}·K^{-1}
c,II/c,I: anomalous region 30.0 to 47.0 K.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation A

$C_{12}H_{10}$ (c) 82WAS/RAD
Biphenyl; Diphenyl
Heat Capacity 300 K, C_p=190 J·mol^{-1}·K^{-1}
Temperature range 180 to 350 K. Data given graphically. Value estimated from graph.
Phase Changes
c,I/liq 343.3 K, ΔH=19900 J·mol^{-1}
ΔS=58.0 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation C(C_p), B(Phase changes)

$C_{12}H_{10}$ (c) 83ATA/SAI
Biphenyl; Diphenyl
Phase Changes
c,III/c,II 16.8 K, ΔH=0.15 J·mol^{-1}
ΔS=0.009 J·mol^{-1}·K^{-1}
Anomalous region: 15.3 to 18.3 K.
c,II/c,I 40.4 K, ΔH=5.02 J·mol^{-1}
ΔS=0.129 J·mol^{-1}·K^{-1}
Anomalous region: 30 to 47 K.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation A

$C_{12}H_{10}$ (c) 83ORO/MRA
Biphenyl; Diphenyl
Heat Capacity 298.15 K, C_p=197.7 J·mol^{-1}·K^{-1}
Temperature range 220 to 475 K. C_p=0.7143 (T/K)−15.3 (220 to 342.2 K) J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 342.2 K, ΔH=18580 J·mol^{-1}
ΔS=54.3 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation A
C_p(liq)=0.4284 (T/K)+122.0 (342.2 to 485 K) J·mol^{-1}·K^{-1}.

$C_{12}H_{10}$ (c) 88SAI/ATA
Biphenyl; Diphenyl
Heat Capacity 298.15 K, C_p=198.17 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, S=209.00 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 16.8 K, ΔH=0.15 J·mol^{-1}
ΔS=0.009 J·mol^{-1}·K^{-1}
Lock-in transition.
c,II/c,I 40.4 K, ΔH=5.02 J·mol^{-1}
ΔS=0.129 J·mol^{-1}·K^{-1}
Twist transition.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation A

$C_{12}H_{10}$ (c) 89CHI/KNI
Biphenyl; Diphenyl
Heat Capacity 298.15 K, C_p=198.39 J·mol^{-1}·K^{-1}
Temperature range 5 to 700 K.
Entropy 298.15 K, S=209.38 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 342.098 K, ΔH=2234.17 J·mol^{-1}
ΔS=6.5307 J·mol^{-1}·K^{-1}
c/g 298.15 K, ΔH=81520 J·mol^{-1}
ΔS=273.42 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation A

$C_{12}H_{10}Hg$ (c) 31SMI/AND2
Diphenylmercury; Mercury diphenyl
Heat Capacity 298.5 K, C_p=225.5 J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 354.8010
Wiswesser Line Notation R-HG-R
Evaluation B

$C_{12}H_{10}N_2$ (c) 1889EYK
Azobenzene
Phase Changes
c/liq 342.2 K, ΔH=22389 J·mol^{-1}
ΔS=65.4 J·mol^{-1}·K^{-1}
Molecular Weight 182.2244
Wiswesser Line Notation RNUNR
Evaluation C

$C_{12}H_{10}N_2$ (c) 74CIN/BER
Azobenzene
Phase Changes
c/liq 340.5 K, $\Delta H = 22368\ J\cdot mol^{-1}$
$\Delta S = 65.59\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 182.2244
Wiswesser Line Notation RNUNR
Evaluation B

$C_{12}H_{10}N_2$ (c) 77SCH/PET
cis-Azobenzene
Heat Capacity 298.15 K, $C_p = 229\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 298 to 333 K. $C_p(c) = 229 + 1.086(T - 298.15\ K)$ J $\cdot mol^{-1}\cdot K^{-1}$ (298 to 333 K).
Molecular Weight 182.2244
Wiswesser Line Notation RNUNR -C
Evaluation B

$C_{12}H_{10}N_2$ (c) 77SCH/PET
trans-Azobenzene
Heat Capacity 298.15 K, $C_p = 219\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 298 to 333 K. $C_p(c) = 219 + 1.029(T - 298.15\ K)$ J $\cdot mol^{-1}\cdot K^{-1}$ (298 to 333 K).
Phase Changes
c/liq 341.8 K, $\Delta H = 22650\ J\cdot mol^{-1}$
Molecular Weight 182.2244
Wiswesser Line Notation RNUNR -T
Evaluation B

$C_{12}H_{10}N_2$ (c) 84VAN/BOU
trans-Azobenzene
Heat Capacity 300 K, $C_p = 229.3\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 90 to 320 K.
Phase Changes
c/liq 341.03 K, $\Delta H = 22520\ J\cdot mol^{-1}$
$\Delta S = 66.0\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 182.2244
Wiswesser Line Notation RNUNR -T
Evaluation B

$C_{12}H_{10}N_2$ (c) 85BOU/DEL
trans-Azobenzene
Heat Capacity 300 K, $C_p = 229.33\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 300 to 400 K.
Phase Changes
c,l/liq 341.06 K, $\Delta H = 22530\ J\cdot mol^{-1}$
$\Delta S = 66.06\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 182.2244
Wiswesser Line Notation RNUNR -T
Evaluation A

$C_{12}H_{10}O$ (c) 73GEI/DZH
o Hydroxybiphenyl
Heat Capacity 298.15 K, $C_p = 235.10\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 12 to 350 K. Complete C_p data in paper deposited at VINITI, No. 4748-72, 24 Aug, 1972.
Entropy 298.15 K, $S = 261.75\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 330.6 K, $\Delta H = 16213\ J\cdot mol^{-1}$
$\Delta S = 49.04\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 170.2104
Wiswesser Line Notation QR BR
Evaluation A

$C_{12}H_{10}O$ (c) 77GEI/KAR
o-Hydroxybiphenyl
Heat Capacity 298.15 K, $C_p = 227.61\ J\cdot mol^{-1}\cdot K^{-1}$
Based on previously published work of authors, not available in detail, on C_p 12 to 370 K.
Entropy 298.15 K, $S = 261.75\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 330.60 K, $\Delta H = 16213\ J\cdot mol^{-1}$
$\Delta S = 49.04\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 170.2104
Wiswesser Line Notation QR BR
Evaluation B

$C_{12}H_{10}O$ (c) 31SMI/AND2
Diphenyl oxide; Diphenyl ether
Heat Capacity 298.5 K, $C_p = 215.9\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 102 to 298 K.
Molecular Weight 170.2104
Wiswesser Line Notation ROR
Evaluation B

$C_{12}H_{10}O$ (c) 51FUR/GIN
Diphenyl oxide; Diphenyl ether
Heat Capacity 298.15 K, $C_p = 216.56\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 18 to 570 K.
Entropy 298.15 K, $S = 233.91\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 300.02 K, $\Delta H = 17216\ J\cdot mol^{-1}$
$\Delta S = 57.38\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 170.2104
Wiswesser Line Notation ROR
Evaluation A

$C_{12}H_{10}O$ (c) 53GIN/FUR
Diphenyl oxide; Diphenyl ether
Heat Capacity 298.15 K, $C_p = 216.56\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 14 to 570 K.
Phase Changes
c/liq 300.03 K, $\Delta H = 17215\ J\cdot mol^{-1}$
$\Delta S = 57.38\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 170.2104
Wiswesser Line Notation ROR
Evaluation A

$C_{12}H_{10}OS$ (c) 31SMI/AND2
Diphenyl sulfoxide
Heat Capacity 298.5 K, $C_p = 239.7\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 102 to 323 K. Value is unsmoothed experimental datum.
Molecular Weight 202.2704
Wiswesser Line Notation OSR&R
Evaluation B

$C_{12}H_{10}O_2$ (c) 86SAI/ATA
p,p′-Biphenol; 4,4′-Dihydroxybiphenyl
Heat Capacity 298.15 K, $C_p = 224.31\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 3 to 315 K.
Entropy 298.15 K, $S = 220.57\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight *186.2098*
Wiswesser Line Notation QR DR DQ
Evaluation A

$C_{12}H_{10}O_2S$ (c) 31SMI/AND2
Diphenyl sulfone
Heat Capacity 298.5 K, C_p=244.3 J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K.
Molecular Weight 218.2698
Wiswesser Line Notation WSR&R
Evaluation B

$C_{12}H_{10}O_4$ (c) 24LAN
Quinhydrone
Heat Capacity 243.4 K, C_p=228.4 J·mol^{-1}·K^{-1}
Temperature range 20 to 244 K. Value is unsmoothed experimental datum.
Molecular Weight 218.2086
Wiswesser Line Notation L6V DVJ &QR DQ
Evaluation B

$C_{12}H_{10}S$ (liq) 31SMI/AND2
Diphenyl sulfide
Heat Capacity 298.5 K, C_p=271.1 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 186.2710
Wiswesser Line Notation RSR
Evaluation B

$C_{12}H_{11}N$ (c,I) 91STE/CHI
2-Aminobiphenyl; [1,1′-biphenyl]-2-amine
Heat Capacity 298.15 K, C_p=221.86 J·mol^{-1}·K^{-1}
Temperature range 5 to 800 K. C_p(liq. 298.15 K)=298.17 J·mol^{-1}·K^{-1}.
Entropy 298.15 K, S=233.48 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 258.00 K, ΔH=0.00 J·mol^{-1}
c,I/liq 322.28 K, ΔH=13987.42 J·mol^{-1}
ΔS=43.40 J·mol^{-1}·K^{-1}
Molecular Weight 169.2256
Wiswesser Line Notation ZR BR
Evaluation A

$C_{12}H_{11}N_3$ (c) 41SAT/SOG2
p-Aminoazobenzene
Heat Capacity 323 K, C_p=276.1 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 197.2390
Wiswesser Line Notation ZR DNUNR
Evaluation C
Same data as 40SAT/SOG3.

$C_{12}H_{12}$ (c) 73GOO
1,8-Dimethylnaphthalene
Heat Capacity 298.15 K, C_p=241.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 156.2268
Wiswesser Line Notation L66J B1 J1
Evaluation B

$C_{12}H_{12}$ (c) 77FIN/MES
1,8-Dimethylnaphthalene
Heat Capacity 298.15 K, C_p=242.80 J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, S=224.72 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 336.33 K, ΔH=46.87 J·mol^{-1}
ΔS=46.86 J·mol^{-1}·K^{-1}
Molecular Weight 156.2268
Wiswesser Line Notation L66J B1 J1
Evaluation A

$C_{12}H_{12}$ (c,I) 88MES/FIN
2,3-Dimethylnaphthalene
Heat Capacity 298.15 K, C_p=216.466 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=225.853 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 226.000 K, ΔH=−0.58 J·mol^{-1}
c,II/c,I 265.000 K, ΔH=−1.08 J·mol^{-1}
c,I/liq 377.496 K, ΔH=19353.29 J·mol^{-1}
ΔS=51.27 J·mol^{-1}·K^{-1}
Molecular Weight 156.2268
Wiswesser Line Notation L66J C1 D1
Evaluation A

$C_{12}H_{12}$ (c) 89SCI/GOD
2,3-Dimethylnaphthalene
Heat Capacity 298 K, C_p=215 J·mol^{-1}·K^{-1}
Temperature range 100 to 350 K. C_p value estimated from graph.
Phase Changes
c,IV/c,III 220 K
c,III/c,II 275 K
c,II/c,I 302 K, ΔH=104 J·mol^{-1}
ΔS=0.35 J·mol^{-1}·K^{-1}
Molecular Weight 156.2268
Wiswesser Line Notation L66J C1 D1
Evaluation B

$C_{12}H_{12}$ (c) 73GOO
2,6-Dimethylnaphthalene
Heat Capacity 298.15 K, C_p=202.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 156.2268
Wiswesser Line Notation L66J C1 H1
Evaluation B

$C_{12}H_{12}$ (c) 77FIN/MES
2,6-Dimethylnaphthalene
Heat Capacity 298.15 K, C_p=203.55 J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, S=227.86 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 383.32 K, ΔH=25056.7 J·mol^{-1}
ΔS=65.37 J·mol^{-1}·K^{-1}
Molecular Weight 156.2268
Wiswesser Line Notation L66J C1 H1
Evaluation A

$C_{12}H_{12}$ (c) 73GOO
2,7-Dimethylnaphthalene
Heat Capacity 298.15 K, C_p=202.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 156.2268
Wiswesser Line Notation L66J C1 I1
Evaluation B

$C_{12}H_{12}$ (c) 77FIN/MES
2,7-Dimethylnaphthalene
Heat Capacity 298.15 K, C_p=204.39 J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, S=228.57 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 368.81 K, ΔH=23351.3 J·mol^{-1}
ΔS=63.32 J·mol^{-1}·K^{-1}
Molecular Weight 156.2268
Wiswesser Line Notation L66J C1 I1
Evaluation A

$C_{12}H_{12}$ (liq) 93CHI/KNI
2,7-Dimethylnaphthalene
Heat Capacity 298.15 K, C_p=251.85 J·mol^{-1}·K^{-1}
Temperature range 298 to 700 K.
Entropy 298.15 K, S=283.36 J·mol^{-1}·K^{-1}
Molecular Weight 156.2268
Wiswesser Line Notation L66J C1 I1
Evaluation A
Values at 298.15 K were calculated with graphically extrapolated heat capacities.

$C_{12}H_{12}Cr$ (c) 69AND/WES
Bis(benzene)chromium
Heat Capacity 298.15 K, C_p=223.93 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=226.23 J·mol^{-1}·K^{-1}
Molecular Weight 208.2228
Wiswesser Line Notation L6ϕJ ϕ-CR- ϕL6ϕJ
Evaluation A

$C_{12}H_{12}CrBr$ (c) 72NIK/SAF
Bis(benzene)chromium bromide
Heat Capacity 298.15 K, C_p=328.4 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S=339.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 234.6 K
Molecular Weight 288.1268
Wiswesser Line Notation L6ϕJ ϕ-CR- ϕL6ϕJ &E
Evaluation B

$C_{12}H_{12}CrCl$ (c) 72NIK/SAF
Bis(benzene)chromium chloride
Heat Capacity 298.15 K, C_p=323.4 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S=335.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 178.75 K, ΔH=1820 J·mol^{-1}
ΔS=10.2 J·mol^{-1}·K^{-1}
Molecular Weight 243.6758
Wiswesser Line Notation L6ϕJ ϕ-CR- ϕL6ϕJ &G
Evaluation B

$C_{12}H_{12}CrI$ (c) 72NIK/SAF
Bis(benzene)chromium iodide
Heat Capacity 298.15 K, C_p=249.6 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S=289.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 240.6 K, ΔH=1695 J·mol^{-1}
ΔS=7.04 J·mol^{-1}·K^{-1}
Molecular Weight 335.1273
Wiswesser Line Notation L6ϕJ ϕ-CR- ϕL6ϕJ &I
Evaluation B

$C_{12}H_{12}FeO$ (c) 81TOM/CUR
Acetylferrocene
Heat Capacity 298 K. C_p=246.0 J·mol^{-1}·K^{-1}
Temperature range 293 to 353 °C. Equation given.
Phase Changes
c/liq 358.7 K
Molecular Weight 228.0732
Wiswesser Line Notation L5ϕJ ϕ-FE- -ϕL5ϕJ AV1
Evaluation B

$C_{12}H_{12}Ge$ (liq) 79LEB/LEI
Diphenylgermane
Heat Capacity 298.15 K, C_p=287.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=337.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 239.44 K, ΔH=11910 J·mol^{-1}
ΔS=49.74 J·mol^{-1}·K^{-1}
Molecular Weight 228.8168
Wiswesser Line Notation R-GE-R
Evaluation A

$C_{12}H_{12}N_2O$ (c) 77KAR/BAZ
4,4′-Diaminodiphenyl oxide; 4,4′-Diaminodiphenyl ether; Bis-(4- aminophenyl)ether
Heat Capacity 300 K, C_p=258.4 J·mol^{-1}·K^{-1}
Temperature range 60 to 400 K.
Entropy 300 K, S=241.0 J·mol^{-1}·K^{-1}
Molecular Weight 200.2396
Wiswesser Line Notation ZR DOR DZ
Evaluation B

$C_{12}H_{12}N_2O$ (c) 78MAR/CIC
4,4′-Diaminodiphenyl oxide; 4,4′-Diaminodiphenyl ether; Bis-(4- aminophenyl)ether
Heat Capacity 298 K, C_p=280.7 J·mol^{-1}·K^{-1}
Temperature range 298 to 502 K.
Phase Changes
c/liq 465.4 K, ΔH=7740 J·mol^{-1}
ΔS=16.6 J·mol^{-1}·K^{-1}
Molecular Weight 200.2396
Wiswesser Line Notation ZR DOR DZ
Evaluation D

$C_{12}H_{12}N_2O$ (c) 87LES/LIC
4,4′-Diaminodiphenyl oxide; 4,4′-Diaminodiphenyl ether; Bis-(4- aminophenyl)ether
Heat Capacity 298 K, C_p=278.2 J·mol^{-1}·K^{-1}
Temperature range 250 to 400 K.
Phase Changes
c/liq 464 K
Molecular Weight 200.2396
Wiswesser Line Notation ZR DOR DZ
Evaluation B

$C_{12}H_{12}N_2O_2S$ (c) 87LES/LIC
4,4′-Diaminodiphenyl sulfone
Heat Capacity 298 K, C_p=314.9 J·mol^{-1}·K^{-1}
Temperature range 250 to 400 K.
Phase Changes
c/liq 451 K
Molecular Weight 248.2990
Wiswesser Line Notation ZR DSWR DZ
Evaluation B

$C_{12}H_{12}N_4$ (c) 41SAT/SOG
2,4-Diaminoazobenzene
Heat Capacity 323 K, C_p=306.7 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value.
Molecular Weight 212.2536
Wiswesser Line Notation ZR CZ DNUNR
Evaluation C
Same data as 40SAT/SOG3.

$C_{12}H_{12}O_4$ (c) 89KIR/CHU
1,4-Dimethylcubane dicarboxylate
Heat Capacity 298.15 K, C_p=251.1 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 437.8 K, ΔH=41000 J·mol^{-1}
ΔS=93.7 J·mol^{-1}·K^{-1}
Molecular Weight 220.2250
Wiswesser Line Notation L444 B4 D4 4ABCD HTJ AVO1 HVO1
Evaluation B

$(C_{12}H_{12}O_4)_n$ (c) 82KAR/SHV2
Poly (butylene terephthalate)
Heat Capacity
Temperature range 60 to 500 K. C_p data given graphically only.
Phase Changes
c/liq 498.0 K, ΔH=31800 J·mol^{-1}
ΔS=64.0 J·mol^{-1}·K^{-1}
Extrapolated to 100% crystallinity.
ΔH=17500 J·mol^{-1}
Actual measurement for 55.5% crystallinity.
Molecular Weight 220.2244
Wiswesser Line Notation /*OVR DVO4*/
Evaluation B

$(C_{12}H_{12}O_4)_n$ (gls) 88CHE/PAN
Poly (butylene terephthalate)
Heat Capacity 280 K, C_p=254 J·mol^{-1}·K^{-1}
Temperature range 210 to 560 K. Data given graphically. C_p (J·mol^{-1}·K^{-1})=0.000713 T^2+0.5203 T+52.16 (220 to 280 K) for semicrystal.
Phase Changes
c,III/c,II 248 K
Glass transition for amorphous sample.
c,II/c,I 320 K
Glass transition for semicrystalline sample.
c,I/liq 518 K
Molecular Weight 220.2244
Wiswesser Line Notation /*OVR DVO4*/
Evaluation B

$C_{12}H_{13}NO_2$ (c) 89ZHA/HUA
4-Methyl-7-dimethylaminocoumarin
Phase Changes
c/liq 416.1 K, ΔH=23915 J·mol^{-1}
ΔS=56.91 J·mol^{-1}·K^{-1}
Molecular Weight 203.2402
Wiswesser Line Notation 166 BOVJ E1 IN1&1
Evaluation B

$C_{12}H_{14}N_4O$ (c) 73KAR/SAP
4,4′-Dihydrazinodiphenyl oxide
Heat Capacity 300 K, C_p=407.81 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=322.63 J·mol^{-1}·K^{-1}
Molecular Weight 230.2688
Wiswesser Line Notation ZMR DOR DMZ
Evaluation B
Assumed -$NHNH_2$ groups are in the 4,4′ positions.

$C_{12}H_{14}N_4O$ (c) 73KAR/SAP
3,3′,4,4′-Tetraaminodiphenyl oxide; 3,3′,4,4′-Tetraaminodiphenyl ether
Heat Capacity 300 K, C_p=320.24 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=295.1 J·mol^{-1}·K^{-1}
Molecular Weight 230.2688
Wiswesser Line Notation ZR BZ DOR CZ DZ
Evaluation B

$C_{12}H_{14}N_4O$ (c) 77KAR/RAB
3,3′,4,4′-Tetraaminodiphenyl oxide; 3,3′,4,4′- Tetraaminodiphenyl ether
Heat Capacity 300 K, C_p=400 J·mol^{-1}·K^{-1}
Temperature range 100 to 700 K. Data given graphically. Value estimated from graph.
Entropy 300 K, S=293.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 402.6 K, ΔH=25301 J·mol^{-1}
ΔS=62.8 J·mol^{-1}·K^{-1}
Molecular Weight 230.2688
Wiswesser Line Notation ZR BZ DOR CZ DZ
Evaluation C(C_p), A, (S,Phase changes).

$C_{12}H_{14}O_4$ (liq) 67CHA/HOR
Diethyl o-phthalate
Heat Capacity 298.15 K, C_p=366.15 J·mol^{-1}·K^{-1}
Temperature range 10 to 360 K. Glass transition temperature about 180 K. Also data for annealed glass and quenched glass 10 to 170 K.
Entropy 298.15 K, S=425.08 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.92 K, ΔH=17984 J·mol^{-1}
ΔS=66.63 J·mol^{-1}·K^{-1}
Molecular Weight 222.2402
Wiswesser Line Notation 2OVR BVO2
Evaluation A

$C_{12}H_{14}O_4$ (liq) 79FUC
Diethyl o-phthalate
Heat Capacity 298.15 K, C_p=357.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 222.2402
Wiswesser Line Notation 2OVR BVO2
Evaluation B

$C_{12}H_{14}O_4$ (liq) 56SMI/DOL
Diethyl p-phthalate; Diethyl terephthalate
Heat Capacity 320 K, C_p=381 J·mol^{-1}·K^{-1}
Temperature range 43 to 75 °C. Equation only.
Phase Changes
c/liq ΔH=24600 J·mol^{-1}
Melting temperature not given. Premelting over a 10 K range was observed.
Molecular Weight 222.2402
Wiswesser Line Notation 2OVR DVO2
Evaluation C

$C_{12}H_{15}NO_2$ (liq) 85KAR/ABD2
Phenylaminoethyl methacrylate
Phase Changes
c/liq 297.5 K, ΔH=25465 J·mol^{-1}
ΔS=85.60 J·mol^{-1}·K^{-1}
Molecular Weight 205.2560
Wiswesser Line Notation 1UY1&VO2MR
Evaluation A

$C_{12}H_{16}$ (liq) 83ORO/MRA
Cyclohexylbenzene
Heat Capacity 198.15 K, C_p=263.2 J·mol^{-1}·K^{-1}
Temperature range 220 to 475 K. $C_p(c)$=0.8803 (T/K)−29.2 (220 to 280.5 K); C_p(liq)=0.6130 (T/K)+80.4 (280.5 to 475 K) J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 280.5 K, ΔH=15270 J·mol^{-1}
ΔS=54.44 J·mol^{-1}·K^{-1}
Molecular Weight 160.2584
Wiswesser Line Notation L6TJ AR
Evaluation A

$C_{12}H_{16}N_2O_2$ (c) 91ABA/DEL
N-Acetylphenylalanine-N′-methylamide(DL); 2-(Acetylamino)-N-methylbenzenepropanamide(DL)
Heat Capacity 298 K, C_p=278.25 J·mol^{-1}·K^{-1}
Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 220.2706
Wiswesser Line Notation 1VMYMV1&1R -DL
Evaluation C

$C_{12}H_{16}N_2O_2$ (c) 91ABA/DEL
N-Acetylphenylalanine-N′-methylamide(L); 2-(Acetylamino)-N-methylbenzenepropanamide(L)
Heat Capacity 298 K, C_p=277.97 J·mol^{-1}·K^{-1}
Data extrapolated to 298 K from values obtained at higher temperatures.
Molecular Weight 220.2706
Wiswesser Line Notation 1VMYVM1&1R -L
Evaluation C

$C_{13}H_{18}O_2$ (c) 88COL/JIM
Pentamethylbenzoic acid
Heat Capacity 298.15 K, C_p=249.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 192.2572
Wiswesser Line Notation QVR B1 C1 D1 E1 F1
Evaluation B

$C_{12}H_{18}$ (c,I) 30HUF/PAR
Hexamethylbenzene
Heat Capacity 294.6 K, C_p=254.8 J·mol^{-1}·K^{-1}
Temperature range 85 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=309.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 82.38 J·mol^{-1}·K^{-1}.
Phase Changes
c,III/c,II 108 K, ΔH=1017 J·mol^{-1}
ΔS=9.5 J·mol^{-1}·K^{-1}
c,II/c,I 151 K, ΔH=155 J·mol^{-1}
ΔS=1.0 J·mol^{-1}·K^{-1}
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation B(C_p),C(S)

$C_{12}H_{18}$ (c,II) 32SPA/THO
Hexamethylbenzene
Heat Capacity 303 K, C_p=258.5 J·mol^{-1}·K^{-1}
Temperature range 30 to 200 °C.
Phase Changes
c,II/c,I 383.7 K, ΔH=1766 J·mol^{-1}
ΔS=4.60 J·mol^{-1}·K^{-1}
c,I/liq 438.7 K, ΔH=20640 J·mol^{-1}
ΔS=47.0 J·mol^{-1}·K^{-1}
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation B

$C_{12}H_{18}$ (liq) 47KUR
Hexamethylbenzene
Heat Capacity 455 K, C_p=370.7 J·mol^{-1}·K^{-1}
Temperature range 183 to 256 °C, mean C_p, two temperatures.
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation D

$C_{12}H_{18}$ (c) 56MOM/SUC
Hexamethylbenzene
Heat Capacity 293.81 K, C_p=256.1 J·mol^{-1}·K^{-1}
Temperature range 273 to 443 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 383.55 K, ΔH=1841 J·mol^{-1}
ΔS=4.81 J·mol^{-1}·K^{-1}
c,I/liq 438.35 K, ΔH=20585 J·mol^{-1}
ΔS=46.86 J·mol^{-1}·K^{-1}
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation B

$C_{12}H_{18}$ (c,I) 65FRA/AST
Hexamethylbenzene
Heat Capacity 298.15 K, C_p=245.64 J·mol^{-1}·K^{-1}
Temperature range 13 to 340 K.
Entropy 298.15 K, S=306.31 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 116.48 K, ΔH=1128.4 J·mol^{-1}
ΔS=10.08 J·mol^{-1}·K^{-1}
Entropy obtained as difference of integral of observed C_p over range 115 to 128 K, and integral of extrapolated C_p data.
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation A

$C_{12}H_{18}$ (c) 82ATA/GYC
Hexamethylbenzene
Heat Capacity 300 K, C_p=252.11 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 300 K, S=302.81 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 117.5 K, ΔH=990 J·mol^{-1}
ΔS=8.3 J·mol^{-1}·K^{-1}
First order transition.
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation A
An additional thermal anomaly producing a hump in the heat capacity curve with a maximum of 50 J·mol^{-1}·K^{-1} at 128 K is hidden behind the first order transition.

$C_{12}H_{18}$ (c) 85YOS/FU
Hexamethylbenzene
Phase Changes
c,II/c,I 115.5 K, ΔH=1103 J·mol^{-1}
ΔS=9.55 J·mol^{-1}·K^{-1}
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation A

$C_{12}H_{18}$ (c) 88PET/TS
Hexamethylbenzene
Phase Changes
c,II/c,I 384.0 K, ΔH=1500 J·mol^{-1}
ΔS=3.9 J·mol^{-1}·K^{-1}
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation A

$C_{12}H_{18}$ (c) 89COL/JIM
Hexamethylbenzene
Heat Capacity 298.15 K, C_p=243.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation C

$C_{12}H_{18}$ (c) 92FUJ/INA
Hexamethylbenzene
Phase Changes
c,III/c,II 117.5 K, ΔH=1100 J·mol^{-1}
ΔS=9.3 J·mol^{-1}·K^{-1}
From 82ATA/GYO
c,III/c,I 382 K
c,I/liq 439 K
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation A

$C_{12}H_{18}$ (liq) 48TSC
n-Hexylbenzene
Heat Capacity 293 K, C_p=248 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 162.2742
Wiswesser Line Notation 6R
Evaluation C

$C_{12}H_{18}$ (liq) 89LAI/ROD
trans,trans,cis-1,5,9-Cyclododecatriene
Heat Capacity 298.15 K, C_p=287.76 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 162.2742
Wiswesser Line Notation L-12- AU EU IUTJ -TTC
Evaluation B

$C_{12}H_{18}$ (liq) 63GUD/CAM
1,4:5,8-Dimethanodecalin; 1,4:5,8-Dimethanodecahydronaphthalene
Heat Capacity 313 K, C_p=334.3 J·mol^{-1}·K^{-1}
Temperature range 313 to 423 K.
Molecular Weight 162.2742
Wiswesser Line Notation L D5 C555 A D-TJ
Evaluation D
Compound assumed to be 1,4:5,8-Dimethanodecalin isomer.

$C_{12}H_{18}Be_4O_{13}$ (c) 47JAF
Beryllium oxyacetate
Heat Capacity 298.95 K, C_p=553.1 J·mol^{-1}·K^{-1}
Temperature range 297 to 332 K. Unsmoothed experimental datum.
Molecular Weight 406.3151
Wiswesser Line Notation OV1 6 .BE 4 &O
Evaluation C

$C_{12}H_{18}Be_4O_{13}$ (c) 55MOM/SEK
Beryllium oxyacetate
Heat Capacity 298.85 K, C_p=514.6 J·mol^{-1}·K^{-1}
Temperature range 273 to 370 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 315 K
Lambda type transition at 315 K. Transitions also indicated at 305, 350 and 398 K.
c,I/liq 421 K. ΔH=27196 J·mol^{-1}
ΔS=48.5 J·mol^{-1}·K^{-1}
Molecular Weight 406.3151
Wiswesser Line Notation OV1 6 .BE 4 &O
Evaluation B(C_p), A(Phase changes)

$C_{12}H_{18}CuO_4$ (c) 92RIB/FER
Bis(3-methylpentane-2,4-dionato)copper(II)
Phase Changes
c/g 430 K, ΔH=132700 J·mol^{-1}
Molecular Weight 289.8178
Wiswesser Line Notation D6O-CU-O ADJ D1 E1 F1 B-& BD6O-CU-O ADJ D1 E1 F1
Evaluation A

$C_{12}H_{18}O$ (c) 92ABB/JIM
1-Adamantyl methyl ketone
Heat Capacity 298.15 K, C_p=217.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 178.2736
Wiswesser Line Notation L66 B6/B-H/DI A B- C 1B ITJ FV1
Evaluation B

$C_{12}H_{18}O_2$ (liq) 77KAR/SAP
Acetophenone diethyl ketal
Heat Capacity 298 K, C_p=210 J·mol^{-1}·K^{-1}
Temperature range 60 to 340 K. C_p estimated from equation: C_p=(475) (0.71198−0.000908T).
Molecular Weight 194.2730
Wiswesser Line Notation 2OX1&O2&R
Evaluation D

$C_{12}H_{18}O_2$ (gls) 78KAR/SAP
Acetophenone diethyl ketal
Entropy 298.15 K, S=364.3 J·mol^{-1}·K^{-1}
Molecular Weight 194.2730
Wiswesser Line Notation 2OX1&O2&R
Evaluation A
T(glass)=173.2 K.

$C_{12}H_{18}O_2$ (c) 92ABB/JIM2
Adamantane-1-carboxylic acid methyl ester
Heat Capacity 298.15 K, C_p=264.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 194.2730
Wiswesser Line Notation L66 B6 /B-H/ A B- C 1B ITJ FVO1
Evaluation B

$C_{12}H_{20}$ (liq) 63GUD/CAM
Perhydromethylcyclopentadiene dimer
Heat Capacity 313 K, C_p=292.2 J·mol^{-1}·K^{-1}
Temperature range 313 to 523 K.
Molecular Weight 164.2900
Wiswesser Line Notation L B545TJ X1 X1
Evaluation C

$C_{12}H_{20}$ (liq) 62GOL/BEL
Tricyclo[6.2.1.1^{3,6}]dodecane
Heat Capacity 311 K, C_p=279.9 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 164.2900
Wiswesser Line Notation L59 D5 A D-TJ
Evaluation C

$C_{12}H_{20}BrN$ (c) 89VAN/WHI
6-Phenylhexylammonium bromide
Phase Changes
c,II/c,I 334 K, $\Delta H = 14400\ J \cdot mol^{-1}$
$\Delta S = 5.2\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 258.2007
Wiswesser Line Notation Z6R &EH
Evaluation A

$C_{12}H_{20}ClN$ (c) 89VAN/WHI
6-Phenylhexylammonium chloride
Phase Changes
c,IV/c,III 319 K, $\Delta H = 40\ J \cdot mol^{-1}$
$\Delta S = 0.02\ J \cdot mol^{-1} \cdot K^{-1}$
c,III/c,II 338 K, $\Delta H = 1170\ J \cdot mol^{-1}$
$\Delta S = 0.41\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I 345 K, $\Delta H = 550\ J \cdot mol^{-1}$
$\Delta S = 0.19\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 213.7497
Wiswesser Line Notation Z6R &GH
Evaluation A

$C_{12}H_{20}N_2O_3$ (c) 89VAN/WHI
6-Phenylhexylammonium nitrate
Phase Changes
c,II/c,I 325 K, $\Delta H = 21700\ J \cdot mol^{-1}$
$\Delta S = 7.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 240.3016
Wiswesser Line Notation Z6R &WNQ
Evaluation A

$(C_{12}H_{20}O_4)_n$ (c) 58WUN/DOL
Poly(ethylenesebacate)
Heat Capacity 298 K, $C_p = 469\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 256 to 408 K. Value per repeating monomer units.
Phase Changes
c/liq 342 K
Molecular Weight 228.2876
Wiswesser Line Notation /*VO2OV8*/
Evaluation C

$C_{12}H_{20}O_6$ (liq) 86NIL/WAD
Tripropionin
Heat Capacity 298.15 K, $C_p = 481.3\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 260.2864
Wiswesser Line Notation 2VO1YOV2&1OV2
Evaluation A

$C_{12}H_{22}$ (liq) 62GOL/BEL
Isopropylhydroindan
Heat Capacity 311 K, $C_p = 329.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperatures 100, 200, 300 °F.
Molecular Weight 166.3058
Wiswesser Line Notation L56TJ XY1&1
Evaluation C

$C_{12}H_{22}$ (liq) 63GUD/CAM
Isopropylhydroindan
Heat Capacity 313 K, $C_p = 327.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 423 K.
Molecular Weight 166.3058
Wiswesser Line Notation L56TJ XY1&1
Evaluation C

$C_{12}H_{22}$ (liq) 62GOL/BEL
α-Ethyldecalin
Heat Capacity 311 K, $C_p = 303.3\ J \cdot mol^{-1} \cdot K^{-1}$
Temperatures 100, 200, 300 °F.
Molecular Weight 166.3058
Wiswesser Line Notation L66TJ B2
Evaluation C

$C_{12}H_{22}$ (liq) 63GUD/CAM
α-Ethyldecalin
Heat Capacity 313 K, $C_p = 305.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 483 K.
Molecular Weight 166.3058
Wiswesser Line Notation L66TJ B2
Evaluation C

$C_{12}H_{22}$ (liq) 62GOL/BEL
β-Ethyldecalin
Heat Capacity 311 K, $C_p = 290.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperatures 100, 200, 300 °F.
Molecular Weight 166.3058
Wiswesser Line Notation L66TJ C2
Evaluation C

$C_{12}H_{22}$ (liq) 63GUD/CAM
β-Ethyldecalin
Heat Capacity 313 K, $C_p = 292.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 483 K.
Molecular Weight 166.3058
Wiswesser Line Notation L66TJ C2
Evaluation C

$C_{12}H_{22}$ (liq) 63GUD/CAM
Dimethyldecalin
Heat Capacity 313 K, $C_p = 303.3\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 483 K.
Molecular Weight 166.3058
Wiswesser Line Notation L66TJ X1 X1
Evaluation C

$C_{12}H_{22}$ (liq) 63GUD/CAM
Ethyldecalin
Heat Capacity 313 K, $C_p = 318.8\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 423 K.
Molecular Weight 166.3058
Wiswesser Line Notation L66TJ X2
Evaluation C

$C_{12}H_{22}$ (liq) 62GOL/BEL
Bicyclohexyl
Heat Capacity 311 K, $C_p = 300.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperatures 100, 200, 300 °F.
Molecular Weight 166.3058
Wiswesser Line Notation L6TJ A- AL6TJ
Evaluation C

$C_{12}H_{22}$ (liq) 63GUD/CAM
Bicyclohexyl
Heat Capacity 313 K, C_p=300 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 166.3058
Wiswesser Line Notation L6TJ A- AL6TJ
Evaluation C

$C_{12}H_{22}$ (liq) 83ORO/MRA
Bicyclohexyl
Heat Capacity 298.15 K, C_p=283.0 J·mol^{-1}·K^{-1}
Temperature range 220 to 475 K. C_p=0.7589 (T/K)+56.7 (277.2 to 475 K) J·mol^{-1}·K^{-1}.
Phase Changes

c,IV/c,III	256.1 K,	ΔH=1540 J·mol^{-1}
c,III/c,II	267.5 K,	ΔH=740 J·mol^{-1}
c,II/c,I	273.5 K,	ΔH=7080 J·mol^{-1}
c,I/liq	277.2 K,	ΔH=6780 J·mol^{-1}

Molecular Weight 166.3058
Wiswesser Line Notation L6TJ A- AL6TJ
Evaluation A

$C_{12}H_{22}$ (liq) 92HOR/KLA
Bicyclohexyl
Phase Changes

c,IV/c,III	256.5 K,	ΔH=1350 J·mol^{-1}
		ΔS=5.3 J·mol^{-1}·K^{-1}
c,III/c,II	267.0 K,	ΔH=320 J·mol^{-1}
		ΔS=1.2 J·mol^{-1}·K^{-1}
c,II/c,I	273.6 K,	ΔH=7090 J·mol^{-1}
		ΔS=25.9 J·mol^{-1}·K^{-1}
c,I/liq	277.4 K,	ΔH=6610 J·mol^{-1}
		ΔS=23.8 J·mol^{-1}·K^{-1}

Crystal/isotropic liquid transition.
Molecular Weight 166.3058
Wiswesser Line Notation L6TJ A- AL6TJ
Evaluation A
DSC heating curve.

$C_{12}H_{22}O_2$ (liq) 85KAR/ABD
Octyl methacrylate
Heat Capacity 298.15 K, C_p=386.0 J·mol^{-1}·K^{-1}
Temperature range 230 to 350 K. C_p (J·kg^{-1}·K^{-1})=1261.8+2.2971 T. C_p data calculated from equation.
Phase Changes
c/liq 230.3 K
Molecular Weight 198.3046
Wiswesser Line Notation 8OVY1&U1
Evaluation B

$C_{12}H_{22}O_2$ (liq) 85KAR/ABD2
Octyl methacrylate
Phase Changes
c/liq 230.3 K, ΔH=24085 J·mol^{-1}
ΔS=104.6 J·mol^{-1}·K^{-1}
Molecular Weight 198.3046
Wiswesser Line Notation 8OVY1&U1
Evaluation A

$C_{12}H_{22}O_2$ (liq) 85KAR/SAI
Octyl methacrylate
Heat Capacity 298.15 K, C_p=386.2 J·mol^{-1}·K^{-1}
Temperature range 90 to 350 K. C_p(c)=199.31+5.22T J/kg· K (95 to 205 K); C_p(liq)=1261.84+2.30T J/kg· K (230.3 to 350 K). C_p data calculated from equation.
Phase Changes
c/liq 230.3 K
Molecular Weight 198.3046
Wiswesser Line Notation 8OVY1&U1
Evaluation B

$C_{12}H_{22}O_2$ (liq) 85KAR/ABD2
Nonyl acrylate
Phase Changes

c/liq	236.5 K,	ΔH=23362 J·mol^{-1}
		ΔS=98.8 J·mol^{-1}·K^{-1}

Molecular Weight 198.3046
Wiswesser Line Notation 9OV1U1
Evaluation A

$C_{12}H_{22}O_2$ (liq) 85KAR/SAI
Nonyl acrylate
Heat Capacity 298.15 K, C_p=417.9 J·mol^{-1}·K^{-1}
Temperature range 90 to 350 K. C_p(c)=85.37+6.51 T J/kg· K (98 to 210 K); C_p(liq)=398.84+5.73T J/kg· K (236.5 to 350 K). C_p data calculated from equation.
Phase Changes
c/liq 236.5 K
Molecular Weight 198.3046
Wiswesser Line Notation 9OV1U1
Evaluation B

$C_{12}H_{22}O_4$ (liq) 89KHO/PUL
Dibutyl succinate
Heat Capacity 298.15 K, C_p=436.24 J·mol^{-1}·K^{-1}
Temperature range 90 to 400 K.
Entropy 298.15 K, S=548.44 J·mol^{-1}·K^{-1}
Phase Changes

c/liq	244.13 K,	ΔH=29211 J·mol^{-1}
		ΔS=119.60 J·mol^{-1}·K^{-1}

Molecular Weight 230.3034
Wiswesser Line Notation 4OV2VO4
Evaluation A
T(glass)=155.5 K.

$C_{12}H_{22}O_4$ (c) 74CIN/BER
Dodecanedioic acid
Phase Changes

c/liq	402.5 K,	ΔH=50564 J·mol^{-1}
		ΔS=125.60 J·mol^{-1}·K^{-1}

Molecular Weight 230.3034
Wiswesser Line Notation QV10VQ
Evaluation B

$2C_{12}H_{22}O_4Pb$ (c) 76ADE/SIM
Lead(II) n-hexanoate
Phase Changes

c/liq	335.9 K,	$\Delta H = 6020\ J \cdot mol^{-1}$
		$\Delta S = 18.0\ J \cdot mol^{-1} \cdot K^{-1}$

Crystal-smectic.

liq/liq	338.5 K,	$\Delta H = 15800\ J \cdot mol^{-1}$
		$\Delta S = 46.4\ J \cdot mol^{-1} \cdot K^{-1}$

Smectic-isomorphous.

liq/liq	350.2 K,	$\Delta H = 1300\ J \cdot mol^{-1}$
		$\Delta S = 3.8\ J \cdot mol^{-1} \cdot K^{-1}$

Isomorphous-liquid.
Molecular Weight 437.5034
Wiswesser Line Notation OV5 2 .PB
Evaluation B

$C_{12}H_{22}O_4Zn$ (c) 78KON/RUF
Zinc(II) n-hexanoate
Phase Changes

c,III/c,II	353 K,	$\Delta H = 7000\ J \cdot mol^{-1}$
c,II/c,I	378 K,	$\Delta H = 6400\ J \cdot mol^{-1}$
c,I/liq	418 K,	$\Delta H = 26000\ J \cdot mol^{-1}$
		$\Delta S = 62\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 295.6834
Wiswesser Line Notation OV5 2 .ZN
Evaluation B

$(C_{12}H_{22}O_5)_n$ (c) 91YIN/LIU
Ethyl cellulose
Heat Capacity 298 K, $C_p = 392.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 338 K. C_p value reported at 298 K is 1.594 J/g· K.
Molecular Weight 246.3028
Wiswesser Line Notation /T5OTJ B* CO2 DO2 EO* F1O2/
Evaluation B

$C_{12}H_{22}O_6$ (liq) 82BAB/RAB
Oligoethylene butylene glycol adipate; 1,4-Butylene glycol-ethylene glycol-adipic acid oligomer
Heat Capacity 298.15 K, $C_p = 482.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 330 K. $C_p = 1.839\ kJ \cdot kg^{-1} \cdot K^{-1}$ at 298.15 K.
Entropy 298.15 K, $S = 471.1\ J \cdot mol^{-1} \cdot K^{-1}$
$S° = 1.796\ kJ \cdot kg^{-1} \cdot K^{-1}$ at 298.15 K.
Phase Changes

gls/liq	207 K,	$\Delta H = 11565\ J \cdot mol^{-1}$
		$\Delta S = 55.87\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 262.3022
Wiswesser Line Notation Q4OV4VO2Q
Evaluation A
Data for glassy oligomer to liquid oligomer.

$C_{12}H_{22}O_6$ (liq) 82BAB/RAB
Oligoethylene butylene glycol adipate; 1,4-Butylene glycol-ethylene glycol-adipic acid oligomer
Heat Capacity 298.15 K, $C_p = 482.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 330 K. $C_p = 1.839\ kJ \cdot kg^{-1} \cdot K^{-1}$ at 298.15 K.
Entropy 298.15 K, $S = 527.0\ J \cdot mol^{-1} \cdot K^{-1}$
$S° = 2.009\ kJ \cdot kg^{-1} \cdot K^{-1}$ at 298.15 K.
Phase Changes

c,I/liq	290.7 K,	$\Delta H = 32709\ J \cdot mol^{-1}$
		$\Delta S = 112.5\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 262.3022
Wiswesser Line Notation Q4OV4VO2Q
Evaluation A
Data for crystalline oligomer to liquid oligomer.

$C_{12}H_{22}O_{11}$ (c) 03MAG
Sucrose; Cane sugar
Heat Capacity 298 K, $C_p = 431.1\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature. C_p given as 0.301 $cal \cdot g^{-1} \cdot K^{-1}$.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ B1Q CQ DQ EQ FO- BT5OTJ B1Q CQ DQ E1Q -A&BD -B&CEF -A&BD -B&CE
Evaluation D

$C_{12}H_{22}O_{11}$ (c) 33PAR/HUF
Sucrose; Cane sugar
Heat Capacity 297.0 K, $C_p = 422.50\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 94 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, $S = 360.2\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, 113.2 $J \cdot mol^{-1} \cdot K^{-1}$.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ B1Q CQ DQ EQ FO- BT5OTJ B1Q CQ DQ E1Q -A&BD -B&CEF -A&BD -B&CE
Evaluation B(C_p), C(S)

$C_{12}H_{22}O_{11}$ (c) 50AND/HIC
Sucrose; Cane sugar
Heat Capacity 298.15 K, $C_p = 425.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 298 to 363 K.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ B1Q CQ DQ EQ FO- BT5OTJ B1Q CQ DQ E1Q -A&BD -B&CEF -A&BD -B&CE
Evaluation B

$C_{12}H_{22}O_{11}$ (c) 89FIN/FRA
Sucrose; Cane sugar
Heat Capacity 300 K, $C_p = 430\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature. T(glass)=330 K.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ B1Q CQ DQ EQ FO- BT5OTJ B1Q CQ DQ E1Q -A&BD -B&CEF -A&BD -B&CE
Evaluation B

$C_{12}H_{22}O_{11}$ (c) 93PUT/BOE
Sucrose; Cane sugar
Heat Capacity 298.15 K, $C_p = 424.30\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 340 K.
Entropy 298.15 K, $S = 392.40\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ B1Q CQ DQ EQ FO- BT5OTJ B1Q CQ DQ E1Q -A&BD -B&CEF -A&BD -B&CE
Evaluation A

$C_{12}H_{22}O_{11}$ (c) 03MAC
Maltose
Heat Capacity 298 K, $C_p = 461.2\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature. C_p given as 0.322 $cal \cdot g^{-1} \cdot K^{-1}$.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF -A&BCE -B&DF
Evaluation D

$C_{12}H_{22}O_{11}$ (c) 81KAW/NIE
Maltose
Heat Capacity 300 K, $C_p = 435\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 270 to 325 K. C_p given as 1.27 $J \cdot g^{-1} \cdot K^{-1}$ at 300 K
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF -A&BCE -B&DF
Evaluation B

$C_{12}H_{22}O_{11}$ (c) 03MAG
Lactose; Milk sugar
Heat Capacity 298 K, C_p=412.5 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.288 cal·g^{-1}·K^{-1}.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF -A&BCE -B&DF
Evaluation D

$C_{12}H_{22}O_{11}$ (c) 36FUR/STE
β-Lactose
Heat Capacity 298.44 K, C_p=408.27 J·mol^{-1}·K^{-1}
Temperature range 83 to 298 K. Value is unsmoothed experimental datum.
Entropy 298 K, S=403.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 26.00 cal·mol^{-1}·K^{-1}.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF -A&BCE -B&DF
Evaluation B(C_p),C(S)

$C_{12}H_{22}O_{11}$ (c) 41AND/STE
β-Lactose
Heat Capacity 289.44 K, C_p=399.78 J·mol^{-1}·K^{-1}
Temperature range 65 to 290 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=386.2 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 94.6 J·mol^{-1}·K^{-1}.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF -A&BCE -B&DF
Evaluation B(C_p),C(S)

$C_{12}H_{22}O_{11}$ (c) 81KAW/NIS
Lactose; Milk sugar
Heat Capacity 300 K, C_p=418 J·mol^{-1}·K^{-1}
Temperature range 270 to 325 K. C_p given as 1.22 J·g^{-1}·K^{-1} at 300 K.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF -A&BCE -B&DF
Evaluation B

$C_{12}H_{22}O_{11}\cdot H_2O$ (c) 41AND/STE
α-Lactose monohydrate
Heat Capacity 297.42 K, C_p=439.57 J·mol^{-1}·K^{-1}
Temperature range 60 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=414.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 101.3 J·mol^{-1}·K^{-1}.
Molecular Weight 360.3144
Wiswesser Line Notation T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&BCE -B&DF -A&C -B&BDEF &QH
Evaluation B(C_p),C(S)

$C_{12}H_{22}O_{11}\cdot H_2O$ (c) 41AND/STE
β-Maltose monohydrate
Heat Capacity 296.27 K, C_p=450.70 J·mol^{-1}·K^{-1}
Temperature range 60 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=417.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 101.3 J·mol^{-1}·K^{-1}.
Molecular Weight 360.3144
Wiswesser Line Notation T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF -A&BCE -B&DF &QH
Evaluation B(C_p),C(S)

$C_{12}H_{23}O_2Tl$ (c) 76MEI/SEY
Thallium n-dodecanoate
Phase Changes

c,III/c,II	312 K,	ΔH=3807 J·mol^{-1}
		ΔS=12.1 J·mol^{-1}·K^{-1}
c,II/c,I	354 K,	ΔH=2427 J·mol^{-1}
		ΔS=6.69 J·mol^{-1}·K^{-1}
liq/liq	471 K,	ΔH=1925 J·mol^{-1}
		ΔS=4.10 J·mol^{-1}·K^{-1}

Mesophase-isotropic.

c,I/liq	398 K,	ΔH=5858 J·mol^{-1}
		ΔS=14.2 J·mol^{-1}·K^{-1}

Solid-mesophase.
Molecular Weight 403.6825
Wiswesser Line Notation OV11 .TL
Evaluation B

$C_{12}H_{23}O_2Tl$ (c) 87LOP/WES
Thallium n-dodecanoate
Heat Capacity 298.15 K, C_p=471.84 J·mol^{-1}·K^{-1}
Temperature range 7 to 470 K.
Entropy 298.15 K, S=451.06 J·mol^{-1}·K^{-1}
Phase Changes

c,VI/c,V	283.0 K,	ΔH=1829 J·mol^{-1}
		ΔS=6.49 J·mol^{-1}·K^{-1}
c,V/c,IV	285.2 K,	ΔH=2087 J·mol^{-1}
		ΔS=7.32 J·mol^{-1}·K^{-1}
c,IV/c,III	293.6 K,	ΔH=1413 J·mol^{-1}
		ΔS=4.82 J·mol^{-1}·K^{-1}
c,III/c,II	312.3 K	ΔH=4490 J·mol^{-1}
		ΔS=14.38 J·mol^{-1}·K^{-1}.
c,II/c,I	356.6 K,	ΔH=2054 J·mol^{-1}
		ΔS=5.74 J·mol^{-1}·K^{-1}
c,I/liq	400.1 K	ΔH=5454 J·mol^{-1}
		ΔS=13.64 J·mol^{-1}·K^{-1}

Solid-mesophase.

liq/liq	471.6 K,	ΔH=1971 J·mol^{-1}
		ΔS=4.16 J·mol^{-1}·K^{-1}

Mesophase-isotropic liquid.
Molecular Weight 403.6825
Wiswesser Line Notation OV11 .TL
Evaluation A

$C_{12}H_{24}$ (liq) 57MCC/FIN2
1-Dodecene
Heat Capacity 298.15 K, C_p=360.66 J·mol^{-1}·K^{-1}
Temperature range 11 to 360 K.
Entropy 298.15 K, S=484.80 J·mol^{-1}·K^{-1}
Does not include S_0.
Phase Changes

c,II/c,I	212.9 K,	ΔH=4552 J·mol^{-1}
		ΔS=21.38 J·mol^{-1}·K^{-1}
c,I/liq	237.93 K,	ΔH=19907 J·mol^{-1}
		ΔS=83.67 J·mol^{-1}·K^{-1}

Molecular Weight 168.3216
Wiswesser Line Notation 11U1
Evaluation A

$C_{12}H_{24}N_2O_2$ (c) 53WIL/DOL
N,N'-Di-n-propyladipamide
Heat Capacity 393 K, C_p=468.1 J·mol^{-1}·K^{-1}
Temperature range 393 to 583 K.
Phase Changes

c/liq	452 K,	ΔH=36110 J·mol^{-1}
		ΔS=79.9 J·mol^{-1}·K^{-1}

Molecular Weight 228.3338
Wiswesser Line Notation 3MV4VM3
Evaluation C

$C_{12}H_{24}O_2$ (c) 1885STO/WIL
Dodecanoic acid; Lauric acid
Heat Capacity 279 K, C_p=381 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C. Mean value 0 to 12 °C.
Phase Changes
c/liq 327 K, ΔH=44940 J·mol^{-1}
ΔS=137 J·mol^{-1}·K^{-1}
Molecular Weight 200.3204
Wiswesser Line Notation QV11
Evaluation D

$C_{12}H_{24}O_2$ (c) 24GAR/RAN
Dodecanoic acid; Lauric acid
Heat Capacity 301 K, C_p=428.9 J·mol^{-1}·K^{-1}
Temperature range 18 to 78 °C. Mean value 19 to 39 °C.
Phase Changes
c/liq 316.9 K, ΔH=36650 J·mol^{-1}
ΔS=115.7 J·mol^{-1}·K^{-1}
Molecular Weight 200.3204
Wiswesser Line Notation QV11
Evaluation B

$C_{12}H_{24}O_2$ (c) 82SCH/MIL2
Dodecanoic acid; Lauric acid
Heat Capacity 298.15 K, C_p=404.28 J·mol^{-1}·K^{-1}
Temperature range 80 to 345 K.
Phase Changes
c,I/liq 316.98 K, ΔH=36295 J·mol^{-1}
ΔS=114.51 J·mol^{-1}·K^{-1}
Molecular Weight 200.3204
Wiswesser Line Notation QV11
Evaluation B

$C_{12}H_{26}$ (liq) 31HUF/PAR
n-Dodecane
Heat Capacity 297.7 K, C_p=371.1 J·mol^{-1}·K^{-1}
Temperature range 93 to 298 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=497.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 105.1 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 263.5 K, ΔH=36581 J·mol^{-1}
ΔS=138.8 J·mol^{-1}·K^{-1}
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B(C_p),C(S)

$C_{12}H_{26}$ (liq) 54FIN/GRO2
n-Dodecane
Heat Capacity 298.15 K, C_p=375.93 J·mol^{-1}·K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=490.66 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 263.59 K, ΔH=36836 J·mol^{-1}
ΔS=139.75 J·mol^{-1}·K^{-1}
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation A

$C_{12}H_{26}$ (liq) 73KAL/WOY
n-Dodecane
Heat Capacity 298.15 K, C_p=370.72 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation A

$C_{12}H_{26}$ (liq) 81GRO/ING
n-Dodecane
Heat Capacity 298.15 K, C_p=374.82 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 82ZAR
n-Dodecane
Heat Capacity 298 K, C_p=374.5 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 84GRO/BEN
n-Dodecane
Heat Capacity 298.15 K, C_p=375.26 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 84KUM/BEN
n-Dodecane
Heat Capacity 298.15 K, C_p=375.30 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 84ROU/GRC
n-Dodecane
Heat Capacity 298.15 K, C_p=374.93 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 85COS/PAT
n-Dodecane
Heat Capacity 298.15 K, C_p=376.91 J·mol^{-1}·K^{-1}
Temperature range 283.15, 298.15, 313.15 K.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 85LAI/ROI
n-Dodecane
Heat Capacity 298.15 K, C_p=373.30 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 86BEN/DAI
n-Dodecane
Heat Capacity 298.15 K, C_p=375.37 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 86TAR/AIC
n-Dodecane
Heat Capacity 298.15 K, C_p=376.00 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 86WIL/LAI
n-Dodecane
Heat Capacity 298.15 K, C_p=373.30 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 88AND/PAT
n-Dodecane
Heat Capacity 298.15 K, C_p=376.46 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 88COS/HUU
n-Dodecane
Heat Capacity 298.15 K, C_p=376.09 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 88PER/AIC
n-Dodecane
Heat Capacity 298.15 K, C_p=376.00 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation A

$C_{12}H_{26}$ (liq) 89LAI/ROD
n-Dodecane
Heat Capacity 298.15 K, C_p=372.12 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 91TRE/COS
n-Dodecane
Heat Capacity 298.15 K, C_p=376.00 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 88COS/HUU
2,2,4,6,6-Pentamethylheptane
Heat Capacity 298.15 K, C_p=350.98 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 1X1&1&1Y1&1X1&1&1
Evaluation B

$C_{12}H_{26}$ (liq) 88PER/AIC
2,2,4,6,6-Pentamethylheptane
Heat Capacity 298.15 K, C_p=350.98 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 1X1&1&1Y1&1X1&1&1
Evaluation A

$C_{12}H_{26}O$ (liq) 79SVE
1-Dodecanol; n-Dodecyl alcohol
Heat Capacity 316 K, C_p=462 J·mol^{-1}·K^{-1}
Temperature range 316 to 486 K.
Phase Changes
liq/g 343.15 K, ΔH=84760 J·mol^{-1}
ΔS=246.74 J·mol^{-1}·K^{-1}
No pressure measurement.
Molecular Weight 186.3368
Wiswesser Line Notation Q12
Evaluation B

$C_{12}H_{26}O$ (liq) 88AND/PAT
1-Dodecanol; n-Dodecyl alcohol
Heat Capacity 298.15 K, C_p=438.42 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 186.3368
Wiswesser Line Notation Q12
Evaluation B

$C_{12}H_{26}O$ (liq) 89KHA/ZYK
1-Dodecanol; n-Dodecyl alcohol
Heat Capacity 303.15 K, C_p=439.4 J·mol^{-1}·K^{-1}
Temperature range 303 to 533 K.
Molecular Weight 186.3368
Wiswesser Line Notation Q12
Evaluation B

$C_{12}H_{26}O_5$ (liq) 82ZAR
Tetrapropylene glycol
Heat Capacity 298 K, C_p=560.0 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 250.3344
Wiswesser Line Notation QYOYOYOYQ
Evaluation B

$C_{12}H_{26}O_7$ (liq) 82ZAR
Hexaethylene glycol
Heat Capacity 298 K, C_p=620.0 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 282.3332
Wiswesser Line Notation Q2O2O2O2O2O2Q
Evaluation B

$C_{12}H_{26}S$ (liq) 82TUT/GAB
1-Dodecanethiol; n-Dodecyl mercaptan
Heat Capacity 300 K, C_p=442.81 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K. C_p=423.01+3.878×10^{-2} T+9.070×10^{-5}T^2.
Molecular Weight 202.3974
Wiswesser Line Notation SH12
Evaluation B

$C_{12}H_{27}O_4P$ (liq) 81NAZ/RUD
Tri-n-butylphosphate
Heat Capacity 298.15 K, C_p=379.4 J·mol^{-1}·K^{-1}
Temperature range 283 to 423 K. C_p given as 1.404 J·g^{-1}·K^{-1} at 20 °C and 1.445 J·g^{-1}·K^{-1} at 30 °C.
Molecular Weight 266.3167
Wiswesser Line Notation OPO4&O4&O4
Evaluation B

$C_{12}H_{28}ClN$ (c) 88VAN/WHI
Di-n-hexylammonium chloride
Heat Capacity 300.92 K, C_p=408.6 J·mol^{-1}·K^{-1}
Temperature range 25 to 350 K. Unsmoothed experimental datum.
Phase Changes
c,III/c,II 115.25 K, ΔH=908 J·mol^{-1}
ΔS=7.89 J·mol^{-1}·K^{-1}
c,II/c,I 279.39 K, ΔH=15950 J·mol^{-1}
ΔS=57.38 J·mol^{-1}·K^{-1}
Molecular Weight 221.8129
Wiswesser Line Notation 6M6 &GH
Evaluation A

$C_{12}H_{28}IN$ (c) 73JOH/MAR
Tetra-n-propylammonium iodide
Heat Capacity 298.15 K, C_p=349.4 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=432.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 218.3 K, ΔH=1350 J·mol^{-1}
ΔS=6.19 J·mol^{-1}·K^{-1}
Molecular Weight 313.2644
Wiswesser Line Notation 3 K3&3&3 &I
Evaluation A

$C_{12}H_{28}O_4Si$ (liq) 85NKI/CHA
Tetrapropyl silicate; Propyl silicate
Heat Capacity 298.15 K, C_p=460.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 264.4363
Wiswesser Line Notation 3O-SI-O3&O3&O3
Evaluation B

$C_{12}H_{30}OSi_2$ (liq) 86DZH/KUL
Hexaethyldisiloxane
Heat Capacity 298.15 K, C_p=460 J·mol^{-1}·K^{-1}
Temperature range 4 to 300 K. C_p(c)=51.15+1.4244T−1.7×10^{-1}T^2 (80 to 170 K); C_p(liq)=282.22+0.626T−1.05×10^{-1}T^2 (200 to 300 K).
Entropy 298.15 K, S=622.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 199.57 K, ΔH=21400 J·mol^{-1}
Molecular Weight 246.5394
Wiswesser Line Notation 2-SI-2&2&O-SI-2&2&2
Evaluation A

$C_{12}H_{30}O_3Si_3$ (liq) 82KUL/LEB
1,1,3,3,5,5-Hexaethylcyclotrisiloxane
Heat Capacity 298.15 K, C_p=535.3 J·mol^{-1}·K^{-1}
Temperature range 14 to 330 K.
Entropy 298.15 K, S=674.4 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 130 K, ΔH=470 J·mol^{-1}
ΔS=3.61 J·mol^{-1}·K^{-1}
Glassy transition.
c,II/c,I 242.3 K, ΔH=11730 J·mol^{-1}
ΔS=48.41 J·mol^{-1}·K^{-1}
c,I/liq 283.41 K, ΔH=11940 J·mol^{-1}
Molecular Weight 306.6237
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 F2
Evaluation A

$C_{12}H_{30}O_3Si_3$ (liq) 84LEB/KUL
1,1,3,3,5,5,-Hexaethylcyclotrisiloxane
Heat Capacity 298.15 K, C_p=535.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S=671.4 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 140–168 K, ΔH=470 J·mol^{-1}
ΔS=2.1 J·mol^{-1}·K^{-1}
Glassy transition.
c,II/c,I 242.3 K, ΔH=11700 J·mol^{-1}
ΔS=48.4 J·mol^{-1}·K^{-1}
c,I/liq 283.24 K, ΔH=11940 J·mol^{-1}
ΔS=42.2 J·mol^{-1}·K^{-1}
Molecular Weight 306.6237
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 F2
Evaluation A

$C_{12}H_{30}O_3Si_3$ (liq) 85DZH/KUL
1,1,3,3,5,5-Hexaethylcyclotrisiloxane
Heat Capacity 298.15 K, C_p=581.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=680.8 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 160 K, ΔH=462 J·mol^{-1}
ΔS=2.9 J·mol^{-1}·K^{-1}
c,II/c,I 242.3 K, ΔH=11824 J·mol^{-1}
ΔS=48.8 J·mol^{-1}·K^{-1}
c,I/liq 280.2 K, ΔH=11424 J·mol^{-1}
ΔS=40.9 J·mol^{-1}·K^{-1}
Molecular Weight 306.6237
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 F2
Evaluation A

$C_{12}H_{30}O_3Si_3$ (liq) 88LEB/KUL
1,1,3,3,5,5-Hexaethylcyclotrisiloxane
Heat Capacity 300 K, C_p=536.53 J·mol^{-1}·K^{-1}
Temperature range 13.4 to 350 K.
Entropy 300 K, S=674.71 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 140–168 K, ΔH=470.0 J·mol^{-1}
ΔS=2.08 J·mol^{-1}·K^{-1}
c,II/c,I 242.4 K, ΔH=11730.8 J·mol^{-1}
ΔS=48.39 J·mol^{-1}·K^{-1}
c,I/liq 283.41 K, ΔH=11940.3 J·mol^{-1}
ΔS=42.07 J·mol^{-1}·K^{-1}
Molecular Weight 306.6237
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 F2
Evaluation A

$C_{12}H_{36}ClCr_3O_{22}$ (c) 71SOR/TAC
Triaquo hexacetate chromate chloride hexahydrate
Heat Capacity 278.084 K, C_p=958.02 J·mol^{-1}·K^{-1}
Temperature range 1.5 to 280 K. Value is unsmoothed experimental datum.
Phase Changes
c,II/c,I 211.4 K, ΔH=3322 J·mol^{-1}
ΔS=13.778 J·mol^{-1}·K^{-1}
Two peaks were observed: at 211.4 K and 215.5 K, ΔH and ΔS give for overall transition.
Molecular Weight 723.8442
Wiswesser Line Notation CR3 O& QH 3 &OV1 6 &G &QH 6
Evaluation A

$C_{12}H_{54}Cr_4N_{12}O_{18}S_3 \cdot 10H_2O$ (c) 72SOR/SEK
Hexahydroxyhexaethylenediamine chromium sulfate decahydrate
Heat Capacity 197.459 K, $C_p = 1001.82\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 1.4 to 200 K. Unsmoothed experimental datum.
Molecular Weight 1138.9442
Wiswesser Line Notation CR 4 &Q 6 &Z2Z 6 &S-O4*3 &QH 1O
Evaluation A

$C_{13}H_8Cl_2O$ (c) 87ECO/BER
p-Dichlorobenzophenone
Heat Capacity
Temperature range 175 to 205 K. Data given graphically.
Phase Changes
c,III/c,II 186.1 K, $\Delta H = 146\ J \cdot mol^{-1}$
c,II/c,I 189.5 K, $\Delta H = 251\ J \cdot mol^{-1}$
Molecular Weight 251.1116
Wiswesser Line Notation GR DVR DG
Evaluation B

$C_{13}H_8N_8O_{15}$ (c) 24TAY/RIN
Tetryl-picric acid complex
Heat Capacity 293 K, $C_p = 433.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 90 to 352 K.
Molecular Weight 516.2508
Wiswesser Line Notation WNN1&R BNW DNW FNW &WNR BQ CNW ENW
Evaluation C

$C_{13}H_8O_2$ (c) 88SAB/ELW
Xanthone
Heat Capacity 298.15 K, $C_p = 226\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Phase Changes
c/liq 449.63 K, $\Delta H = 26120\ J \cdot mol^{-1}$
liq/g 298.15 K, $\Delta H = 98570\ J \cdot mol^{-1}$
Molecular Weight 196.2050
Wiswesser Line Notation T C666 BV IOJ
Evaluation A

$C_{13}H_8OS$ (c) 92SAB/ELW5
Thioxanthone
Phase Changes
c/liq 487.88 K, $\Delta H = 35500\ J \cdot mol^{-1}$
Molecular Weight 212.2656
Wiswesser Line Notation T C666 BS IVJ
Evaluation A

$C_{13}H_9F_3N_2O_2$ (c) 89PIN/GON
2-[3-(trifluoromethyl)-phenyl]amino-3-pyridinecarboxylic acid; Niflumic acid
Heat Capacity 298.15 K, $C_p = 288.3\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 100 to 500 K. $C_p(c) = 0.9T + 20\ J \cdot mol^{-1} \cdot K^{-1}$ (140 to 465 K). C_p value calculated from the equation.
Phase Changes
c/liq 475 K, $\Delta H = 36800\ J \cdot mol^{-1}$
$\Delta S = 77\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 282.2215
Wiswesser Line Notation T6TJ CVQ BMR CXFFF
Evaluation A

$C_{13}H_9N$ (c) 88STE/CHI
7,8-Benzoquinoline
Heat Capacity 298.15 K, $C_p = 206.36\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 500 K.
Entropy 298.15 K, $S = 213.20\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 324.104 K, $\Delta H = 14103\ J \cdot mol^{-1}$
$\Delta S = 43.51\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 179.2208
Wiswesser Line Notation T B666 CNJ
Evaluation A

$C_{13}H_9N$ (c) 89STE/CHI
7,8-Benzoquinoline
Heat Capacity 298.15 K, $C_p = 206.36\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 500 K.
Entropy 298.15 K, $S = 213.20\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 324.104 K, $\Delta H = 14103\ J \cdot mol^{-1}$
$\Delta S = 43.51\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 179.2208
Wiswesser Line Notation T B666 CNJ
Evaluation A

$C_{13}H_9N$ (c) 86STE/CHI
Phenanthridine
Heat Capacity 298.15 K, $C_p = 201.79\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 6 to 450 K.
Entropy 298.15 K, $S = 205.87\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 354.16 K
c,I/liq 379.742 K
Molecular Weight 179.2208
Wiswesser Line Notation T B666 HNJ
Evaluation A

$C_{13}H_9N$ (c) 88STE/CHI
Phenanthridine
Heat Capacity 298.15 K, $C_p = 201.87\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 500 K.
Entropy 298.15 K, $S = 205.91\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 354.0 K, $\Delta H = 20.79\ J \cdot mol^{-1}$
$\Delta S = 0.059\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolated value.
c,I/liq 379.74 K, $\Delta H = 22831\ J \cdot mol^{-1}$
$\Delta S = 60.12\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 179.2208
Wiswesser Line Notation T B666 HNJ
Evaluation A

$C_{13}H_9N$ (c) 89STE/CHI
Phenanthridine
Heat Capacity 298.15 K, $C_p = 201.87\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 500 K.
Entropy 298.15 K, $S = 205.91\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 354.0 K, $\Delta H = 20.79\ J \cdot mol^{-1}$
$\Delta S = 0.059\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolated value.
c,I/liq 379.74 K, $\Delta H = 22831\ J \cdot mol^{-1}$
$\Delta S = 60.12\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 179.2208
Wiswesser Line Notation T B666 HNJ
Evaluation A

$C_{13}H_9N$ (c) 86STE/CHI
Acridine
Heat Capacity 298.15 K, C_p=204.98 J·mol^{-1}·K^{-1}
Temperature range 6 to 450 K.
Entropy 298.15 K, S=208.00 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 383.243 K
Molecular Weight 179.2208
Wiswesser Line Notation T C666 BNJ
Evaluation A

$C_{13}H_9N$ (c) 88STE/CHI
Acridine
Heat Capacity 298.15 K, C_p=205.07 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S=208.03 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 383.242 K, ΔH=20682 J·mol^{-1}
ΔS=53.97 J·mol^{-1}·K^{-1}
Molecular Weight 179.2208
Wiswesser Line Notation T C666 BNJ
Evaluation A

$C_{13}H_9N$ (c) 89STE/CHI
Acridine
Heat Capacity 298.15 K, C_p=205.07 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S=208.03 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 383.242 K, ΔH=20682 J·mol^{-1}
ΔS=53.97 J·mol^{-1}·K^{-1}
Molecular Weight 179.2208
Wiswesser Line Notation T C666 BNJ
Evaluation A

$C_{13}H_{10}$ (c) 44EIB
Fluorene; Diphenylenemethane
Heat Capacity 298.1 K, C_p=189.5 J·mol^{-1}·K^{-1}
Temperature range 25 to 200 °C, equations only, in t °C. C_p(c) =0.2479+0.001233t cal·g^{-1}·C^{-1} (25 to 70 °C); C_p(liq)=0.320 +0.00845t cal·g^{-1}·C^{-1} (114 to 200 °C).
Phase Changes
c/liq 387.0 K, ΔH=19870 J·mol^{-1}
ΔS=51.3 J·mol^{-1}·K^{-1}
Molecular Weight 166.2220
Wiswesser Line Notation L B656 HHJ
Evaluation C

$C_{13}H_{10}$ (c,I) 77FIN/MES
Fluorene: Diphenylenemethane
Heat Capacity 298.15 K, C_p=203.13 J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, S=207.32 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 288 K
Second order transition.
c,I/liq 387.94 K, ΔH=19578.2 J·mol^{-1}
ΔS=50.47 J·mol^{-1}·K^{-1}
Molecular Weight 166.2220
Wiswesser Line Notation L B656 HHJ
Evaluation A

$C_{13}H_{10}N_2$ (liq) 84LEB/BYF
Diphenylcarbodiimide
Heat Capacity 298.15 K, C_p=304.6 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 330 K.
Entropy 298.15 K, S=330.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 287.41 K, ΔH=18550 J·mol^{-1}
ΔS=64.54 J·mol^{-1}·K^{-1}
Molecular Weight 194.2354
Wiswesser Line Notation RNUCUNR
Evaluation A
Data also given for the vitreous state and supercooled liquid from 5 t 287.41. T(glass)=190 ± 1 K.

$C_{13}H_{10}O$ (c) 1889EYF
Benzophenone
Phase Changes
c/liq 321.2 K, ΔH=17669 J·mol^{-1}
ΔS=55.0 J·mol^{-1}·K^{-1}
Molecular Weight 182.2214
Wiswesser Line Notation RVR
Evaluation C

$C_{13}H_{10}O$ (c) 83DEK/VAI
Benzophenone
Heat Capacity 300 K, C_p=224.80 J·mol^{-1}·K^{-1}
Temperature range 80 to 345 K.
Phase Changes
c/liq 321.03 K, ΔH=18194 J·mol^{-1}
ΔS=56.67 J·mol^{-1}·K^{-1}
Molecular Weight 182.2214
Wiswesser Line Notation RVR
Evaluation A
C_p(c)=40.42+0.4252 (T/K)+6.27021×+10^{-4}(T/K)^2 (80 to 290 K) ·mol^{-1}·K^{-1}. C_p(liq)=150.19+0.4576 (T/K) (280 to 350 K) J·mol^{-1}.

$C_{13}H_{10}O_3$ (c) 58SIN/HII
Diphenyl carbonate
Heat Capacity 298.15 K, C_p=263.13 J·mol^{-1}·K^{-1}
Temperature range 15 to 310 K.
Entropy 298.15 K, S=278.40 J·mol^{-1}·K^{-1}
Molecular Weight 214.2202
Wiswesser Line Notation ROVOR
Evaluation A

$C_{13}H_{11}Cl$ (liq) 31SMI/ANI
Diphenylchloromethane
Heat Capacity 298.5 K, C_p=290.4 J mol^{-1} K^{-1}
Temperature range 102 to 311 K. Value is unsmoothed experimenta datum.
Molecular Weight 202.6829
Wiswesser Line Notation GYR&R
Evaluation C

$C_{13}H_{11}N$ (c) 86STE/CH
N-Methylcarbazole
Heat Capacity 298.15 K, C_p=217.84 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=234.30 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 362.490 K
Molecular Weight 181.2366
Wiswesser Line Notation T B656 HNJ H1
Evaluation A

$C_{13}H_{11}N$ (c) 87MES/TOD
N-Methylcarbazole
Heat Capacity 298.15 K, C_p=217.84 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=234.30 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 362.490 K, ΔH=17153.8 J·mol^{-1}
ΔS=47.32 J·mol^{-1}·K^{-1}
Molecular Weight 181.2366
Wiswesser Line Notation T B656 HNJ H1
Evaluation A

$C_{13}H_{11}N$ (c) 88MES/TOD
N-Methylcarbazole
Heat Capacity 298.150 K, C_p=217.838 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S=234.300 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 362.490 K, ΔH=17153.71 J·mol^{-1}
ΔS=47.32 J·mol^{-1}·K^{-1}
Molecular Weight 181.2366
Wiswesser Line Notation T B656 HNJ H1
Evaluation A

$C_{13}H_{11}N$ (c) 90JIM/ROU
N-Methylcarbazole
Heat Capacity 298.15 K, C_p=204.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 181.2366
Wiswesser Line Notation T B656 HNJ H1
Evaluation A

$C_{13}H_{11}N$ (c) 92CAL/MCD
N-Methylcarbazole
Heat Capacity 298.15 K, C_p=218.42 J·mol^{-1}·K^{-1}
Temperature range 4 to 345 K.
Entropy 298.15 K, S=236.05 J·mol^{-1}·K^{-1}
Molecular Weight 181.2366
Wiswesser Line Notation T B656 HNJ H1
Evaluation A

$C_{13}H_{11}NO$ (c) 92SAB/ELW3
Benzanilide
Phase Changes
c/liq 436.49 K, ΔH=29610 J·mol^{-1}
Molecular Weight 197.2360
Wiswesser Line Notation RMVR
Evaluation A

$C_{13}H_{12}$ (c) 1889EYK
Diphenylmethane
Phase Changes
c/liq 299.4 K, ΔH=19050 J·mol^{-1}
Molecular Weight 168.2378
Wiswesser Line Notation R1R
Evaluation C

$C_{13}H_{12}$ (c) 30HUF/PAR
Diphenylmethane
Heat Capacity 282.5 K, C_p=223.8 J·mol^{-1}·K^{-1}
Temperature range 89 to 312 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=239.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 77.86 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 298.3 K, ΔH=18569 J·mol^{-1}
ΔS=62.25 J·mol^{-1}·K^{-1}
Molecular Weight 168.2378
Wiswesser Line Notation R1R
Evaluation B(C_p),C(S)

$C_{13}H_{12}$ (c) 31SMI/AND
Diphenylmethane
Heat Capacity 298.5 K, C_p=233.5 J·mol^{-1}·K^{-1}
Temperature range 102 to 322 K. Value is unsmoothed experimental datum.
Molecular Weight 168.2378
Wiswesser Line Notation R1R
Evaluation C

$C_{13}H_{12}$ (c) 50KUR
Diphenylmethane
Heat Capacity 300 K, C_p=279.9 J·mol^{-1}·K^{-1}
Temperature range 29 to 254 °C.
Molecular Weight 168.2378
Wiswesser Line Notation R1R
Evaluation B

$C_{13}H_{12}$ (c) 56DUF/EVE
Diphenylmethane
Heat Capacity 303 K, C_p=266.1 J·mol^{-1}·K^{-1}
Temperature range 303 to 353 K.
Molecular Weight 168.2378
Wiswesser Line Notation R1R
Evaluation B

$C_{13}H_{12}$ (c) 86CHI/ANN
Diphenylmethane
Phase Changes
c/liq ΔH=19246 J·mol^{-1}
c/g ΔH=83262 J·mol^{-1}
Molecular Weight 168.2378
Wiswesser Line Notation R1R
Evaluation A

$C_{13}H_{12}D_{10}FeN_6S_3$ (c) 86SOR/SHI
Ferrocene d_{10} thiourea clathrate (1:3)
Heat Capacity 300 K, C_p=510 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Data given graphically. Value given is an estimate from graph.
Phase Changes
c,VI/c,V 145.8 K, ΔH=57 J·mol^{-1}
ΔS=0.39 J·mol^{-1}·K^{-1}
c,V/c,IV 160.6 K, ΔH=1762 J·mol^{-1}
ΔS=10.62 J·mol^{-1}·K^{-1}
c,IV/c,III 173.4 K, ΔH=11 J·mol^{-1}
ΔS=0.07 J·mol^{-1}·K^{-1}
c,III/c,II 187.1 K, ΔH=31 J·mol^{-1}
ΔS=0.17 J·mol^{-1}·K^{-1}
c,II/c,I 219.0 K, ΔH=57 J·mol^{-1}
ΔS=0.27 J·mol^{-1}·K^{-1}
Molecular Weight 424.4630
Wiswesser Line Notation L5ϕJ &1A-E/H-2 5 ϕ-FE– ϕL5ϕJ &1A-E/H-2 5 &ZYZUS 3
Evaluation A

$C_{13}H_{12}N_2O$ (c) 87FER/DEL
1,3-Diphenylurea
Phase Changes
c/liq 512.1 K, $\Delta H = 34620\ J \cdot mol^{-1}$
$\Delta S = 66.5\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 212.2506
Wiswesser Line Notation RNVNR
Evaluation A

$C_{13}H_{12}O$ (c) 31SMI/AND
Benzhydrol; Diphenylcarbinol
Heat Capacity 298.5 K, $C_p = 236.8\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 102 to 299 K. Value is unsmoothed experimental datum.
Molecular Weight 184.2372
Wiswesser Line Notation QYR&R
Evaluation C

$C_{13}H_{12}O$ (c) 74CIN/BER
Benzhydrol: Diphenylcarbinol
Phase Changes
c/liq 338.5 K, $\Delta H = 22995\ J \cdot mol^{-1}$
$\Delta S = 67.95\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 184.2372
Wiswesser Line Notation QYR&R
Evaluation B

$C_{13}H_{13}N$ (liq) 1881REI
Methyldiphenylamine
Heat Capacity 298 K, $C_p = 301.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 467 K.
Molecular Weight 183.2524
Wiswesser Line Notation 1NR&R
Evaluation D

$C_{13}H_{14}N_2$ (c) 66ZAL/STR
Bis(4-aminophenyl)methane
Heat Capacity 388 K, $C_p = 227.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 110 to 120 °C, mean value.
Phase Changes
c/liq 366 K
Molecular Weight 198.2670
Wiswesser Line Notation ZR D1R DZ
Evaluation D

$C_{13}H_{14}N_2$ (c) 78MAR/CIO
Bis(4-aminophenyl)methane
Heat Capacity 298 K, $C_p = 66.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 298 to 469 K. Data seem odd; values for solid increase from 66.5 to 606.3 $J \cdot mol^{-1} \cdot K^{-1}$ at 370 K to 463.2 $J \cdot mol^{-1} \cdot K^{-1}$ at 470 K.
Phase Changes
c/liq 363.7 K, $\Delta H = 9225\ J \cdot mol^{-1}$
$\Delta S = 25.4\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 198.2670
Wiswesser Line Notation ZR D1R DZ
Evaluation D

$C_{13}H_{14}N_2$ (c) 87LES/LI(
Bis(4-aminophenyl)methane
Heat Capacity 298 K, $C_p = 270.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 250 to 400 K.
Phase Changes
c/liq 366 K
Molecular Weight 198.2670
Wiswesser Line Notation ZR D1R DZ
Evaluation B

$C_{13}H_{14}N_2O_2$ (c) 86KAR/BA
3,3′-Methylene bis(6-aminophenol)
Heat Capacity 298.15 K, $C_p = 281.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 470 K.
Entropy 298.15 K, $S = 284.6\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 230.2658
Wiswesser Line Notation ZR BQ D1R CQ DZ
Evaluation A

$C_{13}H_{15}N$ (c) 92STE/CH
1,2,3,4-Tetrahydro-9-methylcarbazole
Heat Capacity 298.15 K, $C_p = 241.35\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 460 K. C_p(liq, 298.15 K)=290.62 J/K·mo
C_p value for the liquid at 298.15 K was calculated with graphicall extrapolated data.
Entropy 298.15 K, $S = 260.89\ J \cdot mol^{-1} \cdot K^{-1}$
S(liq, 298.15 K)=302.61 J/K·mol. S value for the liquid at 298.15 I was calculated with graphically extrapolated data.
Phase Changes
c,IV/c,III 103.8 K, $\Delta H = 0.0\ J \cdot mol^{-1}$
c,III/c,II 162.4 K, $\Delta H = 679.3\ J \cdot mol^{-1}$
c,II/c,I 210.4 K, $\Delta H = 0.0\ J \cdot mol^{-1}$
c,I/liq 323.71 K, $\Delta H = 14666.8\ J \cdot mol^{-1}$
Molecular Weight 185.2682
Wiswesser Line Notation T B656 HNT&&J H1
Evaluation A

$C_{13}H_{15}N$ (c,I) 92STE/CHI
1,2,3,4-Tetrahydro-9-methylcarbazole
Heat Capacity 298.15 K, $C_p = 241.35\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 660 K. C_p(liq, 298.15 K)=290.62 J/K·mo extrapolated.
Entropy 298.15 K, $S = 260.89\ J \cdot mol^{-1} \cdot K^{-1}$
S(liq, 298.15 K)=302.61 J/K·mol, extrapolated.
Phase Changes
c,IV/c,III 103.8 K, $\Delta H = 0.0\ J \cdot mol^{-1}$
c,III/c,II 162.4 K, $\Delta H = 679\ J \cdot mol^{-1}$
c,II/c,I 210.4 K, $\Delta H = 0.0\ J \cdot mol^{-1}$
c,I/liq 323.71 K, $\Delta H = 14667\ J \cdot mol^{-1}$
Molecular Weight 185.2682
Wiswesser Line Notation T B656 HNT&&J H1
Evaluation A

$C_{13}H_{15}NO$ (liq) 86ACH/HA
1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl) benzene
Heat Capacity 333 K, $C_p = 382\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 333, 433 K. $C_p = 1.9\ J \cdot g^{-1} \cdot C^{-1}$.
Molecular Weight 201.2676
Wiswesser Line Notation OCNX2&1&R CYU1&1
Evaluation C
98% purity.

$C_{13}H_{15}NO$ (liq) 86ACH/HAS
1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl) benzene
Heat Capacity 333 K, C_p=362 J·mol^{-1}·K^{-1}
Temperature range 333, 433 K. C_p=1.8 J·g^{-1}·C^{-1}.
Molecular Weight 201.2676
Wiswesser Line Notation OCNX2&1&R DYU1&1
Evaluation C
91% purity.

$C_{13}H_{15}NO$ (c) 40CAM/CAM
p-Toluidine-phenol complex; Phenol-p-toluidine complex
Heat Capacity 293 K, C_p=216.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 201.2676
Wiswesser Line Notation ZR D1 &QR
Evaluation C

$C_{13}H_{16}N_2O_3$ (c) 40CAM/CAM
Phenol-urea complex; Urea-phenol complex
Heat Capacity 293 K, C_p=250.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 248.2810
Wiswesser Line Notation ZVZ &QR 2
Evaluation C

$C_{13}H_{18}$ (liq) 81LEE/FIN
1,1,4,6-Tetramethylindan
Heat Capacity 298.15 K, C_p=299.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=348.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 191 K
c,I/liq 273.51 K, ΔH=15742 J·mol^{-1}
Molecular Weight 174.2852
Wiswesser Line Notation L56 T&J B1 B1 F1 I1
Evaluation A

$C_{13}H_{18}$ (liq) 81LEE/FIN
1,1,4,7-Tetramethylindan
Heat Capacity 298.15 K, C_p=302.5 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=343.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 245.553 K, ΔH=11279 J·mol^{-1}
Molecular Weight 174.2852
Wiswesser Line Notation L56 T&J B1 B1 F1 H1
Evaluation A
T(glass)=160 K.

$C_{13}H_{19}NO_2$ (c) 71PRI
Hexyl N-phenylcarbamate
Heat Capacity 298 K, C_p=336.8 J·mol^{-1}·K^{-1}
Temperature range 200 to 390 K. Complete data deposited in VINITI, No. 2713-71, 25 March 1971.
Phase Changes
c/liq 328 K, ΔH=32765 J·mol^{-1}
ΔS=99.9 J·mol^{-1}·K^{-1}
Molecular Weight 221.2986
Wiswesser Line Notation 6OVMR
Evaluation B

$C_{13}H_{20}$ (liq) 48TSC
n-Heptylbenzene
Heat Capacity 294 K, C_p=269 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 176.3010
Wiswesser Line Notation 7R
Evaluation C

$C_{13}H_{20}O$ (liq) 88BAG/GUR
6,10-Dimethyl-4,5,9-undecatrien-2-one
Heat Capacity 313.65 K, C_p=413.4 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 192.3004
Wiswesser Line Notation 1YU3YU1U2V1
Evaluation B

$C_{13}H_{20}O$ (liq) 88BAG/GUR
6,10-Dimethyl-3,5,9-undecatrien-2-one
Heat Capacity 297.85 K, C_p=382.7 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 192.3004
Wiswesser Line Notation 1YU3YU2U1V1
Evaluation B

$C_{13}H_{20}O$ (liq) 88BAG/GUR
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one
Heat Capacity 313.60 K, C_p=388.4 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 192.3004
Wiswesser Line Notation L6 AUTJ A1 B1U1V1 C1 C1
Evaluation B

$C_{13}H_{22}BrN$ (c) 89VAN/WHI
7-Phenylheptylammonium bromide
Phase Changes
c,II/c,I 332 K, ΔH=9300 J·mol^{-1}
ΔS=3.46 J·mol^{-1}·K^{-1}
Molecular Weight 272.2275
Wiswesser Line Notation Z7R &EH
Evaluation A

$C_{13}H_{22}ClN$ (c) 89VAN/WHI
7-Phenylheptylammonium chloride
Phase Changes
c,II/c,I 310 K, ΔH=10100 J·mol^{-1}
ΔS=3.9 J·mol^{-1}·K^{-1}
Molecular Weight 227.7765
Wiswesser Line Notation Z7R &GH
Evaluation A

$C_{13}H_{22}FeN_6S_3$ (c) 81SOR/OGA
Thiourea-ferrocene
Heat Capacity 273.15 K, C_p=447.86 J·mol^{-1}·K^{-1}
Temperature range 13 to 280 K.
Entropy 273.15 K, S=516.05 J·mol^{-1}·K^{-1}
Phase Changes
c,V/c,IV 147.2 K, ΔH=263 J·mol^{-1}
ΔS=1.8 J·mol^{-1}·K^{-1}
c,IV/c,III 159.79 K, ΔH=1473 J·mol^{-1}
ΔS=9.24 J·mol^{-1}·K^{-1}
c,III/c,II 171.4 K, ΔH=14 J·mol^{-1}
ΔS=0.079 J·mol^{-1}·K^{-1}
c,II/c,I 185.5 K, ΔH=35 J·mol^{-1}
ΔS=0.188 J·mol^{-1}·K^{-1}
c,III/c,I 220 K, ΔH=77 J·mol^{-1}
ΔS=0.36 J·mol^{-1}·K^{-1}
Molecular Weight 414.3840
Wiswesser Line Notation L5ϕL ϕ-FE- ϕL5ϕL &ZYZUS 3
Evaluation A

$(C_{13}H_{22}O_8)_n$ (liq) 83SAN/CIO
Diethylene glycol-glycerol-adipate polymer
Heat Capacity 298.15 K, C_p=1287 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K. C_p °(kJ·kg^{-1}·K^{-1})=0.023598T−2.835
Molecular Weight 306.3120
Wiswesser Line Notation /*O2O2OV4VO1YQ71O*/
Evaluation D
Authors did not provide formula for repeating unit of polymer; assumed: diethylene glycol-adipate-glycerol, as repeating unit. The C_p value=1287 J·mol^{-1}·K^{-1} is unrealistic.

$C_{13}H_{24}$ (liq) 62GOL/BEL
α-n-Propyldecalin
Heat Capacity 311 K, C_p=335.6 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 180.3326
Wiswesser Line Notation L66TJ B3
Evaluation C

$C_{13}H_{24}$ (liq) 63GUD/CAM
α-n-Propyldecalin
Heat Capacity 313 K, C_p=337.2 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 180.3326
Wiswesser Line Notation L66TJ B3
Evaluation C

$C_{13}H_{24}$ (liq) 62GOL/BEL
α-Isopropyldecalin
Heat Capacity 311 K, C_p=316.3 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 180.3326
Wiswesser Line Notation L66TJ BY1&1
Evaluation C

$C_{13}H_{24}$ (liq) 63GUD/CAM
α-Isopropyldecalin
Heat Capacity 313 K, C_p=318.4 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 180.3326
Wiswesser Line Notation L66TJ BY1&1
Evaluation C

$C_{13}H_{24}$ (liq) 63GUD/CAM
Isopropyldecalin
Heat Capacity 373 K, C_p=373.6 J·mol^{-1}·K^{-1}
Temperature range 373 to 483 K.
Molecular Weight 180.3326
Wiswesser Line Notation L66TJ XY1&1
Evaluation C

$C_{13}H_{24}$ (liq) 63GUD/CAM
2-Methylbicyclohexyl
Heat Capacity 313 K, C_p=331.4 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 180.3326
Wiswesser Line Notation L6TJ A- BL6TJ A1
Evaluation C

$C_{13}H_{24}$ (liq) 62GOL/BEL
Dicyclohexylmethane
Heat Capacity 311 K, C_p=355.2 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 180.3326
Wiswesser Line Notation L6TJ A1- AL6TJ
Evaluation C

$C_{13}H_{24}$ (liq) 63GUD/CAM
Dicyclohexylmethane
Heat Capacity 313 K, C_p=320.1 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 180.3326
Wiswesser Line Notation L6TJ A1- AL6TJ
Evaluation C

$C_{13}H_{24}O_2$ (liq) 89GUS/BA
Nonyl methacrylate
Heat Capacity 298.15 K, C_p=419.3 J·mol^{-1}·K^{-1}
Temperature range 244 to 315 K. C_p(liq)=2354.676−5.056583
$-0.127035T^2$ J/kg·K (244 to 315 K). C_p=419.3 J/mol·K calculated b
interpolation of experimental data, does not agree with equation give
Molecular Weight 212.3314
Wiswesser Line Notation 9OV1Y1&U1
Evaluation B

$C_{13}H_{24}O_2$ (c) 81LEB/EV
Tridecanolactone
Heat Capacity 298.15 K, C_p=398.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K.
Entropy 298.15 K, S=401.8 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 290.63 K, ΔH=18150 J·mol^{-1}
ΔS=62.45 J·mol^{-1}·K^{-1}
c,I/liq 300.4 K, ΔH=9060 J·mol^{-1}
ΔS=30.2 J·mol^{-1}·K^{-1}
Molecular Weight 212.3314
Wiswesser Line Notation T-14-VOTJ
Evaluation A

$C_{13}H_{24}O_2$ (c) 81LEB/YEV
Tridecanolactone
Heat Capacity 298.15 K, C_p=398.3 J·mol^{-1}·K^{-1}
Temperature range 10.3 to 330 K.
Entropy 298.15 K, S=401.9 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 290.63 K, ΔH=18150 J·mol^{-1}
ΔS=62.3 J·mol^{-1}·K^{-1}
c,I/liq 300.4 K, ΔH=9058 J·mol^{-1}
ΔS=30.2 J·mol^{-1}·K^{-1}
Molecular Weight 212.3314
Wiswesser Line Notation T-14-VOTJ
Evaluation A

$(C_{13}H_{24}O_2)_n$ (c) 81LEB/EVS
Poly(tridecanolactone)
Heat Capacity 298.15 K, C_p=329.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K.
Entropy 298.15 K, S=351.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 229 K
Glass/crystal.
c/liq 368.1 K, ΔH=46000 J·mol^{-1}
ΔS=125 J·mol^{-1}·K^{-1}
Molecular Weight 212.3314
Wiswesser Line Notation /*OV-14-*/
Evaluation A

$C_{13}H_{24}O_4$ (c) 74CIN/BER
Tridecanedioic acid
Phase Changes
c/liq 387.5 K, ΔH=45296 J·mol^{-1}
ΔS=116.9 J·mol^{-1}·K^{-1}
Molecular Weight 244.3302
Wiswesser Line Notation QV11VQ
Evaluation B

$C_{13}H_{25}O_2Tl$ (c) 89ROU/TUR
Thallium tridecanoate
Heat Capacity
Temperature range 345 to 460 K.
Phase Changes
c,V/c,IV 315.0 K, ΔH=790 J·mol^{-1}
ΔS=2.49 J·mol^{-1}·K^{-1}
c,IV/c,III 328.1 K, ΔH=4831 J·mol^{-1}
ΔS=14.72 J·mol^{-1}·K^{-1}
c,III/c,II 332.6 K, ΔH=9312 J·mol^{-1}
ΔS=28.02 J·mol^{-1}·K^{-1}
c,II/c,I 370.1 K, ΔH=2902 J·mol^{-1}
ΔS=7.82 J·mol^{-1}·K^{-1}
c,I/liq 397.9 K, ΔH=6294 J·mol^{-1}
ΔS=15.80 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 417.7093
Wiswesser Line Notation OV12 .TL
Evaluation A
Mesophase-isotropic liquid transition. 464.7 K, ΔH=1871 J/mol, ΔS=3.99 J/mol·K.

$C_{13}H_{26}$ (liq) 49PAR/MOO
n-Heptylcyclohexane
Heat Capacity 298.15 K, C_p=363.2 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.15 K, S=446.9 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 90.04 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 232.8 K, ΔH=22225 J·mol^{-1}
ΔS=95.5 J·mol^{-1}·K^{-1}
Molecular Weight 182.3484
Wiswesser Line Notation L6TJ A7
Evaluation (C_p),C(S)

$C_{13}H_{26}O$ (liq) 88BAG/GUR
6,10-Dimethyl-2-undecanone
Heat Capacity 313.55 K, C_p=428.4 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 198.3478
Wiswesser Line Notation 1Y3Y3V1
Evaluation B

$C_{13}H_{26}O_2$ (c) 82SCH/MIL
Tridecanoic acid
Heat Capacity 298.15 K, C_p=387.6 J·mol^{-1}·K^{-1}
Temperature range 80 to 340 K.
Phase Changes
c,II/c,I 307.1 K, ΔH=8730 J·mol^{-1}
ΔS=28.41 J·mol^{-1}·K^{-1}
c,I/liq 315.01 K, ΔH=33729 J·mol^{-1}
ΔS=107.07 J·mol^{-1}·K^{-1}
Molecular Weight 214.3472
Wiswesser Line Notation QV12
Evaluation B

$C_{13}H_{26}O_2Si_3$ (liq) 84DZH/KUL
1,1,1,3,5,5,5-Heptamethyl-3-phenyltrisiloxane
Heat Capacity 298.15 K C_p=519.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K S=620.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 226.84 K ΔH=18293 J·mol^{-1}
ΔS=80.7 J·mol^{-1}·K^{-1}
Molecular Weight 298.6037
Wiswesser Line Notation 1-SI-1&1&O-SI-1&R&O-SI-1&1&1
Evaluation A

$C_{13}H_{26}O_4$ (c) 65SIL/DAU
1-Monocaprin
Heat Capacity 298 K, C_p=410.0 J·mol^{-1}·K^{-1}
One temperature. β_L form.
Molecular Weight 246.3460
Wiswesser Line Notation Q1YQ1OV9
Evaluation B

$2C_{13}H_{28}$ (liq) 54FIN/GRO2
n-Tridecane
Heat Capacity 298.15 K, C_p=406.89 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=522.87 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 255.0 K, ΔH=7661 J·mol^{-1}
ΔS=30.04 J·mol^{-1}·K^{-1}
c,I/liq 267.79 K, ΔH=28501 J·mol^{-1}
ΔS=106.43 J·mol^{-1}·K^{-1}
Molecular Weight 184.3642
Wiswesser Line Notation 13H
Evaluation A

$C_{13}H_{28}$ (liq) 75WOY/KAL
n-Tridecane
Heat Capacity 303.15 K, C_p=409.40 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 184.3642
Wiswesser Line Notation 13H
Evaluation B

$C_{13}H_{28}$ (c) 86MEE/BEC
Tri(tert-butyl)methane
Heat Capacity 298.15 K, C_p=354.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 184.3642
Wiswesser Line Notation 1X1&1&YX1&1&1X1&1&1
Evaluation B

$C_{13}H_{28}O$ (c) 74MOS/MOU
1-Tridecanol; n-Tridecyl alcohol
Heat Capacity 298.15 K, C_p=378 J·mol^{-1}·K^{-1}
β-form, 276 to 299 K.
Phase Changes
c,β/c,γ 301.6 K, ΔH=3600 J·mol^{-1}
ΔS=11.9 J·mol^{-1}·K^{-1}
c,β/c,α 305.8 K, ΔH=22100 J·mol^{-1}
ΔS=72.3 J·mol^{-1}·K^{-1}
c,γ/c,α 306.6 K, ΔH=18700 J·mol^{-1}
ΔS=61.0 J·mol^{-1}·K^{-1}
c,β/liq 304.6 K, ΔH=45120 J·mol^{-1}
ΔS=148.1 J·mol^{-1}·K^{-1}
c,γ/liq 304.9 K, ΔH=41400 J·mol^{-1}
ΔS=135.8 J·mol^{-1}·K^{-1}
c,α/liq 303.5 K, ΔH=23000 J·mol^{-1}
ΔS=76.8 J·mol^{-1}·K^{-1}.
Molecular Weight 200.3636
Wiswesser Line Notation Q13
Evaluation B

$C_{13}H_{28}O$ (liq) 74MOS/MOU
1-Tridecanol; n-Tridecyl alcohol
Heat Capacity 305 K, C_p=476 J·mol^{-1}·K^{-1}
Temperature range 305 to 346 K.
Molecular Weight 200.3636
Wiswesser Line Notation Q13
Evaluation B

$C_{13}H_{28}O$ (liq) 89KHA/ZYK
1-Tridecanol; n-Tridecyl alcohol
Heat Capacity 313.15 K, C_p=487.5 J·mol^{-1}·K^{-1}
Temperature range 313 to 553 K.
Molecular Weight 200.3636
Wiswesser Line Notation Q13
Evaluation B

$C_{13}H_{28}O$ (liq) 88CAC/CO
5-Butyl-5-nonanol
Heat Capacity 298.15 K, C_p=548.63 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 200.3636
Wiswesser Line Notation QX4&4&4
Evaluation B

$C_{13}H_{28}O$ (c) 83MAS/ST
Tri-tert-butylmethanol
Heat Capacity 298.15 K, C_p=350.6 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.75 J·g^{-1}·K^{-1}.
Phase Changes
c,II/c,I 302.17 K, ΔH=7200 J·mol^{-1}
ΔS=24 J·mol^{-1}·K^{-1}
Solid-plastic.
c/liq 390.15 K, ΔH=3430 J·mol^{-1}
ΔS=8.8 J·mol^{-1}·K^{-1}
Molecular Weight 200.3636
Wiswesser Line Notation QXX1&1&1&X1&1&1&X1&1&1
Evaluation B

$C_{13.5}H_{15}O_{19.5}Mn\cdot 0.19H_2O$ (c) 90MIY/MA
Manganese squarate clathrate
Heat Capacity 299.91 K, C_p=703.2 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. C_p value is unsmoothed experimental datum.
Molecular Weight 492.6782
Wiswesser Line Notation L4VVJ CO CO -MN- &QH 2 3 &QV1 0.75 &QH 0.19
Evaluation A

$C_{14}F_{30}$ (c) 93LEB/BY
n-Perfluorotetradecane
Heat Capacity 298.15 K, C_p=691.16 J·mol^{-1}·K^{-1}
Temperature range 0 to 320 K.
Entropy 298.15 K, S=881.8 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 170.4 K ΔH=2000 J·mol^{-1}
ΔS=11.95 J·mol^{-1}·K^{-1}
c,II/c,I 178.6 K ΔH=3010 J·mol^{-1}
ΔS=17.27 J·mol^{-1}·K^{-1}
Molecular Weight 569.9520
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFXFF-XFFXFFXFFXFFXFFXFFF
Evaluation A

$C_{14}H_7ClO_2$ (c) 92SAP/ELW
2-Chloroanthraquinone
Phase Changes
c/liq 483.02 K, ΔH=38960 J·mol^{-1}
Molecular Weight 242.6611
Wiswesser Line Notation L C666 BV IVJ DG
Evaluation A

$C_{14}H_8Cl_2O_3$ (c) 73SAP/MO
Oxy-p,p'-dibenzoyl chloride
Heat Capacity 300 K, C_p=308.1 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=312.3 J·mol^{-1}·K^{-1}
Molecular Weight 295.1208
Wiswesser Line Notation GVR DOR DVG
Evaluation C
Author's do not specify isomer, assumed to be -p,p' substitution.

$C_{14}H_8O_2$ (c) 17HIL/DUS
Anthraquinone
Heat Capacity 298.15 K, C_p=240.2 J·mol^{-1}·K^{-1}
Temperature range 293 to 593 K. From heat content data.
Phase Changes
c/liq 555 K, ΔH=32570 J·mol^{-1}
ΔS=58.7 J·mol^{-1}·K^{-1}
Molecular Weight 208.2160
Wiswesser Line Notation L C666 BV IVJ
Evaluation C

$C_{14}H_9NO_2$ (c) 77KAR/BAZ
N-Phenylphthalimide
Heat Capacity 300 K, C_p=245.9 J·mol^{-1}·K^{-1}
Temperature range 60 to 400 K.
Entropy 300 K, S=273.0 J·mol^{-1}·K^{-1}
Molecular Weight 223.2306
Wiswesser Line Notation T56 BVNVJ CR
Evaluation B

$C_{14}H_{10}$ (c) 31HUF/PAR
Phenanthrene
Heat Capacity 297.5 K, C_p=233.5 J·mol^{-1}·K^{-1}
Temperature range 93 to 304 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=211.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 65.19 J·mol^{-1}·K^{-1}.
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation B(C_p),C(S)

$C_{14}H_{10}$ (c) 41SCH
Phenanthrene
Heat Capacity 298.1 K, C_p=226.4 J·mol^{-1}·K^{-1}
Temperature range 20 to 200 °C, equations only, in t °C. C_p(c)=0.2440+0.002604t−0.000011t^2 cal·g^{-1}·C^{-1} (20 to 98 °C); C_p(liq)=0.3328+0.0006760t cal·g^{-1}·C^{-1} (98 to 200 °C).
Phase Changes
c/liq 371.7 K, ΔH=17138 J·mol^{-1}
ΔS=46.1 J·mol^{-1}·K^{-1}
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation C

$C_{14}H_{10}$ (c) 44EIB
Phenanthrene
Heat Capacity 298.1 K, C_p=207.1 J·mol^{-1}·K^{-1}
Temperature range 20 to 200 °C, equations only, in t °C. C_p(c)=0.2003+0.00306t cal·g^{-1}·C^{-1} (20 to 98 °C); C_p(liq)=0.292 +0.000923t cal·g^{-1}·C^{-1} (98 to 200 °C).
Phase Changes
c/liq 371.4 K, ΔH=17150 J·mol^{-1}
ΔS=46.2 J·mol^{-1}·K^{-1}
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation C

$C_{14}H_{10}$ (c) 50UEB/ORT
Phenanthrene
Heat Capacity 298.15 K, C_p=134.7 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Phase Changes
c,II/c,I 342 K, ΔH=2600 J·mol^{-1}
ΔS=7.6 J·mol^{-1}·K^{-1}
c,I/liq 373 K, ΔH=18620 J·mol^{-1}
ΔS=49.9 J·mol^{-1}·K^{-1}
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation C

$C_{14}H_{10}$ (c) 64RAS/BAS
Phenanthrene
Heat Capacity 343 K, C_p=267.4 J·mol^{-1}·K^{-1}
Temperature range 343, 404 K.
Phase Changes
c/liq 373.2 K, ΔH=18000 J·mol^{-1}
ΔS=48.2 J·mol^{-1}·K^{-1}
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation B

$C_{14}H_{10}$ (c) 77FIN/MES
Phenanthrene
Heat Capacity 298.15 K, C_p=220.62 J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, S=215.06 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II ~270 K
Second-order glass-type transition.
c,II/c,I 347.5 K, ΔH=218 J·mol^{-1}
ΔS=0.63 J·mol^{-1}·K^{-1}
Lambda transition.
c,I/liq 372.38 K, ΔH=16462.8 J·mol^{-1}
ΔS=44.21 J·mol^{-1}·K^{-1}
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation A

$C_{14}H_{10}$ (c) 87RAI/SIN
Phenanthrene
Phase Changes
c/liq (373) K, ΔH=18627 J·mol^{-1}
ΔS=49.9 J·mol^{-1}·K^{-1}
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation B

$C_{14}H_{10}$ (c) 88PET/TSY
Phenanthrene
Phase Changes
c,II/c,I 332.2 K, ΔH=1000 J·mol^{-1}
ΔS=3.0 J·mol^{-1}·K^{-1}
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation A

$C_{14}H_{10}$ (c) 88TOR/BAR
Phenanthrene
Phase Changes
liq/g 350 K, $\Delta H = 87240\ J \cdot mol^{-1}$
$\Delta S = 249.3\ J \cdot mol^{-1} \cdot K^{-1}$
c/g 298.15 K, $\Delta H = 90900\ J \cdot mol^{-1}$
$\Delta S = 304.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation A

$C_{14}H_{10}$ (c) 90STE/CHI
Phenanthrene
Heat Capacity 298.15 K, $C_p = 220.3\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation B

$C_{14}H_{10}$ (c) 92SAB/ELW3
Phenanthrene
Phase Changes
c/liq 373.81 K, $\Delta H = 15720\ J \cdot mol^{-1}$
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation A

$C_{14}H_{10}$ (c) 17HIL/DUS
Anthracene
Heat Capacity 298.15 K, $C_p = 221.8\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 593 K. From heat content data.
Phase Changes
c/liq 489.7 K, $\Delta H = 28870\ J \cdot mol^{-1}$
$\Delta S = 59.0\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 178.2330
Wiswesser Line Notation L C666J
Evaluation C

$C_{14}H_{10}$ (c) 31HUF/PAR
Anthracene
Heat Capacity 297.2 K, $C_p = 207.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 94 to 297 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, $S = 207.5\ J \cdot mol^{-1} \cdot K^{-1}$
Extrapolation below 90 K, $14.98\ cal \cdot mol^{-1} \cdot K^{-1}$.
Molecular Weight 178.2330
Wiswesser Line Notation L C666J
Evaluation B(C_p),C(S)

$C_{14}H_{10}$ (c) 50UEB/ORT
Anthracene
Heat Capacity 298.15 K, $C_p = 217.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 368 K. Equation only.
Phase Changes
c/liq 490 K, $\Delta H = 28830\ J \cdot mol^{-1}$
$\Delta S = 58.0\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 178.2330
Wiswesser Line Notation L C666J
Evaluation C

$C_{14}H_{10}$ (c) 68GOU/GI
Anthracene
Heat Capacity 298.15 K, $C_p = 210.50\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 520 K. Only 6 points given; summary articl
Entropy 298.15 K, $S = 207.15\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 178.2330
Wiswesser Line Notation L C666J
Evaluation A

$C_{14}H_{10}$ (c) 70GOU/GI
Anthracene
Heat Capacity 298.15 K, $C_p = 210.50\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 500 K.
Entropy 298.15 K, $S = 207.15\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 488.93 K, $\Delta H = 29372\ J \cdot mol^{-1}$
$\Delta S = 60.07\ J \cdot mol^{-1} \cdot K^{-1}$
Note that table of smoothed values indicates $\Delta H_m = 6485\ J\ mol^{-1}$ a
$\Delta S_m = 251\ J \cdot mol^{-1} \cdot K^{-1}$.
Molecular Weight 178.2330
Wiswesser Line Notation L C666J
Evaluation A

$C_{14}H_{10}$ (c) 80RAD/RA
Anthracene
Heat Capacity 298.15 K, $C_p = 211.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 180 to 430 K. Data given graphically. C_p calculat
from equation.
Phase Changes
c,I/liq 490.6 K, $\Delta H = 29000\ J \cdot mol^{-1}$
$\Delta S = 59.1\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 178.2330
Wiswesser Line Notation L C666J
Evaluation B

$C_{14}H_{10}$ (c) 31SMI/AN
Diphenylacetylene; Diphenylethyne
Heat Capacity 298.5 K, $C_p = 225.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 102 to 323 K. Value is unsmoothed experimen
datum.
Molecular Weight 178.2330
Wiswesser Line Notation R1UU1R
Evaluation C

$C_{14}H_{10}$ (c) 50KU
Diphenylacetylene; Diphenylethyne
Heat Capacity 340 K, $C_p = 297.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 65 to 303 °C. Mp 61 °C.
Molecular Weight 178.2330
Wiswesser Line Notation R1UU1R
Evaluation B

$C_{14}H_{10}$ (c) 86CHI/AN
Diphenylacetylene; Diphenylethyne
Phase Changes
c/liq $\Delta H = 20502\ J \cdot mol^{-1}$
c/g $\Delta H = 90374\ J \cdot mol^{-1}$
Molecular Weight 178.2330
Wiswesser Line Notation R1UU1R
Evaluation A

$C_{14}H_{10}O$ (c) 91ELW/SAB
Anthrone
Phase Changes
c/liq 429 K, $\Delta H = 26800\ J \cdot mol^{-1}$
Molecular Weight 194.2324
Wiswesser Line Notation T C666 BV IHJ
Evaluation A

$C_{14}H_{10}O$ (c) 92SAB/ELW4
Anthrone
Phase Changes
c/liq 429 K, $\Delta H = 26800\ J \cdot mol^{-1}$
Slight decomposition at melting.
c/g 298.15 K, $\Delta H = 1037300\ J \cdot mol^{-1}$
Molecular Weight 194.2324
Wiswesser Line Notation T C666 BV IHJ
Evaluation A

$C_{14}H_{10}O_2$ (c) 72BOO/HAU
Benzil; Diphenyl diketone
Phase Changes
c/liq 368.05 K, $\Delta H = 22690\ J \cdot mol^{-1}$
$\Delta S = 61.65\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 210.2318
Wiswesser Line Notation RVVR
Evaluation C

$C_{14}H_{10}O_2$ (c) 77DWO/FUC
Benzil; Diphenyl diketone
Heat Capacity
C_p data given graphically only. Temperature range 60 to 100 K.
Phase Changes
c,II/c,I 84.07 K, $\Delta H = 44.1\ J \cdot mol^{-1}$
$\Delta S = 0.52\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 210.2318
Wiswesser Line Notation RVVR
Evaluation B

$C_{14}H_{10}O_2$ (c) 80AND/CON
Benzil; Diphenyl diketone
Phase Changes
c,I/liq 368.022 K, $\Delta H = 23556\ J \cdot mol^{-1}$
$\Delta S = 64.01\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 210.2318
Wiswesser Line Notation RVVR
Evaluation A

$C_{14}H_{10}O_2$ (c) 83DWO
Benzil; Diphenyl diketone
Heat Capacity 298.15 K, $C_p = 245.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 15 to 300 K.
Entropy 298.15 K, $S = 292.08\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 84.07 K, $\Delta H = 44.1\ J \cdot mol^{-1}$
$\Delta S = 0.52\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 210.2318
Wiswesser Line Notation RVVR
Evaluation A

$C_{14}H_{11}NO_3$ (c) 77KAR/BAZ
Phthalanilic acid
Heat Capacity 300 K, $C_p = 279.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 60 to 400 K.
Entropy 300 K, $S = 322.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 241.2458
Wiswesser Line Notation QVR BVMR
Evaluation B

$C_{14}H_{11}NO_3$ (c) 91WU/XIO
N-Salicylidene-m-aminobenzoic acid
Phase Changes
c/liq 464 K, $\Delta H = 33110\ J \cdot mol^{-1}$
$\Delta S = 71.36\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 241.2458
Wiswesser Line Notation QVR DNU1R DQ
Evaluation A

$C_{14}H_{12}$ (liq) 31SMI/AND
1,1-Diphenylethylene
Heat Capacity 298.5 K, $C_p = 299.2\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 102 to 299 K. Value is unsmoothed experimental datum.
Molecular Weight 180.2488
Wiswesser Line Notation 1UYR&R
Evaluation C

$C_{14}H_{12}$ (c) 79LEE/HOS
9,10-Dihydrophenanthrene
Heat Capacity 298.15 K, $C_p = 243.8\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 350 K.
Entropy 298.15 K, $S = 229.4\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 306.52 K, $\Delta H = 12790\ J \cdot mol^{-1}$
$\Delta S = 41.73\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 180.2488
Wiswesser Line Notation L B666&T&J
Evaluation A

$C_{14}H_{12}$ (c) 87CHI/HOS
9,10-Dihydrophenanthrene
Heat Capacity 298.15 K, $C_p = 243.08\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 350 K.
Entropy 298.15 K, $S = 229.29\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 180.2488
Wiswesser Line Notation L B666&T&J
Evaluation A
Heat capacity and entropy data given for liquid state at 298.15 K: $C_p = 278.04$, $S° = 270.14\ J \cdot mol^{-1} \cdot K^{-1}$.

$C_{14}H_{12}$ (c) 87CHI/HOS2
9,10-Dihydroanthracene
Heat Capacity 298.15 K, $C_p = 219.06\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 500 K.
Entropy 298.15 K, $S = 218.97\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 382.18 K, $\Delta H = 23840\ J \cdot mol^{-1}$
$\Delta S = 62.38\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 180.2488
Wiswesser Line Notation L C666&T&J
Evaluation A

$C_{14}H_{12}$ (c) 30PAR/HUF2
Stilbene
Heat Capacity 292.8 K, C_p=227.2 J·mol^{-1}·K^{-1}
Temperature range 92 to 293 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=251.0 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 82.89 J·mol^{-1}·K^{-1}.
Molecular Weight 180.2488
Wiswesser Line Notation R1U1R
Evaluation B(C_p),C(S)

$C_{14}H_{12}$ (c) 31SMI/AND
Stilbene
Heat Capacity 298.5 K, C_p=232.6 J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 180.2488
Wiswesser Line Notation R1U1R
Evaluation C

$C_{14}H_{12}$ (c) 33FER/THO
Stilbene
Heat Capacity 313 K, C_p=239.1 J·mol^{-1}·K^{-1}
Temperature range 303 to 403 K.
Phase Changes
c/liq 397.55 K, ΔH=27829 J·mol^{-1}
Molecular Weight 180.2488
Wiswesser Line Notation R1U1R
Evaluation C

$C_{14}H_{12}$ (c) 50KUR
Stilbene
Heat Capacity 410 K, C_p=343.1 J·mol^{-1}·K^{-1}
Temperature range 135 to 305 °C. Mp 124.2 °C.
Molecular Weight 180.2488
Wiswesser Line Notation R1U1R
Evaluation B

$C_{14}H_{12}$ (c) 84VAN/BOU
trans-Stilbene
Heat Capacity 298.15 K, C_p=235.0 J·mol^{-1}·K^{-1}
Temperature range 8 to 350 K.
Entropy 298.15 K, S=247.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 398 K, ΔH=27370 J·mol^{-1}
ΔS=68.8 J·mol^{-1}·K^{-1}
Molecular Weight 180.2488
Wiswesser Line Notation R1U1R -T
Evaluation B

$C_{14}H_{12}$ (c) 85BOU/DEL
trans-Stilbene
Heat Capacity 320 K, C_p=251.08 J·mol^{-1}·K^{-1}
Temperature range 320 to 410 K.
Phase Changes
c,I/liq 397.40 K, ΔH=27690 J·mol^{-1}
ΔS=69.6 J·mol^{-1}·K^{-1}
Molecular Weight 180.2488
Wiswesser Line Notation R1U1R -T
Evaluation A

$(C_{14}H_{12}Ge)_n$ (liq) 75LEB/MIL
Polyvinylenediphenylgermane
Heat Capacity 298.15 K, C_p=334.7 J·mol^{-1}·K^{-1}
Temperature range 8 to 324 K.
Entropy 298.15 K, S=323.2 J·mol^{-1}·K^{-1}
Molecular Weight 252.8388
Wiswesser Line Notation /*-GE-R&R&1U1*/
Evaluation A
T(glass)=237 K.

$(C_{14}H_{12}Ge)_n$ (gls) 78LEB/RAB
Polyvinylenediphenylgermyl-α,ω-dihydride
Heat Capacity 298.15 K, C_p=334.7 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S=323.2 J·mol^{-1}·K^{-1}
Highly elastic state.
Molecular Weight 252.8388
Wiswesser Line Notation /*-GE-R&R&1U1*/
Evaluation A
T(glass)=237 K.

$C_{14}H_{12}O_2$ (c) 80AND/CO
Diphenylacetic acid
Phase Changes
c,I/liq 420.441 K, ΔH=31271 J·mol^{-1}
ΔS=74.38 J·mol^{-1}·K^{-1}
Molecular Weight 212.2476
Wiswesser Line Notation QVYR&R
Evaluation A

$C_{14}H_{12}O_4$ (c) 92STE/CH
Naphthalene-2,6-dicarboxylic acid dimethyl ester
Heat Capacity 298.15 K, C_p=283.8 J·mol^{-1}·K^{-1}
Temperature range 310 to 670 K. C/R(c)=0.0960T+5.51 (310 to 464. K); C/R(liq)=0.0635T+26.29 (464.5 to 670 K), R=8.31451 J/l ·mol.
Phase Changes
c/liq 464.5 K, ΔH=53300 J·mol^{-1}
Molecular Weight 244.2464
Wiswesser Line Notation L66J CVO1 HVO1
Evaluation B
Authors give C_p/R=23.1 at 298.15 K which is inconsistent wit equation.

$(C_{14}H_{12}Si)_n$(amorph) 77LEB/EVS
Polyvinylenediphenylsilane
Heat Capacity 298 K, C_p=331.2 J·mol^{-1}·K^{-1}
Temperature range 13 to 334 K. Values per repeating unit. Da deposited VINITI, No. 2360-76, 24 June 1976.
Entropy 298 K, S=298.0 J·mol^{-1}·K^{-1}
Molecular Weight 208.3343
Wiswesser Line Notation /*1U1-SI-*R&R/
Evaluation B

$(C_{14}H_{12}Si)_n$ (gls) 78LEB/RAE
Polyvinylenediphenylsilyl-α,ω-dihydride
Heat Capacity 298.15 K, C_p=331.2 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S=298.0 J·mol^{-1}·K^{-1}
Highly elastic state.
Molecular Weight 208.3343
Wiswesser Line Notation /*1U1-SI-*R&R/
Evaluation A
T(glass)=264 K.

$C_{14}H_{13}N$ (c) 90JIM/ROU
N-Ethylcarbazole
Heat Capacity 298.15 K, C_p=238.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 195.2634
Wiswesser Line Notation T B656 HNJ H2
Evaluation A

$C_{14}H_{14}$ (liq) 87CHI/HOS2
Phenyl-o-tolylmethane
Heat Capacity 298.15 K, C_p=296.58 J·mol^{-1}·K^{-1}
Temperature range 10 to 500 K.
Entropy 298.15 K, S=335.50 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 279.76 K, ΔH=19241 J·mol^{-1}
ΔS=68.78 J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation 1R B1R
Evaluation A

$C_{14}H_{14}$ (liq) 87CHI/HOS
2,2′-Dimethylbiphenyl
Heat Capacity 298.15 K, C_p=298.06 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=332.60 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 293.091 K, ΔH=2279.9 J·mol^{-1}
ΔS=7.78 J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation 1R BR B1
Evaluation A

$C_{14}H_{14}$ (liq) 31SMI/AND
1,1-Diphenylethane
Heat Capacity 298.5 K, C_p=295.0 J·mol^{-1}·K^{-1}
Temperature range 102 to 299 K. Value is unsmoothed experimental datum.
Molecular Weight 182.2646
Wiswesser Line Notation 1YR&R
Evaluation C

$C_{14}H_{14}$ (c) 33FER/THO
1,2-Diphenylethane; Dibenzyl
Heat Capacity 303 K, C_p=257.0 J·mol^{-1}·K^{-1}
Temperature range 303 to 343 K.
Phase Changes
c/liq 324.3 K, ΔH=22573 J·mol^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation R2R
Evaluation C

$C_{14}H_{14}$ (liq) 87CHI/HOS
2-Ethylbiphenyl
Heat Capacity 298.15 K, C_p=302.73 J·mol^{-1}·K^{-1}
Temperature range 5 to 440 K.
Entropy 298.15 K, S=332.69 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 267.076 K, ΔH=2068.0 J·mol^{-1}
ΔS=7.74 J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation 2R BR
Evaluation A

$C_{14}H_{14}$ (liq) 87CHI/HOS
1,2,3,4-Tetrahydrophenanthrene
Heat Capacity 298.15 K, C_p=278.26 J·mol^{-1}·K^{-1}
Temperature range 5 to 430 K.
Entropy 298.15 K, S=286.60 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 282.5 K, ΔH=213 J·mol^{-1}
ΔS=0.75 J·mol^{-1}·K^{-1}
c,II/c,I 298.0 K, ΔH=1344.2 J·mol^{-1}
ΔS=4.44 J·mol^{-1}·K^{-1}
c,I/liq 302.560 K
Molecular Weight 182.2646
Wiswesser Line Notation L B666T&&J
Evaluation A

$C_{14}H_{14}$ (c,II) 87CHI/HOS2
1,2,3,4-Tetrahydroanthracene
Heat Capacity 298.15 K, C_p=247.02 J·mol^{-1}·K^{-1}
Temperature range 10 to 500 K.
Entropy 298.15 K, S=227.12 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 388.0 K, ΔH=2921 J·mol^{-1}
ΔS=7.53 J·mol^{-1}·K^{-1}
c,I/liq 373.245 K, ΔH=19157 J·mol^{-1}
ΔS=51.33 J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation L C666T&&J
Evaluation A

$C_{14}H_{14}$ (c) 30HUF/PAR
1,2-Diphenylethane; Dibenzyl
Heat Capacity 293.6 K, C_p=251.0 J·mol^{-1}·K^{-1}
Temperature range 93 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=270.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 90.37 J·mol^{-1}·K^{-1}.
Molecular Weight 182.2646
Wiswesser Line Notation R2R
Evaluation B(C_p),C(S)

$C_{14}H_{14}$ (c) 31SMI/AND
1,2-Diphenylethane; Dibenzyl
Heat Capacity 298.5 K, C_p=253.6 J·mol^{-1}·K^{-1}
Temperature range 102 to 299 K. Value is unsmoothed experimental datum.
Molecular Weight 182.2646
Wiswesser Line Notation R2R
Evaluation C

$C_{14}H_{14}$ (c) 41SCH
1,2-Diphenylethane; Dibenzyl
Heat Capacity 298.1 K, C_p=251.9 J·mol^{-1}·K^{-1}
Temperature range 20 to 200 °C, equations only in t °C. C_p(c)=0.2867+0.001743t cal·g^{-1}·C^{-1} (20 to 51 °C); C_p(liq)=0.3865+0.0005986t cal·g^{-1}·C^{-1} (51 to −200 °C).
Phase Changes
c/liq 324.4 K, ΔH=23010 J·mol^{-1}
ΔS=70.9 J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation R2R
Evaluation C

$C_{14}H_{14}$ (c) 50KUR
1,2-Diphenylethane; Dibenzyl
Heat Capacity 330 K, C_p=320.1 J·mol^{-1}·K^{-1}
Temperature 54 to 254 °C. M_p=52.8 °C.
Molecular Weight 182.2646
Wiswesser Line Notation R2R
Evaluation B

$C_{14}H_{14}$ (c,I) 88MES/FIN
1,2-Diphenylethane; Dibenzyl
Heat Capacity 298.15 K, C_p=253.764 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=267.391 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 273.150 K, ΔH=2247.55 J·mol^{-1}
ΔS=8.23 J·mol^{-1}·K^{-1}
c,I/liq 324.348 K, ΔH=22730.52 J·mol^{-1}
ΔS=70.08 J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation R2R
Evaluation A

$C_{14}H_{14}FeO_2$ (c) 81TOM/CUR
1,1′-Diacetylferrocene
Heat Capacity 298 K, C_p=289.1 J·mol^{-1}·K^{-1}
Temperature range 293 to 393 K. Equation given.
Phase Changes
c/liq 403.7 K
Molecular Weight 270.1104
Wiswesser Line Notation L5ϕJ AV1 ϕ-FE- -ϕL5ϕJ AV1
Evaluation B

$C_{14}H_{14}Hg$ (c) 31SMI/AND2
Di(p-tolyl)mercury; Mercury di(p-tolyl)
Heat Capacity 298.5 K, C_p=262.3 J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 382.8546
Wiswesser Line Notation 1R D- 2 .HG
Evaluation B

$C_{14}H_{14}N_2O_3$ (liq) 38KRE
p-Azoxyanisole; 4,4′-Dimethoxyazoxybenzene
Heat Capacity 400 K, C_p=569 J·mol^{-1}·K^{-1}
Value a few degrees below anisotropic-isotropic liquid-liquid transition at 409 K.
Molecular Weight 258.2762
Wiswesser Line Notation 1OR DNUNO&R DO1
Evaluation C

$C_{14}H_{14}N_2O_3$ (c) 67BAR/POR
p-Azoxyanisole; 4,4′-Dimethoxyazoxybenzene
Heat Capacity 368 K, C_p=380.3 J·mol^{-1}·K^{-1}
Temperature range 368 to 423 K.
Phase Changes
c,I/liq 390.8 K, ΔH=30367 J·mol^{-1}
ΔS=77.7 J·mol^{-1}·K^{-1}
Solid-nematic transition.
liq/liq 407.1 K, ΔH=736 J·mol^{-1}
ΔS=1.8 J·mol^{-1}·K^{-1}
Nematic liquid-isotropic liquid transition.
Molecular Weight 258.2762
Wiswesser Line Notation 1OR DNUNO&R DO1
Evaluation B

$C_{14}H_{14}N_2O_3$ (c) 82J/
p-Azoxyanisole; 4,4′-Dimethoxyazoxybenzene
Phase Changes
c,III/c,I 250.7 K, ΔH=104.6 J·mol^{-1}
ΔS=0.42 J·mol^{-1}·K^{-1}
c,II/c,I 335.6 K
c,II/liq 377.5 K, ΔH=23891 J·mol^{-1}
ΔS=63.30 J·mol^{-1}·K^{-1}
Crystal II-nematic.
c,I/liq 388.0 K, ΔH=30430 J·mol^{-1}
ΔS=78.41 J·mol^{-1}·K^{-1}
Crystal I-nematic.
liq/liq 406.9 K, ΔH=757 J·mol^{-1}
ΔS=1.84 J·mol^{-1}·K^{-1}
Nematic-isotropic.
Molecular Weight 258.2762
Wiswesser Line Notation 1OR DNUNO&R DO1
Evaluation A

$C_{14}H_{14}N_2O_3$ (c) 90KUZ/V/
p-Azoxyanisole; 4,4′-Dimethoxyazoxybenzene
Phase Changes
c/liq 377.2 K, ΔH=20630 J·mol^{-1}
Crystal to nematic liquid.
liq/liq 411.6 K, ΔH=1334 J·mol^{-1}
Nematic to isotropic liquid.
Molecular Weight 258.2762
Wiswesser Line Notation 1OR DNUNO&R DO1
Evaluation A

$C_{14}H_{14}N_2O_3$ (c) 93ACR/TU
p-Azoxyanisole; 4,4′-Dimethoxyazoxybenzene
Phase Changes
c/liq 391.7 K, ΔH=29300 J·mol^{-1}
c/nematic.
liq/liq 410.7 K, ΔH=1000 J·mol^{-1}
Nematic/liq.
Molecular Weight 258.2762
Wiswesser Line Notation 1OR DNUNO&R DO1
Evaluation A

$(C_{14}H_{15}N_2NaO_3)_n$ (c) 91R(
Poly-L-sodium glutamate· tyrosine copolymer
Heat Capacity 300 K, C_p=353.2 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 314.2727
Wiswesser Line Notation /*VY1R DQ &MVY2VO &-NA- &M*/ -I
Evaluation B

$(C_{14}H_{15}N_2NaO_3)_n$ (c) 93ROL/WU
Poly-L-sodium glutamate· tyrosine copolymer
Heat Capacity 300 K, C_p=353.2 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 314.2727
Wiswesser Line Notation /*VY1R DQ &MVY2VO &-NA- &M*/ -I
Evaluation B

$C_{14}H_{16}FeN_6S_4Se_2$ (c) 92KUL/T
Bis-(2,2′-bi-2-thiazoline)diisoselenocyanato iron(II)
Heat Capacity
Temperature range 115 to 300 K. Data given graphically only.
Phase Changes
c,II/c,I 223 K, ΔH=9100 J·mol^{-1}
ΔS=41.5 J·mol^{-1}·K^{-1}
Molecular Weight 610.3276
Wiswesser Line Notation T5NU CSTJ B- BT5NU CSTJ &-F NC-SE-2
Evaluation B

$C_{14}H_{16}FeN_6S_6$ (c) 92KUL/IYE
Bis-(2,2′-bi-2-thiazoline)diisothiocyanato iron(II)
Heat Capacity
Temperature range 115 to 300 K. Data given graphically only.
Phase Changes
c,II/c,I 183.0 K, ΔH=9540 J·mol^{-1}
ΔS=54.4 J·mol^{-1}·K^{-1}
Molecular Weight 516.5276
Wiswesser Line Notation T5NU CSTJ B- BT5NU CSTJ &-FE- NCS2
Evaluation B

$C_{14}H_{17}NO_2$ (c) 89ZHA/HUA
4-Methyl-7-diethylaminocoumarin
Phase Changes
c/liq 343.8 K, ΔH=17884 J·mol^{-1}
ΔS=46.26 J·mol^{-1}·K^{-1}
Molecular Weight 231.2938
Wiswesser Line Notation T66 BOVJ E1 IN2&2
Evaluation B

$C_{14}H_{18}$ (c) 71BOY/SAN
1,2,3,4,5,6,7,8-Octahydroanthracene
Heat Capacity 327 K, C_p=327.6 J·mol^{-1}·K^{-1}
Temperature range 327 to 390 K. Four temperatures.
Phase Changes
c/liq 346 K, ΔH=17910 J·mol^{-1}
ΔS=51.8 J·mol^{-1}·K^{-1}
Molecular Weight 186.2962
Wiswesser Line Notation L 666 T&TJ
Evaluation C

$C_{14}H_{18}$ (c) 88PET/TSY
1,2,3,4,5,6,7,8-Octahydroanthracene
Phase Changes
c,II/c,I 331.6 K, ΔH=2400 J·mol^{-1}
ΔS=7.2 J·mol^{-1}·K^{-1}
Molecular Weight 186.2962
Wiswesser Line Notation L 666 T&TJ
Evaluation A

$C_{14}H_{16}CrI$ (c) 72NIK/SAF
Bis(toluene)chromium iodide
Heat Capacity 298.15 K, C_p=333.5 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S=328.2 J·mol^{-1}·K^{-1}
Molecular Weight 363.1809
Wiswesser Line Notation L6ϕJ A1 ϕ-CR- ϕL6ϕJ A1 &I
Evaluation B

$C_{14}H_{16}N_2O_2$ (liq) 86ACH/HAS
1,3-Bis-(1-isocyanato-1-methylethyl)benzene
Heat Capacity 333 K, C_p=464 J·mol^{-1}·K^{-1}
Temperature range 333, 433 K. C_p=1.9 J·g^{-1}·C^{-1}.
Molecular Weight 244.2926
Wiswesser Line Notation OCNX2&1&R CXNCO&2&1
Evaluation C
99% purity.

$C_{14}H_{16}N_2O_2$ (c) 86ACH/HAS
1,4-Bis-(1-isocyanato-1-methylethyl)benzene
Heat Capacity 333 K, C_p=415 J·mol^{-1}·K^{-1}
Temperature range 333, 433 K. C_p=1.7 J·g^{-1}·C^{-1}.
Molecular Weight 244.2926
Wiswesser Line Notation OCNX2&1&R DXNCO&2&1
Evaluation C
99% purity.

$C_{14}H_{18}$ (c) 82GAM/CAL
1,2,3,4,5,6,7,8-Octahydroanthracene
Heat Capacity 298.15 K, C_p=277.96 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=248.92 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 331.348 K, ΔH=2514.3 J·mol^{-1}
ΔS=7.59 J·mol^{-1}·K^{-1}
c,I/liq 345.390 K, ΔH=18341.6 J·mol^{-1}
ΔS=53.10 J·mol^{-1}·K^{-1}
Molecular Weight 186.2962
Wiswesser Line Notation L 666 T&TJ
Evaluation A

$C_{14}H_{20}$ (c,III) 78SPI/AND
Diamantane;
Pentacyclo[7.3.1.1^{4,12}.0^{2,7}.0^{6,11}] tetradecane
Heat Capacity 295.56 K, C_p=220.2 J·mol^{-1}·K^{-1}
Temperature range 295 to 540 K. Value is unsmoothed experimental datum.
Phase Changes
c,III/c,II 407.22 K, ΔH=4445 J·mol^{-1}
ΔS=10.92 J·mol^{-1}·K^{-1}
c,II/c,I 440.43 K, ΔH=8960 J·mol^{-1}
ΔS=20.34 J·mol^{-1}·K^{-1}
c,I/liq 517.92 K, ΔH=8646 J·mol^{-1}
ΔS=16.69 J·mol^{-1}·K^{-1}
Molecular Weight 188.3120
Wiswesser Line Notation L666 C6 E6 B C- D G 4ACEF MTJ
Evaluation A

$C_{14}H_{20}$ (c,III) 78WES/MCK
Diamantane;
Pentacyclo[7.3.1.1^{4,12}.0^{2,7}.0^{6,11}] tetradecane
Heat Capacity 298.15 K, C_p=223.22 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K. Data between 350 and 540 K taken from other work.
Entropy 298.15 K, S=200.16 J·mol^{-1}·K^{-1}
Phase Changes
Second order transition between 26 and 36 K, with ΔH=8.4 J mol^{-1}, ΔS=0.33 J·mol^{-1}·K^{-1}.
Molecular Weight 188.3120
Wiswesser Line Notation L666 C6 E6 B C- D G 4ACEF MTJ
Evaluation A

$C_{14}H_{22}$ (liq) 48TSC
n-Octylbenzene
Heat Capacity 295 K, C_p=291 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 234.2 K, ΔH=29957 J·mol^{-1}
Molecular Weight 190.3278
Wiswesser Line Notation 8R
Evaluation C

$C_{14}H_{24}$ (liq) 63GUD/CAM
Perhydrophenanthrene
Heat Capacity 313 K, C_p=330.1 J·mol^{-1}·K^{-1}
Temperature range 313 to 583 K.
Molecular Weight 192.3436
Wiswesser Line Notation L B666TJ
Evaluation C

$C_{14}H_{24}$ (c) 82NUZ
Perhydrophenanthrene
Heat Capacity 298 K, C_p=289.5 J·mol^{-1}·K^{-1}
Temperature range 193 to 403 K.
Phase Changes
c/liq 313 K, ΔH=11155 J·mol^{-1}
ΔS=35.64 J·mol^{-1}·K^{-1}
Molecular Weight 192.3436
Wiswesser Line Notation L B666TJ
Evaluation B
(cat) cis/anti/trans isomer

$C_{14}H_{24}$ (c) 82NUZ
Perhydrophenanthrene
Heat Capacity 298 K, C_p=345.6 J·mol^{-1}·K^{-1}
Temperature range 193 to 403 K.
Phase Changes
c/liq 273 K, ΔH=10481 J·mol^{-1}
ΔS=38.39 J·mol^{-1}·K^{-1}
Molecular Weight 192.3436
Wiswesser Line Notation L B666TJ
Evaluation B
(cst) cis/syn/trans isomer

$C_{14}H_{24}$ (c) 82NUZ
Perhydrophenanthrene
Heat Capacity 298 K, C_p=281.2 J·mol^{-1}·K^{-1}
Temperature range 193 to 403 K.
Phase Changes
c/liq 283 K, ΔH=11832 J·mol^{-1}
ΔS=41.81 J·mol^{-1}·K^{-1}
Molecular Weight 192.3436
Wiswesser Line Notation L B666TJ
Evaluation B
(tat) trans/anti/trans isomer

$C_{14}H_{24}BrN$ (c) 89VAN/WHI
8-Phenyloctylammonium bromide
Phase Changes
c,III/c,II 356 K, ΔH=690 J·mol^{-1}
ΔS=0.23 J·mol^{-1}·K^{-1}
c,II/c,I 379 K, ΔH=12100 J·mol^{-1}
ΔS=3.83 J·mol^{-1}·K^{-1}
Molecular Weight 286.2543
Wiswesser Line Notation Z8R &EH
Evaluation A

$C_{14}H_{24}ClN$ (c) 89VAN/WHI
8 Phenyloctylammonium chloride
Phase Changes
c,III/c,II 332 K, ΔH=7020 J·mol^{-1}
ΔS=2.54 J·mol^{-1}·K^{-1}
c,II/c,I 347 K, ΔH=2850 J·mol^{-1}
ΔS=0.99 J·mol^{-1}·K^{-1}
Molecular Weight 241.8033
Wiswesser Line Notation Z8R &GH
Evaluation A

$C_{14}H_{24}N_2O_3$ (c) 89VAN/WHI
8-Phenyloctylammonium nitrate
Phase Changes
c,II/c,I 334 K, ΔH=23000 J·mol^{-1}
ΔS=8.29 J·mol^{-1}·K^{-1}
Molecular Weight 268.3552
Wiswesser Line Notation Z8R &WNQ
Evaluation A

$C_{14}H_{26}$ (liq) 63GUD/CAI
α-Isobutyldecalin
Heat Capacity 313 K, C_p=358.6 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 194.3594
Wiswesser Line Notation L66TJ B2Y1&1
Evaluation C

$C_{14}H_{26}$ (liq) 62GOL/BI
α-n-Butyldecalin
Heat Capacity 311 K, C_p=356.9 J·mol^{-1}·K^{-1}
Temperature range 100, 200, 300 °F.
Molecular Weight 194.3594
Wiswesser Line Notation L66TJ B4
Evaluation C

$C_{14}H_{26}$ (liq) 63GUD/CA
α-n-Butyldecalin
Heat Capacity 313 K, C_p=361.9 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 194.3594
Wiswesser Line Notation L66TJ B4
Evaluation C

$C_{14}H_{26}$ (liq) 62GOL/BI
α-sec-Butyldecalin
Heat Capacity 311 K, C_p=350.6 J·mol^{-1}·K^{-1}
Temperature range 100, 200, 300 °F.
Molecular Weight 194.3594
Wiswesser Line Notation L66TJ BY2&1
Evaluation C

$C_{14}H_{26}$ (liq) 63GUD/CA
α-sec-Butyldecalin
Heat Capacity 313 K, C_p=352.3 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 194.3594
Wiswesser Line Notation L66TJ BY2&1
Evaluation C

$C_{14}H_{26}$ (liq) 63GUD/CA
tert-Butyldecalin
Heat Capacity 313 K, C_p=352.3 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 194.3594
Wiswesser Line Notation L66TJ XX1&1&1
Evaluation C

$C_{14}H_{26}$ (liq) 63GUD/CA
2-Methylbicyclohexylmethane
Heat Capacity 313 K, C_p=361.1 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 194.3594
Wiswesser Line Notation L6TJ A1- BL6TJ A1
Evaluation C

$C_{14}H_{26}$ (liq) 63GUD/CA
1,2-Dicyclohexylethane
Heat Capacity 313 K, C_p=367.8 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 194.3594
Wiswesser Line Notation L6TJ A2- AL6TJ
Evaluation C

$C_{14}H_{26}$ (liq) 63GUD/CAM
1,1-Dicyclohexylethane
Heat Capacity 313 K, C_p=348.1 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 194.3594
Wiswesser Line Notation L6TJ AY1&- AL6TJ
Evaluation C

$C_{14}H_{26}$ (liq) 63GUD/CAM
2-Ethylbicyclohexyl
Heat Capacity 313 K, C_p=369.0 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 194.3594
Wiswesser Line Notation L6TJA- BL6TJ A2
Evaluation C

$C_{14}H_{26}O$ (liq) 87MIL/FEN
2-(1,2-Dimethylpropyl)-5,6-dimethylheptenal
Heat Capacity 323.15 K, C_p=419.03 J·mol^{-1}·K^{-1}
Temperature range 323.15 to 428.15 K.
Molecular Weight 210.3588
Wiswesser Line Notation 1YYYVH&U2YY
Evaluation A

$C_{14}H_{26}O$ (liq) 87MIL/FEN
2-Pentylnonenal
Heat Capacity 323.15 K, C_p=435.35 J·mol^{-1}·K^{-1}
Temperature range 323.15 to 428.15 K.
Molecular Weight 210.3588
Wiswesser Line Notation VHY5&U7
Evaluation A

$C_{14}H_{26}O_2$ (liq) 85KAR/ABD
Decyl methacrylate
Heat Capacity 298.15 K, C_p=452.9 J·mol^{-1}·K^{-1}
Temperature range 250 to 350 K. Equation only. C_p (J·kg^{-1}·K^{-1})=1098.7+3.0251 T. C_p data calculated from equation.
Phase Changes
c/liq 250.7 K
Molecular Weight 226.3582
Wiswesser Line Notation 10OVY1&U1
Evaluation B

$C_{14}H_{26}O_2$ (liq) 85KAR/ABD2
Decyl methacrylate
Phase Changes
c/liq 250.7 K. ΔH=30548 J·mol^{-1}
ΔS=121.9 J·mol^{-1}·K^{-1}
Molecular Weight 226.3582
Wiswesser Line Notation 10OVY1&U1
Evaluation A

$C_{14}H_{26}O_2$ (liq) 85KAR/SAI
Decyl methacrylate
Heat Capacity 298.15 K. C_p=452.5 J·mol^{-1}·K^{-1}
Temperature range 90 to 350 K. C_p(c)=266.05+4.78T J/kg·K (93 to 230 K); C_p(liq)=1098.69+3.02T J/kg·K (250.7 to 350 K). C_p data calculated from equation.
Phase Changes
c/liq 250.7 K
Molecular Weight 226.3582
Wiswesser Line Notation 10OVY1&U1
Evaluation B

$C_{14}H_{26}O_4Pb$ (c,II) 78ADE/SIM
Lead(II) heptanoate; Lead(II) oenanthate
Heat Capacity 345 K, C_p=770 J·mol^{-1}·K^{-1}
Mean value, 341 to 351 K. Data only graphically for c, IV. Data also for c,I, 363 to 371 K and liquid, 413 to 453 K.
Phase Changes
c,IV/c,III 36.6 K, ΔH=17100 J·mol^{-1}
ΔS=51 J·mol^{-1}·K^{-1}
c,II, c,II, c,I are mesophases.
c,III/c,II 356.8 K, ΔH=8500 J·mol^{-1}
ΔS=24 J·mol^{-1}·K^{-1}
c,II/c,I 361.3 K, ΔH=9700 J·mol^{-1}
ΔS=27 J·mol^{-1}·K^{-1}
c,I/liq 374.7 K, ΔH=1400 J·mol^{-1}
ΔS=3.7 J·mol^{-1}·K^{-1}
Molecular Weight 465.5570
Wiswesser Line Notation OV6 2.PB
Evaluation C

$C_{14}H_{27}O_2Tl$ (c) 76MEI/SEY
Thallium tetradecanoate
Phase Changes
c,III/,cII 313 K, ΔH=11715 J·mol^{-1}
ΔS=37.2 J·mol^{-1}·K^{-1}
c,II/c,I 371 K, ΔH=3138 J·mol^{-1}
ΔS=8.37 J·mol^{-1}·K^{-1}
c,I/liq 393 K, ΔH=5439 J·mol^{-1}
ΔS=13.4 J·mol^{-1}·K^{-1}
Solid-mesophase.
liq/liq 460 K, ΔH=1632 J·mol^{-1}
ΔS=3.56 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
Molecular Weight 431.7361
Wiswesser Line Notation OV13 .TL
Evaluation B

$C_{14}H_{27}O_2Tl$ (c) 87NGE/WES
Thallium tetradecanoate
Heat Capacity 298.15 K, C_p=438.25 J·mol^{-1}·K^{-1}
Temperature range 10 to 460 K.
Entropy 298.15 K, S=473.84 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 318.2 K, ΔH=15099 J·mol^{-1}
ΔS=47.39 J·mol^{-1}·K^{-1}
c,II/c,I 378.0 K, ΔH=2877 J·mol^{-1}
ΔS=7.65 J·mol^{-1}·K^{-1}
c,I/liq 396.3 K, ΔH=6269 J·mol^{-1}
ΔS=15.80 J·mol^{-1}·K^{-1}
Solid-mesophase.
liq/liq 460.7 K, ΔH=1671 J·mol^{-1}
ΔS=3.66 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
Molecular Weight 431.7361
Wiswesser Line Notation OV13 .TL
Evaluation A

$C_{14}H_{28}O$ (c) 79SUN/SVE
2-Tetradecanone; n-Dodecyl methyl ketone
Heat Capacity 298.15 K, C_p=415.2 J·mol^{-1}·K^{-1}
Temperature range 278 to 338 K. Equations only.
Phase Changes
c/liq 306.7 K, ΔH=49120 J·mol^{-1}
ΔS=160.2 J·mol^{-1}·K^{-1}
Molecular Weight 212.3746
Wiswesser Line Notation 12V1
Evaluation B

$C_{14}H_{28}O_2$ (liq) 34KIN/GAR
Ethyl dodecanoate; Ethyl laurate
Phase Changes
c/liq 271.45 K, ΔH=9312 J·mol^{-1}
Molecular Weight 228.3740
Wiswesser Line Notation 11VO2
Evaluation B
Data on the specific heat is given at or near the phase transition.

$C_{14}H_{28}O_2$ (c) 1885STO/WIL
Tetradecanoic acid; Myristic acid
Heat Capacity 298 K, C_p=523 J·mol^{-1}·K^{-1}
Temperature range 0 to 100 °C.
Phase Changes
c/liq 317 K, ΔH=36280 J·mol^{-1}
ΔS=114 J·mol^{-1}·K^{-1}
Molecular Weight 228.3740
Wiswesser Line Notation QV13
Evaluation D

$C_{14}H_{28}O_2$ (c) 82SCH/MIL2
Tetradecanoic acid; Myristic acid
Heat Capacity 298.15 K, C_p=432.01 J·mol^{-1}·K^{-1}
Temperature range 80 to 345 K.
Phase Changes
c,I/liq 327.32 K, ΔH=45100 J mol^{-1}
ΔS=137.79 J·mol^{-1}·K^{-1}
Molecular Weight 228.3740
Wiswesser Line Notation QV13
Evaluation B

$C_{14}H_{30}$ (liq) 34PAR/LIG
n-Tetradecane
Heat Capacity 290.6 K, C_p=434.3 J·mol^{-1}·K^{-1}
Temperature range 93 to 291 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=562.3 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 120.2 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 194 K, ΔH=182.4 J·mol^{-1}
ΔS=0.94 J·mol^{-1}·K^{-1}
c,I/liq 288.7 K, ΔH=44267 J·mol^{-1}
ΔS=153.3 J·mol^{-1}·K^{-1}
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B(C_p),C(S)

$C_{14}H_{30}$ (liq) 54FIN/GRO2
n-Tetradecane
Heat Capacity 298.15 K, C_p=438.44 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=555.43 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 279.03 K, ΔH=45070 J·mol^{-1}
ΔS=161.52 J·mol^{-1}·K^{-1}
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation A

$C_{14}H_{30}$ (liq) 82ZAR
n-Tetradecane
Heat Capacity 298 K, C_p=436.0 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 84GRI/ANI
n-Tetradecane
Heat Capacity 296.20 K, C_p=435.1 J·mol^{-1}·K^{-1}
Temperature range 296 to 433 K. Unsmoothed experimental datun given as 2.193 kJ/kg·K.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 84GRO/BEI
n-Tetradecane
Heat Capacity 298.15 K, C_p=436.40 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 84GRO/INC
n-Tetradecane
Heat Capacity 298.15 K, C_p=436.52 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 84ROU/GRC
n-Tetradecane
Heat Capacity 298.15 K, C_p=436.91 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 85BAL/BRA
n-Tetradecane
Heat Capacity 298.15 K, C_p=433.53 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 85LAI/ROU
n-Tetradecane
Heat Capacity 298.15 K, C_p=434.20 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 85LAI/WIL
n Tetradecane
Heat Capacity 298.15 K, C_p=434.20 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation A

$C_{14}H_{30}$ (liq) 86WIL/LA
n-Tetradecane
Heat Capacity 298.15 K, C_p=433.98 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 87WIL/ING
n-Tetradecane
Heat Capacity 298.15 K, C_p=434.16 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 88COS/HUU
n-Tetradecane
Heat Capacity 298.15 K, C_p=438.01 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 88PER/AIC
n-Tetradecane
Heat Capacity 298.15 K, C_p=438.01 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation A

$C_{14}H_{30}$ (liq) 88PIN/BRA
n-Tetradecane
Heat Capacity 298.15 K, C_p=433.53 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 89WIL/LAI
n-Tetradecane
Heat Capacity 298.15 K, C_p=434.20 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 91TRE/COS
n-Tetradecane
Heat Capacity 298.15 K, C_p=438.28 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}O$ (c) 74MOS/MOU
1-Tetradecanol; n-Tetradecyl alcohol
Heat Capacity 298.15 K, C_p=388 J·mol^{-1}·K^{-1}
α-form, 386 to 303 K.
Phase Changes
c,β/c,γ 306 K, ΔH=1800 J·mol^{-1}; ΔS=5.9 J·mol^{-1}·K^{-1}
c,β/c,α 311.2 K, ΔH=23800 J·mol^{-1}; ΔS=76.5 J·mol^{-1}·K^{-1}
c,γ/c,α 311.6 K, ΔH=22000 J·mol^{-1}; ΔS=70.6 J·mol^{-1}·K^{-1}
c,β/liq 311.0 K, ΔH=49510 J·mol^{-1}; ΔS=159.2 J·mol^{-1}·K^{-1}
c,γ/liq 311.2 K, ΔH=47000 J·mol^{-1}; ΔS=151.0 J·mol^{-1}·K^{-1}
c,α/liq 310.8 K, ΔH=25100 J·mol^{-1}; ΔS=80.8 J·mol^{-1}·K^{-1}.
Molecular Weight 214.3904
Wiswesser Line Notation Q14
Evaluation B

$C_{14}H_{30}O$ (c) 74MOS/MOU
1-Tetradecanol; n-Tetradecyl alcohol
Heat Capacity 312 K, C_p=506 J·mol^{-1}·K^{-1}
Temperature range 312 to 346 K.
Molecular Weight 214.3904
Wiswesser Line Notation Q14
Evaluation B

$C_{14}H_{30}S$ (liq) 82TUT/GAB
1-Tetradecanethiol; n-Tetradecyl mercaptan
Heat Capacity 300 K, C_p=501.57 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K. C_p=480.72+4.157×10^{-2}T+9.310×10^{-5}T^2.
Molecular Weight 230.4510
Wiswesser Line Notation SH14
Evaluation B

$C_{14}H_{30}O$ (liq) 89KHA/ZYK
1-Tetradecanol; n-Tetradecyl alcohol
Heat Capacity 313.15 K, C_p=516.0 J·mol^{-1}·K^{-1}
Temperature range 313 to 563 K.
Molecular Weight 214.3904
Wiswesser Line Notation Q14
Evaluation B

$C_{14}H_{30}O$ (c) 92STE/CHI
1-Tetradecanol; n-Tetradecyl alcohol
Heat Capacity 298.15 K, C_p=426.5 J·mol^{-1}·K^{-1}
Temperature range 274 to 564 K. C/R(c)=0.360T−56.06 (269 to 311 K); C/R(liq)=0.159T+13.618 (311 to 379 K), R=8.31451 J/K·mol.
Phase Changes
c/liq 311 K, ΔH=49400 J·mol^{-1}
Molecular Weight 214.3904
Wiswesser Line Notation Q14
Evaluation A

$C_{14}H_{34}$ (liq) 63GUD/CAM
9-Methylperhydrofluorene
Heat Capacity 313 K, C_p=323.4 J·mol^{-1}·K^{-1}
Temperature range 313 to 583 K.
Molecular Weight 202.4226
Wiswesser Line Notation L B656TJ H1
Evaluation C

$C_{14}H_{34}Br_2N_2$ (c) 74BUR/VER
1,2-Bis(triethylammonium)ethane dibromide
Heat Capacity 298 K, C_p=411.7 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
Molecular Weight 390.2440
Wiswesser Line Notation 2K2&2&2K2&2&2 &E &E
Evaluation B

$C_{14}H_{36}CdCl_4N_2$ (c) 83WHI/DAV
Bis(n-heptylammonium)tetrachlorocadmate
Heat Capacity 298.15 K, C_p=633.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 325 K.
Entropy 298.15 K, S=779.0 J·mol^{-1}·K^{-1}
Phase Changes
c.III/c.II 250.00 K, ΔH=17630 J·mol^{-1}; ΔS=71.38 J·mol^{-1}·K^{-1}
c.II/c.I 316.74 K, ΔH=5060 J·mol^{-1}; ΔS=16.0 J·mol^{-1}·K^{-1}
Molecular Weight 486.6738
Wiswesser Line Notation 7ZH 2 .CD G4
Evaluation A

$C_{14}H_{36}N_2MnCl_4$ (c) 83WHI/DAV
Bis(n-heptylammonium)tetrachloromanganate
Heat Capacity 298.15 K, C_p=653.0 J·mol^{-1}·K^{-1}
Temperature range 10 to 325 K.
Entropy 298.15 K, S=772.9 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 247.95 K, ΔH=16930 J·mol^{-1}
ΔS=68.2 J·mol^{-1}·K^{-1}
c,II/c,I 313.8 K, ΔH=10197 J·mol^{-1}
ΔS=32.5 J·mol^{-1}·K^{-1}
Molecular Weight 398.5688
Wiswesser Line Notation 7ZH 2 .MN G4
Evaluation A

$C_{15}H_{10}N_2O_2$ (c) 66ZAL/STR
4,4′-Diphenylmethane diisocyanate
Heat Capacity 334 K, C_p=244.8 J·mol^{-1}·K^{-1}
Temperature range 46 to 78 °C, mean value.
Molecular Weight 250.2562
Wiswesser Line Notation OCNR D1R DNCO
Evaluation D
State not given; assumed solid.

$C_{15}H_{10}N_2O_2$ (c) 77LEB/EVS3
4,4′-Diphenylmethane diisocyanate
Heat Capacity 298.15 K, C_p=307.0 J·mol^{-1}·K^{-1}
Temperature range 12 to 355 K. Data deposited VINITI, No 4328-76, 14 December 1976.
Entropy 298.15 K, S=332.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 313.57 K, ΔH=27300 J·mol^{-1}
ΔS=87.1 J·mol^{-1}·K^{-1}
Molecular Weight 250.2562
Wiswesser Line Notation OCNR D1R DNCO
Evaluation A

$C_{15}H_{10}N_2O_2$ (c) 77LEB/RAB4
4,4′-Diphenylmethane diisocyanate
Heat Capacity 300 K, C_p=313 J·mol^{-1}·K^{-1}
Temperature range 13 to 400 K. Data given graphically. Value estimated from graph.
Entropy 298.15 K, S=332.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 313.57 K, ΔH=27300 J·mol^{-1}
ΔS=87.1 J·mol^{-1}·K^{-1}
Molecular Weight 250.2562
Wiswesser Line Notation OCNR D1R DNCO
Evaluation C(C_p); A(S, Phase changes)

$(C_{15}H_{10}N_2O_2)_n$ (gls) 77LEB/RAB4
Polyisocyanurate
Heat Capacity 300 K, C_p=300 J·mol^{-1}·K^{-1}
Temperature range 13 to 400 K. Data given graphically. Value estimated from graph.
Entropy 298.15 K, S=294 J·mol^{-1}·K^{-1}
Molecular Weight 250.2562
Wiswesser Line Notation /T4NVNVTJ A* CR D1R D*/
Evaluation C(C_p), A(S)

$C_{15}H_{11}ClN_2O$ (c) 92CHA/ELM
Nordazepam;
7-Chloro-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one
Phase Changes
c,IV/liq 214.2 K, ΔH=33620 J·mol^{-1}
c,III/liq 216.0 K, ΔH=27400 J·mol^{-1}
c,II/liq 216.7 K, ΔH=34000 J·mol^{-1}
c,I/liq 221.3 K, ΔH=24450 J·mol^{-1}
Molecular Weight 270.7177
Wiswesser Line Notation T76 BMV DH ENJ FR IG
Evaluation A

$C_{15}H_{11}N_3O_7$ (c) 79FAR/SHA
Indene picric acid
Phase Changes
c/liq 366.7 K, ΔH=25100 J·mol^{-1}
ΔS=68.5 J·mol^{-1}·K^{-1}
Molecular Weight 345.2678
Wiswesser Line Notation L56 BHJ &WNR BQ CNW ENW
Evaluation B

$C_{15}H_{12}$ (c) 88CHI/HOS
4-Methylphenanthrene
Heat Capacity 298.15 K, C_p=263.13 J·mol^{-1}·K^{-1}
Temperature range 10 to 500 K. Value is a graphical extrapolation.
Entropy 298.15 K, S=244.55 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 182.0 K, ΔH=22.4 J·mol^{-1}
ΔS=0.12 J·mol^{-1}·K^{-1}
Extrapolated value.
c,II/c,I 295 K, ΔH=33.3 J·mol^{-1}
ΔS=0.11 J·mol^{-1}·K^{-1}
Extrapolated value.
c,I/liq 324.925 K, ΔH=14039 J·mol^{-1}
ΔS=43.21 J·mol^{-1}·K^{-1}
Molecular Weight 192.2598
Wiswesser Line Notation L B666J C1
Evaluation A

$C_{15}H_{12}$ (c) 89CHI/HOS
4-Methylphenanthrene
Heat Capacity 298.15 K, C_p=263.13 J·mol^{-1}·K^{-1}
Temperature range 10 to 500 K. Value is a graphical extrapolation.
Entropy 298.15 K, S=244.55 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 182.0 K, ΔH=22.4 J·mol^{-1}
ΔS=0.12 J·mol^{-1}·K^{-1}
Extrapolated value.
c,II/c,I 295.0 K, ΔH=33.3 J·mol^{-1}
ΔS=0.11 J·mol^{-1}·K^{-1}
Extrapolated value.
c,I/liq 324.925 K, ΔH=14039 J·mol^{-1}
ΔS=43.21 J·mol^{-1}·K^{-1}
Molecular Weight 192.2598
Wiswesser Line Notation L B666J C1
Evaluation A

$C_{15}H_{15}Co_3S_2$ (c) 71SOR/KOS
Tris-(cyclopentadienylcobalt)disulfide
Phase Changes
c,II/c,I 192.5 K, ΔH=5253.4 J·mol^{-1}
ΔS=28.894 J·mol^{-1}·K^{-1}
Molecular Weight 436.2031
Wiswesser Line Notation L5ϕJ ϕ-CO– 3 &S 2
Evaluation A

$C_{15}H_{15}Y$ (c) 82SHE/KAM
Tricyclopentadienyl yttrium
Heat Capacity 298.15 K, C_p=289.0 J·mol^{-1}·K^{-1}
Temperature range 4.5 to 300 K.
Entropy 298.15 K, S=301.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 265–280 K
Order-disorder transition.
Molecular Weight 284.1894
Wiswesser Line Notation L5ϕJ ϕ-Y- ϕL5ϕJ &ϕL5ϕJ
Evaluation A

$C_{15}H_{16}$ (liq) 56MCE
p-Isopropylbiphenyl
Heat Capacity 422 K, C_p=421.3 J·mol^{-1}·K^{-1}
Temperature range 300 to 600 °C.
Molecular Weight 196.2914
Wiswesser Line Notation 1Y1&R DR
Evaluation C
Quoted in 58WAL/BRO.

$C_{15}H_{16}$ (liq) 63VAR/KOP
Isopropylbiphenyl
Heat Capacity 295 K, C_p=343.9 J·mol^{-1}·K^{-1}
Temperature range 293 to 670 K. Value is unsmoothed experimental datum.
Molecular Weight 196.2914
Wiswesser Line Notation 1Y1&R XR
Evaluation B
Probably the para isomer.

$C_{15}H_{16}$ (liq) 64VUK/RAS
Isopropylbiphenyl
Heat Capacity 298 K, C_p=338.5 J·mol^{-1}·K^{-1}
Temperature range 38 to 212 °C.
Molecular Weight 196.2914
Wiswesser Line Notation 1Y1&R XR
Evaluation C
Probably the para isomer.

$C_{15}H_{16}N_2O_3$ (liq) 38KRE
p-Azoxyanisoylphenetole
Heat Capacity 420 K, C_p=594 J·mol^{-1}·K^{-1}
Value a few degrees below anisotropic-isotropic liquid-liquid transition at 428 K.
Molecular Weight 272.3030
Wiswesser Line Notation 2OR DNO&UNR DO1
Evaluation C

$C_{15}H_{16}O$ (c) 57MAS
p-α-Cumylphenol
Phase Changes
c/liq 346.40 K, ΔH=21677 J·mol^{-1}
Molecular Weight 212.2908
Wiswesser Line Notation QR DX1&1&R
Evaluation A

$C_{15}H_{16}O_2$ (c) 85NOV/TSV
4,4′-Dihydroxydiphenyl-2,2-propane
Heat Capacity 298.15 K, C_p=287.72 J·mol^{-1}·K^{-1}
Temperature range 14 to 480 K.
Entropy 298.15 K, S=287.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 433 K, ΔH=30100 J·mol^{-1}
ΔS=69.6 J·mol^{-1}·K^{-1}
Molecular Weight 228.2902
Wiswesser Line Notation QR DX1&1&R DQ
Evaluation A

$C_{15}H_{21}AlO_6$ (c) 81TEG/FER
Aluminum acetylacetonate
Heat Capacity 298 K, C_p=321.4 J·mol^{-1}·K^{-1}
Temperature range 4.2 to 450 K.
Entropy 298 K, S=479.1 J·mol^{-1}·K^{-1}
Molecular Weight 324.3088
Wiswesser Line Notation D6O-AL-O ADJ D1 F1 B-& BD6O-AL-O ADJ D1 F1 B-& BD60-AL-O ADJ D1 F1
Evaluation B

$C_{15}H_{21}AlO_6$ (c) 86GRI/LAZ
Aluminum acetylacetonate
Phase Changes
c/liq 466.7 K, ΔH=33700 J·mol^{-1}
ΔS=72.1 J·mol^{-1}·K^{-1}
Molecular Weight 324.3088
Wiswesser Line Notation D6O-AL-O ADJ D1 F1 B-& BD6O-AL-O ADJ D1 F1 B-& BD60-AL-O ADJ D1 F1
Evaluation A

$C_{15}H_{21}CrO_6$ (c) 86GRI/LAZ
Chromium acetylacetonate
Phase Changes
c/liq 481.9 K, ΔH=34000 J·mol^{-1}
ΔS=69.5 J·mol^{-1}·K^{-1}
Molecular Weight 349.3233
Wiswesser Line Notation D6O-CR-O ADJ D1 F1 B-& BD6O-CR-O ADJ D1 F1 B-& BD6O-CR-O ADJ D1 F1
Evaluation A

$C_{15}H_{21}FeO_6$ (c) 87ZHI/KAR
Iron (III) acetylacetonate
Heat Capacity 298.15 K, C_p=429.9 J·mol^{-1}·K^{-1}
Temperature range 13 to 310 K.
Entropy 298.15 K, S=526.5 J·mol^{-1}·K^{-1}
Molecular Weight 353.1743
Wiswesser Line Notation D6O-FE-O ADJ D1 F1 B-& BD6O-FE-O ADJ D1 F1 B-& BD6O-FE-O ADJ D1 F1
Evaluation A

$(C_{15}H_{21}N_3O\cdot HBr)_n$ (c) 91ROL
Poly-L-lysine hydrobromide· phenylalanine copolymer
Heat Capacity 300 K, C_p=366.5 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 356.2617
Wiswesser Line Notation /*VY4Z &EH &MVYM*&1R/ -L
Evaluation B

$(C_{15}H_{21}N_3O\cdot HBr)_n$ (c) 93ROL/WUN
Poly-L-lysine hydrobromide· phenylalanine copolymer
Heat Capacity 300 K, C_p=366.5 J·mol^{-1}·K^{-1}
Temperature range 220 to 390 K.
Molecular Weight 356.2617
Wiswesser Line Notation /*VY4Z &EH &MVYM*&1R/ -L
Evaluation B

$C_{15}H_{26}$ (liq) 63GUD/CAM
1,3-Dicyclopentylcyclopentane
Heat Capacity 313 K, C_p=363.6 J·mol^{-1}·K^{-1}
Temperature range 313 to 583 K.
Molecular Weight 206.3704
Wiswesser Line Notation L5TJ A CL5TJ A- AL5TJ
Evaluation C

$C_{15}H_{26}BrN$ (c) 89VAN/WHI
9-Phenylnonylammonium bromide
Phase Changes
c,II/c,I 309 K, $\Delta H = 8930\ J \cdot mol^{-1}$
$\Delta S = 3.48\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 300.2811
Wiswesser Line Notation Z9R &EH
Evaluation A

$C_{15}H_{26}ClN$ (c) 89VAN/WHI
9-Phenylnonylammonium chloride
Phase Changes
c,III/c,II 320 K, $\Delta H = 10000\ J \cdot mol^{-1}$
$\Delta S = 3.82\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I 331 K, $\Delta H = 7590\ J \cdot mol^{-1}$
$\Delta S = 2.54\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 255.8301
Wiswesser Line Notation Z9R &GH
Evaluation A

$C_{15}H_{26}O_6$ (liq) 76PHI/MAT
Tributyrin; Glyceryl tributyrate
Heat Capacity 313 K, $C_p = 569\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 413 K.
Molecular Weight 302.3668
Wiswesser Line Notation 3VO1YOV3&1OV3
Evaluation C

$C_{15}H_{26}O_6$ (liq) 86NIL/WAD
Tributyrin; Glyceryl tributyrate
Heat Capacity 298.15 K, $C_p = 555.3\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 302.3668
Wiswesser Line Notation 3VO1YOV3&1OV3
Evaluation A

$C_{15}H_{28}$ (liq) 63GUD/CAM
2-Isopropylbicyclohexyl
Heat Capacity 313 K, $C_p = 418.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 483 K.
Molecular Weight 208.3862
Wiswesser Line Notation L6TJ A- BL6TJ AY1&1
Evaluation C

$C_{15}H_{28}$ (liq) 63GUD/CAM
2-Ethylbicyclohexylmethane
Heat Capacity 313 K, $C_p = 384.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 483 K.
Molecular Weight 208.3862
Wiswesser Line Notation L6TJ A- BL6TJ A2
Evaluation C

$C_{15}H_{28}$ (liq) 63GUD/CAM
Cyclohexyl(ethylcyclohexyl)methane
Heat Capacity 313 K, $C_p = 402.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 483 K.
Molecular Weight 208.3862
Wiswesser Line Notation L6TJ A1- XL6TJ A2
Evaluation C

$C_{15}H_{28}$ (liq) 62GOL/BE
1,2-Dicyclohexylpropane
Heat Capacity 422 K, $C_p = 497.9\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 208.3862
Wiswesser Line Notation L6TJ AY1&1- AL6TJ
Evaluation C

$C_{15}H_{28}$ (liq) 63GUD/CAM
1,2-Dicyclohexylpropane
Heat Capacity 313 K, $C_p = 398.3\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 583 K.
Molecular Weight 208.3862
Wiswesser Line Notation L6TJ AY1&1- AL6TJ
Evaluation C

$C_{15}H_{28}$ (liq) 62GOL/BE
Cyclohexyl(2-ethylcyclohexyl)methane
Heat Capacity 311 K, $C_p = 411.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperatures 100, 200, 300 °F.
Molecular Weight 208.3862
Wiswesser Line Notation L6TJ B2 A1- AL6TJ
Evaluation C

$C_{15}H_{28}$ (liq) 62GOL/BE
Isopropylbicyclohexyl
Heat Capacity 311 K, $C_p = 417.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperatures 100, 200, 300 °F.
Molecular Weight 208.3862
Wiswesser Line Notation L6TJ XY1&1 A- AL6TJ
Evaluation C

$C_{15}H_{28}O$ (liq) 88BAG/GU
3,7,11-Trimethyl-1-dodecyn-3-ol
Heat Capacity 313.15 K, $C_p = 574.4\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 224.3856
Wiswesser Line Notation 1Y3Y3XQ1UU1
Evaluation B

$C_{15}H_{28}O_2$ (c) 81LEB/YE
Pentadecanolactone
Heat Capacity 298.15 K, $C_p = 444.3\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 13.8 to 330 K.
Entropy 298.15 K, $S = 482.8\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 282.98 K, $\Delta H = 27301\ J \cdot mol^{-1}$
$\Delta S = 96.2\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 308.5 K, $\Delta H = 6979\ J \cdot mol^{-1}$
$\Delta S = 22.6\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 240.3850
Wiswesser Line Notation T-16-VOTJ
Evaluation A

$C_{15}H_{28}O_2$ (c) 83YEV/LEB
Pentadecanolactone
Heat Capacity 298.15 K, C_p=444.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S=482.9 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 282.98 K, ΔH=27300 J·mol^{-1}
ΔS=96.3 J·mol^{-1}·K^{-1}
c,I/liq 308.5 K, ΔH=6980 J·mol^{-1}
ΔS=22.6 J·mol^{-1}·K^{-1}
c,I″/c,I′ 193 K, ΔH=0 J·mol^{-1}
ΔS=0 J·mol^{-1}·K^{-1}
Molecular Weight 240.3850
Wiswesser Line Notation T-16-VOTJ
Evaluation A
Thermodynamic functions are also given for the c,I′ and the c,I″ states from 5 to 282.98 K.

$(C_{15}H_{28}O_2)_n$ (c) 83YEV/LEB
Polypentadecanolactone
Heat Capacity 298.15 K, C_p=369.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 370.4 K.
Entropy 298.15 K, S=397.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 370.4 K, ΔH=56000 J·mol^{-1}
ΔS=151 J·mol^{-1}·K^{-1}
100% crystallinity
gls/h.e. 251 K, ΔH=0 J·mol^{-1}
ΔS=0 J·mol^{-1}·K^{-1}
Glass to high-elastic state.
Molecular Weight 240.3850
Wiswesser Line Notation /*MV14*/
Evaluation A

$C_{15}H_{30}$ (liq) 65MES/TOD2
n-Decylcyclopentane
Heat Capacity 298.15 K, C_p=426.52 J·mol^{-1}·K^{-1}
Temperature range 12 to 370 K.
Entropy 298.15 K, S=538.52 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 251.02 K, ΔH=33125 J·mol^{-1}
ΔS=132.0 J·mol^{-1}·K^{-1}
Molecular Weight 210.4020
Wiswesser Line Notation L5TJ A10
Evaluation A

$C_{15}H_{30}O$ (c) 79SUN/SVE
2-Pentadecanone; Tridecyl methyl ketone
Heat Capacity 298.15 K, C_p=426.8 J·mol^{-1}·K^{-1}
Temperature range 285 to 343 K. Equations only.
Phase Changes
c/liq 312.2 K, ΔH=54570 J·mol^{-1}
ΔS=174.8 J·mol^{-1}·K^{-1}
Molecular Weight 226.4014
Wiswesser Line Notation 13V1
Evaluation B

$C_{15}H_{30}O_2$ (c) 82SCH/MIL
Pentadecanoic acid
Heat Capacity 298.15 K, C_p=443.28 J·mol^{-1}·K^{-1}
Temperature range 80 to 345 K.
Phase Changes
c,II/c,I 318.7 K, ΔH=8123 J·mol^{-1}
ΔS=25.47 J·mol^{-1}·K^{-1}
c,I/liq 325.68 K, ΔH=41526 J·mol^{-1}
ΔS=127.50 J·mol^{-1}·K^{-1}
Molecular Weight 242.4008
Wiswesser Line Notation QV14
Evaluation B

$C_{15}H_{30}O_2$ (liq) 79FUC
Methyl tetradecanoate; Methyl myristate
Heat Capacity 298.15 K, C_p=505.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 242.4008
Wiswesser Line Notation 13VO1
Evaluation B

$C_{15}H_{30}O_4$ (c) 65SIL/DAU
2-Monolaurin
Heat Capacity 298 K, C_p=436.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 274.3996
Wiswesser Line Notation Q1Y1QOV11
Evaluation B

$C_{15}H_{30}O_4$ (c) 65SIL/DAU
1-Monolaurin
Heat Capacity 298 K, C_p=447.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 274.3996
Wiswesser Line Notation Q1YQOV11
Evaluation B
β_L form.

$C_{15}H_{32}$ (liq) 54FIN/GRO2
n-Pentadecane
Heat Capacity 298.15 K, C_p=469.95 J·mol^{-1}·K^{-1}
Temperature range 12 to 310 K.
Entropy 298.15 K, S=587.52 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 270.9 K, ΔH=9167 J·mol^{-1}
ΔS=33.84 J·mol^{-1}·K^{-1}
c,I/liq 283.11 K, ΔH=34593 J·mol^{-1}
ΔS=122.19 J·mol^{-1}·K^{-1}
Molecular Weight 212.4178
Wiswesser Line Notation 15H
Evaluation A

$C_{15}H_{32}$ (liq) 81GRO/ING
n-Pentadecane
Heat Capacity 298.15 K, C_p=467.81 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 212.4178
Wiswesser Line Notation 15H
Evaluation B

$C_{15}H_{32}$ (liq) 88COS/HUU
n-Pentadecane
Heat Capacity 298.15 K, C_p=468.81 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 212.4178
Wiswesser Line Notation 15H
Evaluation B

$C_{15}H_{32}$ (liq) 91TRE/COS
n-Pentadecane
Heat Capacity 298.15 K, C_p=470.48 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 212.4178
Wiswesser Line Notation 15H
Evaluation B

$C_{15}H_{32}O$ (c) 74MOS/MOU
1-Pentadecanol; n-Pentadecyl alcohol
Heat Capacity 298.15 K, C_p=400 J·mol^{-1}·K^{-1}
Temperature range 295 to 308 K.
Phase Changes
c,β/c,α 316.2 K, ΔH=23650 J·mol^{-1}
ΔS=74.8 J·mol^{-1}·K^{-1}
c,β/liq 316.6 K, ΔH=54720 J·mol^{-1}
ΔS=172.8 J·mol^{-1}·K^{-1}
c,α/liq 316.9 K, ΔH=30350 J·mol^{-1}
ΔS=95.8 J·mol^{-1}·K^{-1}
Molecular Weight 228.4172
Wiswesser Line Notation Q15
Evaluation B

$C_{15}H_{32}O$ (c) 74MOS/MOU
1-Pentadecanol; n-Pentadecyl alcohol
Heat Capacity 318 K, C_p=535 J·mol^{-1}·K^{-1}
Temperature range 318 to 346 K.
Molecular Weight 228.4172
Wiswesser Line Notation Q15
Evaluation B

$C_{15}H_{32}O$ (c) 82VAS/PET
1-Pentadecanol; n-Pentadecyl alcohol
Heat Capacity 358 K, C_p=537.3 J·mol^{-1}·K^{-1}
Temperature range 358 to 608 K.
Molecular Weight 228.4172
Wiswesser Line Notation Q15
Evaluation B

$C_{15}H_{32}O$ (liq) 89KHA/ZYK
1-Pentadecanol; n-Pentadecyl alcohol
Heat Capacity 323.15 K, C_p=567.4 J·mol^{-1}·K^{-1}
Temperature range 323 to 573 K.
Molecular Weight 228.4172
Wiswesser Line Notation Q15
Evaluation B

$C_{15}H_{32}O_6$ (liq) 82ZAR
Pentapropylene glycol
Heat Capacity 298 K, C_p=685.6 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 308.4142
Wiswesser Line Notation QYOYOYOYOYQ
Evaluation B

$C_{15}H_{36}Br_2N_2$ (c) 74BUR/VER
1,3-Bis(triethylammonium)propane dibromide
Heat Capacity 298 K, C_p=439.3 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
Molecular Weight 404.2708
Wiswesser Line Notation 2K2&2&3K2&2&2 &E &E
Evaluation B

$C_{16}F_{34}$ (c) 93LEB/BYK
n-Perfluorohexadecane
Heat Capacity 298.15 K, C_p=772.5 J·mol^{-1}·K^{-1}
Temperature range 0 to 320 K.
Entropy 298.15 K, S=990.0 J·mol^{-1}·K^{-1}
Phase Changes
c,IV/c,III 175.47 K ΔH=870 J·mol^{-1}
ΔS=4.97 J·mol^{-1}·K^{-1}
c,III/c,II 177.34 K ΔH=1880 J·mol^{-1}
ΔS=10.68 J·mol^{-1}·K^{-1}
Molecular Weight 838.1216
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFXFF-XFXFFXFFXFFXFFXFFXFFXFFXFFF
Evaluation A

$C_{16}H_6O_7$ (c) 73KAR/MOC
Bis-(3-phthalyl anhydride) ether
Heat Capacity 300 K, C_p=311.8 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=319.2 J·mol^{-1}·K^{-1}
Molecular Weight 310.2192
Wiswesser Line Notation T56 BVOVJ GO- GT56 BVOVJ
Evaluation A

$C_{16}H_6O_8S$ (c) 73KAR/MOC
Bis-(3-phthalyl anhydride) sulfone
Heat Capacity 300 K, C_p=360.0 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=360.7 J·mol^{-1}·K^{-1}
Molecular Weight 358.2786
Wiswesser Line Notation T56 BVOVJ GSW- GT56 BVOVJ
Evaluation A

$(C_{16}H_8D_8)_n$ (gls) 83LEB/SMI
Polystyrene-polystyrene-d_8 copolymer
Heat Capacity 298.15 K, C_p=279.1 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S=291.4 J·mol^{-1}·K^{-1}
Molecular Weight 216.3656
Wiswesser Line Notation /*YR&1*/ &/*YR&1*/ &1/2-BCDEF/4/H-2 8
Evaluation A

$C_{16}H_8N_4$ (c) 79BOE/WES
Naphthalene-tetracyanoethylene adduct
Heat Capacity
Temperature range 5 to 300 K. Data graphically only.
Phase Changes
c,III/c,II 160 K, ΔS=5.10 J·mol^{-1}·K^{-1}
Bifurcated peak. Transition region 150 to 172.5 K.
c,II/c,I 222 K, ΔS=5.02 J·mol^{-1}·K^{-1}
Extended transition. Transition region 172.5 to 240 K.
Molecular Weight 256.2600
Wiswesser Line Notation L66J &NCYCN&UYCN&CN
Evaluation A

$C_{16}H_8N_4$ (c) 80BOE/WES

Naphthalene-tetracyanoethylene adduct

Heat Capacity 298.15 K, C_p=328.7 J·mol^{-1}·K^{-1}

Temperature range 5 to 300 K.

Entropy 298.15 K, S=384.3 J·mol^{-1}·K^{-1}

Phase Changes

c,III/c,II 160 K, ΔH=822.6 J·mol^{-1}; ΔS=5.10 J·mol^{-1}·K^{-1}

c,II/c,I 240 K, ΔH=1029 J·mol^{-1}; ΔS=5.02 J·mol^{-1}·K^{-1}

c,III/c,II:

region from 150 to 172.5 K;

c,II/c,I:

region from 172.5 to 240 K.

Molecular Weight 256.2600

Wiswesser Line Notation L66J &NCYCN&UYCN&CN

Evaluation A

$C_{16}H_{10}$ (c) 71WON/WES

Fluoranthene; Idryl; 1,2-Benzacenaphthene

Heat Capacity 298.15 K, C_p=230.25 J·mol^{-1}·K^{-1}

Temperature range 5 to 427 K.

Entropy 298.15 K, S=230.58 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 383.36 K, ΔH=18728 J·mol^{-1}; ΔS=48.85 J·mol^{-1}·K^{-1}

Molecular Weight 202.2550

Wiswesser Line Notation L C6566 1A PJ

Evaluation A

$C_{16}H_{10}$ (c) 34JAC/PAR

Pyrene; Benzo(d.e.f)phenanthrene

Heat Capacity 291.1 K, C_p=227.65 J·mol^{-1}·K^{-1}

Temperature range 94 to 292 K. Value is unsmoothed experimental datum.

Entropy 298.1 K, S=215.1 J·mol^{-1}·K^{-1}

Extrapolation below 90 K, 59.79 J·mol^{-1}·K^{-1}. Hump in C_p curve around 116 K, probably 2nd order transition. ΔH=100 J·mol^{-1}.

Molecular Weight 202.2550

Wiswesser Line Notation L666 B6 2AB PJ

Evaluation B(C_p),C(S)

$C_{16}H_{10}$ (c) 71WON/WES

Pyrene; Benzo(d,e,f)phenanthrene

Heat Capacity 298.15 K, C_p=229.70 J·mol^{-1}·K^{-1}

Temperature range 5 to 484 K.

Entropy 298.15 K, S=224.89 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 120.8 K, ΔH=289 J·mol^{-1}; ΔS=2.30 J·mol^{-1}·K^{-1}

c,I/liq 423.81 K, ΔH=17364 J·mol^{-1}; ΔS=40.97 J·mol^{-1}·K^{-1}

Molecular Weight 202.2550

Wiswesser Line Notation L666 B6 2AB PJ

Evaluation A

$C_{16}H_{10}$ (c) 80SMI/STE

Pyrene; Benzo(d,e,f)phenanthrene

Heat Capacity 298.15 K, C_p=229.36 J·mol^{-1}·K^{-1}

One temperature.

Molecular Weight 202.2550

Wiswesser Line Notation L666 B6 2AB PJ

Evaluation C

$(C_{16}H_{10}Ge)_n$ (gls) 77LEB/RAB

Polydiphenyldiethynylgermanium

Heat Capacity 298.15 K, C_p=279.4 J·mol^{-1}·K^{-1}

Temperature range 50 to 325 K.

Molecular Weight 274.8650

Wiswesser Line Notation /*1UU1-GE-R&R&1UU1*/

Evaluation B

$(C_{16}H_{10}Si)_n$ (c) 73LEB/TSV2

Polydiphenyldiethynylsilane

Heat Capacity 300 K, C_p=309.2 J·mol^{-1}·K^{-1}

Temperature range 10 to 300 K.

Entropy 300 K, S=286.6 J·mol^{-1}·K^{-1}

Molecular Weight 230.3405

Wiswesser Line Notation /*1UU1-SI-R&R&1UU1*/

Evaluation A

$(C_{16}H_{10}Si)_n$ (c) 74MIL/LEB

Polydiphenyldiethynylsilane

Heat Capacity 300 K, C_p=309.2 J·mol^{-1}·K^{-1}

Temperature range 300 to 330 K.

Entropy 300 K, S=286.6 J·mol^{-1}·K^{-1}

Molecular Weight 230.3405

Wiswesser Line Notation /*1UU1-SI-R&R&1UU1*/

Evaluation B

$C_{16}H_{11}N_3O_6$ (c) 80RAD/RAD

Naphthalene-1,3,5-trinitrobenzene adduct

Heat Capacity 298.15 K, C_p=233.5 J·mol^{-1}·K^{-1}

Temperature range 220 to 400 K. Data given graphically. C_p calculated from equation.

Phase Changes

c,III/c,II 220 K, ΔH=1700 J·mol^{-1}; ΔS=7.22 J·mol^{-1}·K^{-1}

c,II/c,I 424.5 K, ΔH=1598 J·mol^{-1}; ΔS=3.77 J·mol^{-1}·K^{-1}

c,I/liq 430.8 K, ΔH=31900 J·mol^{-1}; ΔS=74.05 J·mol^{-1}·K^{-1}

Molecular Weight 341.2794

Wiswesser Line Notation L66J &WNR CNW ENW

Evaluation B

$C_{16}H_{11}N_3O_7$ (c) 79FAR/SHA

Naphthalene picric acid

Phase Changes

c/liq 426.2 K, ΔH=34700 J·mol^{-1}; ΔS=81.4 J·mol^{-1}·K^{-1}

Molecular Weight 357.2788

Wiswesser Line Notation L66J &WNR BQ CNW ENW

Evaluation B

$C_{16}H_{12}Ge$ (c) 75LEB/MIL4

Diethynyldiphenylgermane

Heat Capacity 298.15 K, C_p=305.4 J·mol^{-1}·K^{-1}

Temperature range 8.4 to 326 K. Deposited in VINITI, No 605-75, 10 March 1975.

Entropy 298.15 K, S=356.9 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 319.94 K, ΔH=20100 J·mol^{-1}; ΔS=62.80 J·mol^{-1}·K^{-1}

Molecular Weight 276.8608

Wiswesser Line Notation 1UU1-GE-R&R&1UU1

Evaluation A

$C_{16}H_{12}Ge$ (c) 75LEB/MIL2
Diethynyldiphenylgermane
Heat Capacity 300 K, C_p=307.1 J·mol^{-1}·K^{-1}
Temperature range 8 to 326 K.
Entropy 300 K, S=358.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 319.94 K, ΔH=20100 J·mol^{-1}
ΔS=62.80 J·mol^{-1}·K^{-1}
Molecular Weight 276.8608
Wiswesser Line Notation 1UU1-GE-R&R&1UU1
Evaluation A

$C_{16}H_{12}Ge$ (c) 75LEB/MIL6
Diethynyldiphenylgermane
Heat Capacity 298.15 K, C_p=305.4 J·mol^{-1}·K^{-1}
Temperature range 10 to 325 K.
Entropy 298.15 K, S=356.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 319.94 K, ΔH=20100 J·mol^{-1}
ΔS=62.8 J·mol^{-1}·K^{-1}
Molecular Weight 276.8608
Wiswesser Line Notation 1UU1-GE-R&R&1UU1
Evaluation A

$C_{16}H_{12}N_7$ (c) 84ABR/BAI
Tetramethylammonium hexacyanotrimethylenecyclopropanide
Heat Capacity 295 K, C_p=442.6 J·mol^{-1}·K^{-1}
Temperature range 233 to 393 K.
Phase Changes
c,II/c,I 363.7 K, ΔH=1350 J·mol^{-1}
ΔS=3.4 J·mol^{-1}·K^{-1}
Molecular Weight 302.3177
Wiswesser Line Notation L3YYYJ AU1CN&CN BU1CN&CN CU1CN&CN &K1&1&1
Evaluation B
Treated as a second-order transition, the phase change gives a heat capacity discontinuity of 56 J·mol^{-1}·K^{-1} at 363.7 K.

$C_{16}H_{12}O_2$ (c) 30PAR/HUF2
Dibenzoylethylene
Heat Capacity 291.9 K, C_p=286.6 J·mol^{-1}·K^{-1}
Temperature range 89 to 292 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=319.2 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 104.1 J·mol^{-1}·K^{-1}.
Molecular Weight 236.2696
Wiswesser Line Notation RV1U1VR
Evaluation B(C_p),C(S)

$C_{16}H_{14}Si$ (c) 74MIL/LEB
Diphenyldiethynylsilane
Heat Capacity 298.15 K, C_p=312.5 J·mol^{-1}·K^{-1}
Temperature range 50 to 330 K.
Entropy 298.15 K, S=357.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 316.24 K, ΔH=19673 J·mol^{-1}
Molecular Weight 232.3563
Wiswesser Line Notation 1UU1-SI-R&R&1UU1
Evaluation A

$C_{16}H_{12}Si$ (c) 77MIL/LEB
Diphenyldiethynylsilane
Heat Capacity 298.15 K, C_p=305.2 J·mol^{-1}·K^{-1}
Temperature range 10 to 326 K.
Entropy 298.15 K, S=345.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 209 K
Crystal-glass transition.
c,I/liq 316.72 K, ΔH=22360 J·mol^{-1}
ΔS=70.60 J·mol^{-1}·K^{-1}
Molecular Weight 232.3563
Wiswesser Line Notation 1UU1-SI-R&R&1UU1
Evaluation A

$C_{16}H_{14}$ (c,II) 93CHI/KNI2
4,5,9,10-Tetrahydropyrene
Heat Capacity 298.15 K, C_p=257.12 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S=247.77 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 319.9 K, ΔH=3670.9 J·mol^{-1}
c,II/c,I 385.1 K, ΔH=261.1 J·mol^{-1}
c,I/liq 412.725 K, ΔH=17093.8 J·mol^{-1}
Molecular Weight 206.2866
Wiswesser Line Notation L666 B6 2AB PT&T&J
Evaluation A

$C_{16}H_{14}O_2$ (c,I) 30PAR/HUF2
1,2-Dibenzoylethane
Heat Capacity 296.0 K, C_p=291.2 J·mol^{-1}·K^{-1}
Temperature range 93 to 296 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=324.79 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 103.7 J·mol^{-1}·K^{-1}.
Phase Changes
c,II/c,I 187 K, ΔH=218 J·mol^{-1}
ΔS=1.17 J·mol^{-1}·K^{-1}
Molecular Weight 238.2854
Wiswesser Line Notation RV2VR
Evaluation B(C_p),C(S)

$C_{16}H_{14}O_2$ (c) 32SPA/THO
1,2-Dibenzoylethane
Heat Capacity 303 K, C_p=302.1 J·mol^{-1}·K^{-1}
Temperature range 30 to 190 °C.
Phase Changes
c/liq 418.6 K, ΔH=38982 J·mol^{-1}
ΔS=93.1 J·mol^{-1}·K^{-1}
Molecular Weight 238.2854
Wiswesser Line Notation RV2VR
Evaluation B

$(C_{16}H_{14}O_3)_n$ (c) 62DAI/EVA7
Poly(4,4′-dioxyphenyl-2,2′-propane carbonate); Lexan polycarbonate
Heat Capacity 298.15 K, C_p=300.3 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 298.15 K, S=315.1 J·mol^{-1}·K^{-1}
Molecular Weight 254.2848
Wiswesser Line Notation /*VOR DX1&1&R DO*/
Evaluation A

$(C_{16}H_{14}O_3)_n$ (c) 63ORE/KAR
Poly(4,4′-dioxyphenyl-2,2′-propane carbonate); Lexan polycarbonate
Heat Capacity
Temperature range 80 to 570 K. C_p data given graphically only.
Phase Changes
gls/liq 450–520 K, $\Delta H = 5894\ J \cdot mol^{-1}$
Amorphous powder sample.
gls/liq 450–520 K, $\Delta H = 8235\ J \cdot mol^{-1}$
Solvent crystallized sample.
(24% crystallinity).
Molecular Weight 254.2848
Wiswesser Line Notation /*VOR DX1&1&R DO*/
Evaluation B
T(glass)=410 to 415 K.

$C_{16}H_{15}N$ (c) 91ASA/SOR
4′-Propylbiphenyl-4-carbonitrile
Heat Capacity 298.15 K, $C_p = 302.97\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 380 K.
Entropy 298.15 K, $S = 324.774\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 338.77 K, $\Delta H = 22700\ J \cdot mol^{-1}$
$\Delta S = 67.0\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 221.3012
Wiswesser Line Notation NCR DR D3
Evaluation A

$C_{16}H_{15}NO_3$ (c) 87BYK/KIP
3-Phenyl-5-phenoxymethyl-2-oxazolidinone
Heat Capacity 298.15 K, $C_p = 310.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 0 to 330 K.
Entropy 298.15 K, $S = 330.0\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 269.2994
Wiswesser Line Notation T5NVOTJ AR D1OR
Evaluation A

$C_{16}H_{16}$ (c,II) 93CHI/KNI2
1,2,3,6,7,8-Hexahydropyrene
Heat Capacity 298.15 K, $C_p = 255.54\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 700 K.
Entropy 298.15 K, $S = 236.26\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 377.00 K, $\Delta H = 9979.1\ J \cdot mol^{-1}$
c,I/liq 407.635 K, $\Delta H = 18093.2\ J \cdot mol^{-1}$
Molecular Weight 208.3024
Wiswesser Line Notation L666 B6 2AB P&T&TJ
Evaluation A

$C_{16}H_{16}$ (c) 69SHI/MCN
2,2-Metaparacyclophane
Heat Capacity 300 K, $C_p = 261.5\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 208.3024
Wiswesser Line Notation L E6 B-10-6 E-&T&J
Evaluation B

$C_{16}H_{16}$ (c) 69SHI/MCN
2,2-Metacyclophane
Heat Capacity 300 K, $C_p = 240.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 300, 318 K.
Molecular Weight 208.3024
Wiswesser Line Notation L E6 B-10-6 E-&T&J
Evaluation B

$C_{16}H_{16}$ (c) 69SHI/MCN
2,2-Paracyclophane; Cyclo-di-p-xylene
Heat Capacity 300 K, $C_p = 248.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 300, 318 K.
Molecular Weight 208.3024
Wiswesser Line Notation L F6 C-12-6 A B F- F-&T&J
Evaluation A

$C_{16}H_{16}$ (c) 70AND/WES
2,2-Paracyclophane; Cyclo-di-p-xylene
Heat Capacity 298.15 K, $C_p = 252.34\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 10 to 350 K.
Entropy 298.15 K, $S = 265.68\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
Second order transition between 30 and 60 K.
Molecular Weight 208.3024
Wiswesser Line Notation L F6 C-12-6 A B F- F-&T&J
Evaluation A

$C_{16}H_{16}$ (c) 73ROD/WES
2,2-Paracyclophane; Cyclo-di-p-xylene
Heat Capacity 298.15 K, $C_p = 252.7\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature. C_p given as $0.290\ cal \cdot K^{-1} \cdot g^{-1}$.
Molecular Weight 208.3024
Wiswesser Line Notation L F6 C-12-6 A B F- F-&T&J
Evaluation A

$C_{16}H_{16}N_2O_2$ (c) 67BAR/POR
Anisaldazine
Heat Capacity
C_p data given graphically only. Temperature range 313 to 500 K.
Phase Changes
c/liq 442.0 K, $\Delta H = 29750\ J \cdot mol^{-1}$
$\Delta S = 67.3\ J \cdot mol^{-1} \cdot K^{-1}$
Solid-nematic transition.
liq/liq 453.6 K, $\Delta H = 661\ J \cdot mol^{-1}$
$\Delta S = 1.5\ J \cdot mol^{-1} \cdot K^{-1}$
Nematic-isotropic transition.
Molecular Weight 268.3146
Wiswesser Line Notation 1OR D1UNNU1R DO1
Evaluation B

$C_{16}H_{18}N_2O_3$ (liq) 38KRE
p-Azoxyphenetole; 4,4′-Diethoxyazoxybenzene
Heat Capacity 430 K, $C_p = 607\ J \cdot mol^{-1} \cdot K^{-1}$
Value a few degrees below anisotropic-isotropic liquid–liquid transition at 436 K.
Molecular Weight 286.3298
Wiswesser Line Notation 2OR DNUNO&R DO2
Evaluation C

$C_{16}H_{18}N_2O_3$ (c) 93ACR/TUC
p-Azoxyphenetole; 4,4′-Diethoxyazoxybenzene
Phase Changes
c/liq 406.5 K, $\Delta H = 27000\ J \cdot mol^{-1}$
c/nematic.
liq/liq 438.5 K, $\Delta H = 1700\ J \cdot mol^{-1}$
Nematic/liq.
Molecular Weight 286.3298
Wiswesser Line Notation 2OR DNUNO&R DO2
Evaluation A

$C_{16}H_{18}N_4O_4$ (c) 73KAR/SAP3
3,3-Bis(4-carboxyphenyl)phthalide dihydrazide
Heat Capacity 298 K, C_p=460.2 J·mol^{-1}·K^{-1}
Temperature range 20 to 298 K.
Entropy 298 K, S=441.4 J·mol^{-1}·K^{-1}
Molecular Weight 330.3426
Wiswesser Line Notation T56BVO EHJ ER DVMZ &ER DVMZ
Evaluation B

$C_{16}H_{18}N_8$ (c) 73KAR/SAP3
1,3-Bis[5-(o-aminophenyl)-1,2,4-trizaole-3-yl]benzene
Heat Capacity 298 K, C_p=433.0 J·mol^{-1}·K^{-1}
Temperature range 20 to 298 K.
Entropy 298 K, S=408.9 J·mol^{-1}·K^{-1}
Molecular Weight 322.3718
Wiswesser Line Notation ZR B- CT5NN DMJ ER C- CT5NN DMJ ER BZ
Evaluation B

$C_{16}H_{20}Cr$ (liq) 72NIK/SAF
Bis(ethylbenzene)chromium
Heat Capacity 298.15 K, C_p=393.3 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S=406.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 275.6 K
Molecular Weight 264.3300
Wiswesser Line Notation L6ϕJ A2ϕ-CR- ϕL6ϕJ A2
Evaluation B
Data also given for glassy phase from 60 to 190 K.

$C_{16}H_{20}CrI$ (c) 72NIK/SAF
Bis(m-xylene)chromium iodide
Heat Capacity 298.15 K, C_p=353.3 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S=370.1 J·mol^{-1}·K^{-1}
Molecular Weight 391.2345
Wiswesser Line Notation L6ϕJ A1 C1ϕ-CR- ϕL6ϕJ A1 C1 &I
Evaluation B

$C_{16}H_{20}N_2$ (c) 84BER/BEC2
Tetracyclopropylsuccinonitrile
Heat Capacity 298.15 K, C_p=321.8 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 390 K, ΔH=22301 J·mol^{-1}
Molecular Weight 240.3474
Wiswesser Line Notation
Evaluation B

$C_{16}H_{22}OSi_2$ (liq) 83DZH/KUL
1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane
Heat Capacity 298.15 K, C_p=508.1 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Phase Changes
c/liq 250 K
Molecular Weight 286.5202
Wiswesser Line Notation 1-SI-1&R&O-SI-1&1&R
Evaluation A
T(glass)=167 K.

$C_{16}H_{22}OSi_2$ (liq) 86DZH/KUI
1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane
Heat Capacity 298.15 K, C_p=508.1 J·mol^{-1}·K^{-1}
Temperature range 4 to 300 K. C_p(c)=40.76+1.51T−5.428×10^{-4}T (90 to 160 K); C_p(liq)=382.004−3.75×10^{-2}T+1.5144×10^{-3}T^2 (17(to 300 K).
Entropy 298.15 K, S=559.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 251 K
Molecular Weight 286.5202
Wiswesser Line Notation 1-SI-1&R&O-SI-1&1&R
Evaluation A
T(glass)=167 K.

$C_{16}H_{22}O_3Si_3$ (c) 82KUL/DZF
Diphenyltetramethylcyclotrisiloxane
Heat Capacity 298.15 K, C_p=463.6 J·mol^{-1}·K^{-1}
Temperature range 4.2 to 370 K. Data given graphically except for dat at 298.15 K.
Entropy 298.15 K, S=528.0 J·mol^{-1}·K^{-1}
Phase Changes
c,l/liq 337.98 K, ΔH=22192 J·mol^{-1}
ΔS=65.7 J·mol^{-1}·K^{-1}
Molecular Weight 346.6045
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ AR AR C1 C1 E1 E1
Evaluation B

$C_{16}H_{22}O_4$ (liq) 69RAB/MAR
Dibutyl o-phthalate
Heat Capacity 300 K, C_p=477.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 360 K.
Entropy 300 K, S=933.0 J·mol^{-1}·K^{-1}
Molecular Weight 278.3474
Wiswesser Line Notation 4OVR BVO4
Evaluation C
Glass transition at 173.5 K; ΔH=1238 J·mol^{-1}, ΔS=4.77 J·mol^{-1}·K^{-1}.

$C_{16}H_{22}O_4$ (c) 70MAR/RAB
Dibutyl o-phthalate
Heat Capacity 300 K, C_p=477.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 360 K.
Entropy 300 K, S=514.6 J·mol^{-1}·K^{-1}
Molecular Weight 278.3474
Wiswesser Line Notation 4OVR BVO4
Evaluation B
T(glass)=173.5 °C.

$C_{16}H_{22}O_4$ (liq) 85RAB/NOV
Dibutyl o-phthalate
Heat Capacity 298.15 K, C_p=476.0 J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K.
Entropy 298.15 K, S=561.1 J·mol^{-1}·K^{-1}
Molecular Weight 278.3474
Wiswesser Line Notation 4OVR BVO4
Evaluation A
Data given for glassy state from 10 to 170 K. T(glass)=173.5 K.

$C_{16}H_{22}O_{11}$ (c) 44CLA/STE
α-Glucose pentaacetate (D)
Heat Capacity 298 K, C_p=491.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 390.3432
Wiswesser Line Notation T6OTJ BOV1 COV1 DOV1 EOV1 F1OV -A&BCE -B&DF
Evaluation C

$C_{16}H_{22}O_{11}$ (c) 44CLA/STE
β-Glucose pentaacetate (D)
Heat Capacity 298 K, C_p=498.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 390.3432
Wiswesser Line Notation T6OTJ BOV1 COV1 DOV1 EOV1 F1OV1 -A&CE -B&BDF
Evaluation C

$C_{16}H_{24}Si_8O_{12}$ (c) 85PAN/KOZ
Octa(vinylsilasesquioxane)
Heat Capacity 300 K, C_p=760 J·mol^{-1}·K^{-1}
Temperature range 160 to 300 K. C_p value estimated from graphical data.
Phase Changes
c,II/c,I 229.6 K, ΔH=9200 J·mol^{-1}
ΔS=40.0 J·mol^{-1}·K^{-1}
Molecular Weight 633.0424
Wiswesser Line Notation T16 /-SIO-O-SI-O/ 4J C1U1 C1U1 G1U1 G1U1 K1U1 K1U1 O1U1 O1U1
Evaluation C(C_p), B(Phase changes)

$C_{16}H_{25}NO_2$ (c) 71PRI
Nonyl N-phenylcarbamate
Heat Capacity 298.15 K, C_p=471.1 J·mol^{-1}·K^{-1}
Temperature range 200 to 390 K. Complete data deposited in VINITI, No. 2713-71, 25 March 1971.
Phase Changes
c/liq 327 K, ΔH=28054 J·mol^{-1}
ΔS=85.8 J·mol^{-1}·K^{-1}
Molecular Weight 263.3790
Wiswesser Line Notation 9OVMR
Evaluation B

$C_{16}H_{26}$ (liq) 63GUD/CAM
1-Cyclohexyl-3-methylhydroindan
Heat Capacity 313 K, C_p=400.7 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 218.3814
Wiswesser Line Notation L56TJ B1 D- AL6TJ
Evaluation C

$C_{16}H_{27}N$ (c) 91ASA/SOR
trans,trans-4′-Propylbicyclohexyl-4-carbonitrile
Heat Capacity 298.15 K, C_p=349.77 J·mol^{-1}·K^{-1}
Temperature range 5 to 380 K.
Entropy 298.15 K, S=355.407 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 330.73 K, ΔH=27000 J·mol^{-1}
ΔS=81.7 J·mol^{-1}·K^{-1}
Crystal to nematic liquid.
liq/liq 353.80 K, ΔH=1800 J·mol^{-1}
ΔS=5.0 J·mol^{-1}·K^{-1}
Nematic to isotropic liquid.
Molecular Weight 234.1906
Wiswesser Line Notation L6TJ DCN A- -L6TJ D3
Evaluation A
The metastable phase exhibits the phase sequence I to N to S(I) to S(II) to C on cooling. ΔH(329.62, S(I) to N)=5400 J·mol^{-1}; ΔS=16.4 J·mol^{-1}·K^{-1}.

$C_{16}H_{28}$ (liq) 63GUD/CAM
2-Ethylperhydrophenanthrene
Heat Capacity 313 K, C_p=402.9 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 220.3972
Wiswesser Line Notation L B666 TJ E2
Evaluation C

$C_{16}H_{28}BrN$ (c) 89VAN/WHI
10-Phenyldecylammonium bromide
Phase Changes
c,III/c,II 323 K, ΔH=14200 J·mol^{-1}
ΔS=5.3 J·mol^{-1}·K^{-1}
c,II/c,I 369 K, ΔH=16000 J·mol^{-1}
ΔS=5.2 J·mol^{-1}·K^{-1}
Molecular Weight 314.3079
Wiswesser Line Notation Z10R &EH
Evaluation A

$C_{16}H_{28}ClN$ (c) 89VAN/WHI
10-Phenyldecylammonium chloride
Phase Changes
c,III/c,II 357 K, ΔH=17700 J·mol^{-1}
ΔS=6.0 J·mol^{-1}·K^{-1}
c,II/c,I 368 K, ΔH=7200 J·mol^{-1}
ΔS=2.4 J·mol^{-1}·K^{-1}
Molecular Weight 269.8569
Wiswesser Line Notation Z10R &GH
Evaluation A

$(C_{16}H_{28}O_8)_n$ (liq) 83SAN/CIO
Diethylene glycol-trimethylolpropane-adipate polymer
Heat Capacity 298.15 K, C_p=659 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K. C_p(kJ·kg^{-1}·K^{-1}) =0.016882T−3.143.
Molecular Weight 348.3924
Wiswesser Line Notation /*O2O2OV4VO1X2&1Q&1O*/
Evaluation D
Authors did not provide formula for repeating unit of polymer; we have assumed: diethylene glycol-adipate-trimethylolpropane, as repeating unit.

$C_{16}H_{30}$ (liq) 63GUD/CAM
Cyclohexyl(isopropylcyclohexyl)methane
Heat Capacity 313 K, C_p=428.9 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 222.4130
Wiswesser Line Notation L6TJ A1- AL6TJ XY1&1
Evaluation C

$C_{16}H_{30}$ (liq) 63GUD/CAM
1,3-Dicyclohexylbutane
Heat Capacity 313 K, C_p=359.4 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 222.4130
Wiswesser Line Notation L6TJ AY1&2- AL6TJ
Evaluation C

$C_{16}H_{30}Br_2N_2$ (c,II) 74BUR/VER
1,2-Bis(methyldiallylammonium)ethane dibromide
Heat Capacity 298 K, C_p=465.3 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
Phase Changes
c,II/c,I 371 K, ΔH=3010 J·mol^{-1}
ΔS=8.1 J·mol^{-1}·K^{-1}
Temperature range 370 to 372 K.
Molecular Weight 410.2344
Wiswesser Line Notation 1U2K1&2U1&2K1&2U1&2U1 E2
Evaluation B

$C_{16}H_{30}HgO_4$ (liq) 78ADE
Mercuric octanoate; Mercuric caprylate
Heat Capacity 410 K, C_p=635.5 J·mol^{-1}·K^{-1}
Temperature range 420 to 425 K. Mean value. Data graphically only for solid.
Phase Changes
c/liq 387.2 K, ΔH=61500 J·mol^{-1}
ΔS=158.8 J·mol^{-1}·K^{-1}
Molecular Weight 487.0006
Wiswesser Line Notation OV7 2 .HG
Evaluation C

$C_{16}H_{30}O_4Pb$ (c) 76ADE/SIM
Lead(II) n-octanoate
Phase Changes
c/liq 352.5 K, ΔH=30000 J·mol^{-1}
ΔS=89 J·mol^{-1}·K^{-1}
Crystal-smectic.
liq/liq 356.2 K, ΔH=7900 J·mol^{-1}
ΔS=24.7 J·mol^{-1}·K^{-1}
Smectic-isomorphous.
liq/liq 381.2 K, ΔH=1200 J·mol^{-1}
ΔS=3.1 J·mol^{-1}·K^{-1}
Isomorphous-liquid.
Molecular Weight 493.6106
Wiswesser Line Notation OV7 2 .PB
Evaluation B

$C_{16}H_{30}O_4Zn$ (c) 78KON/RUF
Zinc(II) n-octanoate
Phase Changes
c,III/c,II 373 K, ΔH=1400 J·mol^{-1}
c,II/c,I 379 K, ΔH=9200 J·mol^{-1}
c,I/liq 413 K, ΔH=43000 J·mol^{-1}
ΔS=104 J·mol^{-1}·K^{-1}
Molecular Weight 351.7906
Wiswesser Line Notation OV7 2 .ZN
Evaluation B

$C_{16}H_{31}NaO_2$ (c) 59WIR/DRO
δ-Sodium palmitate
Heat Capacity 298.15 K, C_p=449.4 J·mol^{-1}·K^{-1}
Temperature range 58 to 298 K.
Entropy 298.15 K, S=474.5 J·mol^{-1}·K^{-1}
Extrapolation below 50 K, 55.19 J·mol^{-1}·K^{-1}.
Molecular Weight 278.4095
Wiswesser Line Notation OV15 .NA
Evaluation B
Sample with 0.12 mol H_2O. Correction of 5.0 J·mol^{-1}·K^{-1} for H_2O gives S=469.4 J·mol^{-1}·K^{-1} for anhydrous salt.

$C_{16}H_{31}NaO_2$ (c) 59WIR/DRC
ω-Sodium palmitate
Heat Capacity 298.15 K, C_p=495.0 J·mol^{-1}·K^{-1}
Temperature range 58 to 298 K.
Entropy 298.15 K, S=476.1 J·mol^{-1}·K^{-1}
Extrapolation below 50 K, 53.76 J·mol^{-1}·K^{-1}.
Molecular Weight 278.4095
Wiswesser Line Notation OV15 .NA
Evaluation B
Sample with 0.017 mol H_2O. Correction of 0.8 J·mol^{-1}·K^{-1} for H_2O gives S=475.3 J·mol^{-1}·K^{-1} for anhydrous salt.

$C_{16}H_{31}NaO_2$·0.01H_2O (c) 59WIR/DRC
β-Sodium palmitate
Heat Capacity 298.15 K, C_p=462.8 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=472.8 J·mol^{-1}·K^{-1}
Molecular Weight 278.5896
Wiswesser Line Notation OV15 .NA &QH 0.01
Evaluation A

$C_{16}H_{31}NaO_2$·0.409H_2O (c) 59WIR/DRC
β-Sodium palmitate
Heat Capacity 298.15 K, C_p=481.2 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=499.2 J·mol^{-1}·K^{-1}
Molecular Weight 285.7777
Wiswesser Line Notation OV15 .NA &QH 0.409
Evaluation A

$C_{16}H_{31}NaO_2$·0.482H_2O (c) 59WIR/DRO
ϵ-Sodium palmitate
Heat Capacity 298.15 K, C_p=476.6 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 298.15 K, S=500.8 J·mol^{-1}·K^{-1}
Extrapolation below 50 K, 58.12 J·mol^{-1}·K^{-1}.
Molecular Weight 287.0928
Wiswesser Line Notation OV15 .NA &QH 0.482
Evaluation A

$C_{16}H_{31}NaO_2$·0.715H_2O (c) 59WIR/DRO
ϵ-Sodium palmitate
Heat Capacity 298.15 K, C_p=501.7 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=518.4 J·mol^{-1}·K^{-1}
Molecular Weight 291.2904
Wiswesser Line Notation OV15 .NA &QH 0.715
Evaluation A

$C_{16}H_{31}O_2Tl$ (c) 76MEI/SEY
Thallium hexadecanoate
Phase Changes
liq/liq 450 K, ΔH=1381 J·mol^{-1}
ΔS=3.05 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
c,II/c,I 327 K, ΔH=10878 J·mol^{-1}
ΔS=33.5 J·mol^{-1}·K^{-1}
c,I/liq 390 K, ΔH=8786 J·mol^{-1}
ΔS=22.2 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 459.7897
Wiswesser Line Notation OV15 .TL
Evaluation B

$C_{16}H_{32}$ (liq) 57MCC/FIN2
1-Hexadecene
Heat Capacity 298.15 K, C_p=488.88 J·mol^{-1}·K^{-1}
Temperature range 11 to 360 K.
Entropy 298.15 K, S=587.90 J·mol^{-1}·K^{-1}
Does not include S_0.
Phase Changes
c/liq 277.51 K, ΔH=30192 J·mol^{-1}
ΔS=108.80 J·mol^{-1}·K^{-1}
Molecular Weight 224.4288
Wiswesser Line Notation 15U1
Evaluation A

$C_{16}H_{32}$ (liq) 90MES/TOD
1-Hexadecene
Heat Capacity 298.15 K, C_p=485.83 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S=613.88 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 217.7 K, ΔH=0.0 J·mol^{-1}
c,II/c,I 249.2 K, ΔH=3869.57 J·mol^{-1}
ΔS=15.53 J·mol^{-1}·K^{-1}
c,I/liq 277.396 K, ΔH=30099.36 J·mol^{-1}
ΔS=108.51 J·mol^{-1}·K^{-1}
Molecular Weight 224.4288
Wiswesser Line Notation 15U1
Evaluation A

$C_{16}H_{32}$ (liq) 65FIN/MES
n-Decylcyclohexane
Heat Capacity 298.15 K, C_p=452.25 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S=540.15 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 271.43 K, ΔH=38597 J·mol^{-1}
ΔS=142.20 J·mol^{-1}·K^{-1}
Molecular Weight 224.4288
Wiswesser Line Notation L6TJ A10
Evaluation A

$C_{16}H_{32}O_2$ (c) 25PAR/KEL
Hexadecanoic acid; Palmitic acid
Heat Capacity 292.5 K, C_p=462.3 J·mol^{-1}·K^{-1}
Temperature range 88 to 293 K. Value is unsmoothed experimental datum.
Entropy 298.1 K, S=543.5 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 214.2 J·mol^{-1}·K^{-1}.
Molecular Weight 256.4276
Wiswesser Line Notation QV15
Evaluation B(C_p),C(S)

$C_{16}H_{32}O_2$ (c) 29PAR/KEL
Hexadecanoic acid; Palmitic acid
Entropy 298.1 K, S=475.7 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 146.4 J·mol^{-1}·K^{-1}. Revision of previous data.
Molecular Weight 256.4276
Wiswesser Line Notation QV15
Evaluation C

$C_{16}H_{32}O_2$ (c) 52WAR/SIN
Hexadecanoic acid; Palmitic acid
Heat Capacity 298 K, C_p=448 J·mol^{-1}·K^{-1}
Temperature range 183 to 365 K. Three temperatures, each for solid and liquid and equations. C form.
Entropy 298.6 K, S=438.65 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 106.7 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 335.73 K, ΔH=54894 J·mol^{-1}
ΔS=163.5 J·mol^{-1}·K^{-1}
Molecular Weight 256.4276
Wiswesser Line Notation QV15
Evaluation 1CB(C_p),C(S)

$C_{16}H_{32}O_2$ (c) 56WIR/DRO
Hexadecanoic acid; Palmitic acid
Heat Capacity 298.15 K, C_p=460.66 J·mol^{-1}·K^{-1}
Temperature range 15 to 302 K.
Entropy 298.15 K, S=452.37 J·mol^{-1}·K^{-1}
Molecular Weight 256.4276
Wiswesser Line Notation QV15
Evaluation A

$C_{16}H_{32}O_2$ (c) 67PAC
Hexadecanoic acid; Palmitic acid
Heat Capacity 373 K, C_p=678 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 336 K, ΔH=54935 J·mol^{-1}
ΔS=163.5 J·mol^{-1}·K^{-1}
Molecular Weight 256.4276
Wiswesser Line Notation QV15
Evaluation C

$C_{16}H_{32}O_2$ (c) 82SCH/MIL2
Hexadecanoic acid; Palmitic acid
Heat Capacity 298.15 K, C_p=463.36 J·mol^{-1}·K^{-1}
Temperature range 80 to 345 K.
Phase Changes
c,I/liq 335.66 K, ΔH=53711 J·mol^{-1}
ΔS=160.02 J·mol^{-1}·K^{-1}
Molecular Weight 256.4276
Wiswesser Line Notation QV15
Evaluation B

$C_{16}H_{34}$ (liq) 88COS/HUU
2,2,4,4,6,8,8-Heptamethylnonane
Heat Capacity 298.15 K, C_p=458.80 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 1X1&1&1X1&1&1Y1&1X1&1&1
Evaluation B

$C_{16}H_{34}$ (liq) 88PER/AIC
2,2,4,4,6,8,8-Heptamethylnonane
Heat Capacity 298.15 K, C_p=458.80 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 1X1&1&1X1&1&1Y1&1X1&1&1
Evaluation A

$C_{16}H_{34}$ (liq) 49PAR/MOO
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=504.2 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.15 K, S=626.8 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 116.6 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 291.1 K, ΔH=51543 J·mol^{-1}
ΔS=177.1 J·mol^{-1}·K^{-1}
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B(C_p),C(S)

$C_{16}H_{34}$ (liq) 54FIN/GRO2
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=501.45 J·mol^{-1}·K^{-1}
Temperature range 12 to 320 K.
Entropy 298.15 K, S=586.18 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 291.34 K, ΔH=53359 J·mol^{-1}
ΔS=183.15 J·mol^{-1}·K^{-1}
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation A

$C_{16}H_{34}$ (liq) 62GOL/BEL
n-Hexadecane; Cetane
Heat Capacity 311 K, C_p=484.9 J·mol^{-1}·K^{-1}
Temperature range 100, 200, 300 °F.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation C

$C_{16}H_{34}$ (liq) 73KAL/WOY
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=504.58 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation A

$C_{16}H_{34}$ (liq) 74DIA/REN
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=501.6 J·mol^{-1}·K^{-1}
Temperature range 300 to 324 K.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation A

$C_{16}H_{34}$ (liq) 74PET/TER
n-Hexadecane; Cetane
Heat Capacity 297.79 K, C_p=499 J·mol^{-1}·K^{-1}
Temperature range 297 to 471 K. Value is unsmoothed experimental datum.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 81GRO/ING
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=499.97 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 82ZAF
n-Hexadecane; Cetane
Heat Capacity 298 K, C_p=498.3 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 85LAI/ROU
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=496.45 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 86TAR/AIC
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=499.62 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 86WIL/LAI
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=495.73 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 88AND/PAT
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=499.62 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 88COS/HUU
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=500.21 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 88PER/AIC
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=500.21 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 89LAI/ROL
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=497.16 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation A

$C_{16}H_{34}$ (liq) 91BAN/GAR
n-Hexadecane; Cetane
Heat Capacity 313.15 K, C_p=512.37 J·mol^{-1}·K^{-1}
Temperature range 313 to 373 K. p=0.1 MPa.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 91CLA/LET
n-Hexadecane; Cetane
Phase Changes
c/liq 292.1 K, ΔH=47545 J·mol^{-1}
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation A

$C_{16}H_{34}$ (liq) 91TRE/COS
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p=499.72 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}O$ (c) 1889EYK
n-Cetyl alcohol; 1-Hexadecanol
Phase Changes
c/liq 320 K, ΔH=34727 J·mol^{-1}
ΔS=108.5 J·mol^{-1}·K^{-1}
Molecular Weight 242.4440
Wiswesser Line Notation Q16
Evaluation C

$C_{16}H_{34}O$ (c) 56PAR/KEN
n-Cetyl alcohol; 1-Hexadecanol
Heat Capacity 290 K, C_p=441.24 J·mol^{-1}·K^{-1}
Temperature range 80 to 290 K.
Entropy 298.1 K, S=451.9 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 115.3 J·mol^{-1}·K^{-1}.
Molecular Weight 242.4440
Wiswesser Line Notation Q16
Evaluation B(C_p),C(S)

$C_{16}H_{34}O$ (c) 74MOS/MOU
n-Cetyl alcohol; 1-Hexadecanol
Heat Capacity 298.15 K, C_p=422 J·mol^{-1}·K^{-1}
Temperature range 293 to 311 K.
Phase Changes
c,γ/c,α 322.2 K, ΔH=23700 J·mol^{-1}
ΔS=73.6 J·mol^{-1}·K^{-1}
c,γ/liq 322.2 K, ΔH=58380 J·mol^{-1}
ΔS=181.2 J·mol^{-1}·K^{-1}
c,α/liq 322.3 K, ΔH=33600 J·mol^{-1}
ΔS=104.3 J·mol^{-1}·K^{-1}
Molecular Weight 242.4440
Wiswesser Line Notation Q16
Evaluation B

$C_{16}H_{34}O$ (liq) 74MOS/MOU
n-Cetyl alcohol; 1-Hexadecanol
Heat Capacity 323 K, C_p=524 J·mol^{-1}·K^{-1}
Temperature range 323 to 346 K.
Molecular Weight 242.4440
Wiswesser Line Notation Q16
Evaluation B

$C_{16}H_{34}O$ (c) 88PET/TSY
n-Cetyl alcohol; 1-Hexadecanol
Phase Changes
c,III/c,II 308.9 K, ΔH=12500 J·mol^{-1}
ΔS=40.4 J·mol^{-1}·K^{-1}
c,II/c,I 310.4 K, ΔH=5200 J·mol^{-1}
ΔS=16.8 J·mol^{-1}·K^{-1}
Molecular Weight 242.4440
Wiswesser Line Notation Q16
Evaluation A

$C_{16}H_{34}O$ (liq) 89KHA/ZYK
n-Cetyl alcohol; 1-Hexadecanol
Heat Capacity 333.15 K, C_p=618.2 J·mol^{-1}·K^{-1}
Temperature range 333 to 583 K.
Molecular Weight 242.4440
Wiswesser Line Notation Q16
Evaluation B

$C_{16}H_{34}S$ (liq) 82TUT/GAB
1-Hexadecanethiol; n-Hexadecyl mercaptan
Heat Capacity 300 K, C_p=574.22 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K. C_p=553.16+4.153×10^{-2}T +9.560×10^{-5}T^2.
Molecular Weight 258.5046
Wiswesser Line Notation SH16
Evaluation B

$C_{16}H_{35}N$ (liq) 87MIL/FEN
N,N-Dimethyl-2-pentylnonylamine
Heat Capacity 323.15 K, C_p=537.98 J·mol^{-1}·K^{-1}
Temperature range 323.15 to 423.15 K.
Molecular Weight 241.4592
Wiswesser Line Notation 7Y5&1N1&1
Evaluation A

$C_{16}H_{35}N$ (liq) 93STE/CHI2
Di-n-octylamine
Heat Capacity 298.15 K, C_p=507.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 241.4592
Wiswesser Line Notation 8M8
Evaluation A

$C_{16}H_{36}BrN$ (c) 73VIS/SOM
Tetra-n-butylammonium bromide
Heat Capacity 298.15 K, C_p=412 J·mol^{-1}·K^{-1}
Temperature range 278 to 328 K.
Molecular Weight 322.3711
Wiswesser Line Notation 4K4&4&4 E
Evaluation B

$C_{16}H_{36}BrN$ (c,III) 74BUR/VER
Tetra-n-butylammonium bromide
Heat Capacity 298 K, C_p=447.8 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
Phase Changes
c,IV/c,III 293 K, ΔH=67 J·mol^{-1}
ΔS=0.2 J·mol^{-1}·K^{-1}
Temperature range 293 to 295 K. ΔH maximum value.
c,III/c,II 367 K, ΔH=1630 J·mol^{-1}
ΔS=4.4 J·mol^{-1}·K^{-1}
Temperature range 366.0 to 369 K.
c,II/c,I 383 K, ΔH=335 J·mol^{-1}
ΔS=0.9 J·mol^{-1}·K^{-1}
Temperature range 382 to 383.5 K.
c/liq 395 K, ΔH=16150 J·mol^{-1}
ΔS=40.89 J·mol^{-1}·K^{-1}
Molecular Weight 322.3711
Wiswesser Line Notation 4K4&4&4 E
Evaluation B

$C_{16}H_{36}ClN$ (c) 88VAN/WHI
Di-n-octylammonium chloride
Heat Capacity 298.24 K, C_p=550.2 J·mol^{-1}·K^{-1}
Temperature range 25 to 350 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 297.70 K, ΔH=33610 J·mol^{-1}
ΔS=112.97 J·mol^{-1}·K^{-1}
Molecular Weight 277.9201
Wiswesser Line Notation 8M8 &GH
Evaluation A

$C_{16}H_{36}N_4$ (c) 87KUL/KIP
cis-(5,12)-7,7,14,14-Hexamethyl-1,4,8,11-tetraazacyclotetradecane
Heat Capacity 298.15 K, C_p=444.9 J·mol^{-1}·K^{-1}
Temperature range 0 to 330 K.
Entropy 298.15 K, S=443.1 J·mol^{-1}·K^{-1}
Molecular Weight 284.4872
Wiswesser Line Notation L14N DN HN KNTJ E1 G1 G1 L1 N1 N1
Evaluation A

$C_{16}H_{36}O_4Si$ (liq) 85NKI/CHA
Tetrabutyl silicate; Butyl silicate
Heat Capacity 298.15 K, C_p=580.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 320.5435
Wiswesser Line Notation 4O-SI-O4&O4&O4
Evaluation B

$C_{16}H_{36}O_4Ti$ (liq) 79SAM/GRI
Tetrabutoxytitanium
Heat Capacity 353 K, C_p=711 J·mol^{-1}·K^{-1}
Temperature range 333 to 453 K.
Molecular Weight 340.3580
Wiswesser Line Notation 4O-TI-O4&O4&O4
Evaluation C

$C_{16}H_{38}Br_2N_2$ (c,II) 74BUR/VER
1,4-Bis(triethylammonium)butane dibromide
Heat Capacity 298 K, C_p=462.3 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
Phase Changes
c,II/c,I 518 K, ΔH=50200 J·mol^{-1}
ΔS=96.9 J·mol^{-1}·K^{-1}
Temperature range 503 to 530 K.
Molecular Weight 418.2976
Wiswesser Line Notation 2K2&2&4K2&2&2 E 2
Evaluation B

$C_{16}H_{40}CdCl_4N_2$ (c) 85RIC/CA
Bis-octylammonium tetrachlorocadmium
Phase Changes
c,III/c,II 269 K, ΔH=14500 J·mol^{-1}
ΔS=54 J·mol^{-1}·K^{-1}
c,II/c,I 308 K, ΔH=5100 J·mol^{-1}
ΔS=16.7 J·mol^{-1}·K^{-1}
Molecular Weight 514.7274
Wiswesser Line Notation -8-ZH 2 .CD G4
Evaluation B

$C_{16}H_{40}Cl_4N_2Ni$ (c,I) 79LAN/WE
Bis-(tetraethylammonium) tetrachloronickelate
Heat Capacity 298.15 K, C_p=634.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=775.42 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,I 222.4 K, ΔH=8732 J·mol^{-1}
ΔS=38.32 J·mol^{-1}·K^{-1}
Two transitions, c,III/c,II at 222.1 K and c,II/c,I at 222.7 K. ΔH an
ΔS are the sum of the two transitions.
Molecular Weight 461.0174
Wiswesser Line Notation 2K2&2&2 2 NI G4
Evaluation A

$C_{16}H_{40}Cl_4N_2Zn$ (c,I) 79LAN/WE
Bis-(tetraethylammonium) tetrachlorozincate
Heat Capacity 298.15 K, C_p=640.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S=759.48 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,I 228.4 K, ΔH=9556 J·mol^{-1}
ΔS=41.67 J·mol^{-1}·K^{-1}
Two transitions, c,III/c,II at 227.9 K and c,II/c,I at 228.9 K. ΔH an
ΔS are the sum of the two transitions.
Molecular Weight 467.6974
Wiswesser Line Notation 2K2&2&2 2 ZN G4
Evaluation A

$C_{16}H_{40}D_4Si_4$ (liq) 87DZH/KU
Octaethylcyclotetrasiloxane
Heat Capacity 298.15 K, C_p=746.8 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=909.3 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 134 K
c,II/c,I 208.16 K, ΔH=12219 J·mol^{-1}
ΔS=58.69 J·mol^{-1}·K^{-1}
c,I/liq 213.35 K, ΔH=13705 J·mol^{-1}
ΔS=64.38 J·mol^{-1}·K^{-1}
Molecular Weight 352.8972
Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI- OTJ A2 A2 C2 C2 E
E2 G2 G2
Evaluation A

$C_{17}H_6O_7$ (c) 73KAR/MO
Bis-(3-phthalyl anhydride) ketone
Heat Capacity 300 K, C_p=318.7 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S=350.2 J·mol^{-1}·K^{-1}
Molecular Weight 322.2302
Wiswesser Line Notation T56 BVOVJ GV- GT56 BVOVJ
Evaluation A

$C_{17}H_{12}$ (c) 79FAR/SHA
1,2-Benzofluorene
Phase Changes
c,II/c,I 399.9 K, $\Delta H = 3800\ J \cdot mol^{-1}$
c/liq 462.8 K, $\Delta H = 18400\ J \cdot mol^{-1}$
$\Delta S = 39.7\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 216.2818
Wiswesser Line Notation L D6 B566 CHJ
Evaluation B

$C_{17}H_{12}$ (c) 79FAR/SHA
2,3-Benzofluorene
Phase Changes
c/liq 489.7 K, $\Delta H = 23400\ J \cdot mol^{-1}$
$\Delta S = 47.8\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 216.2818
Wiswesser Line Notation L D6 B656 LHJ
Evaluation B

$C_{17}H_{14}FeO$ (c) 81TOM/CUR
Benzoylferrocene
Heat Capacity 298 K, $C_p = 387.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 293 to 363 K. Equation given.
Phase Changes
c/liq 384.2 K
Molecular Weight 290.1440
Wiswesser Line Notation L5ϕJ ϕ-FE- -ϕL5ϕJ AVR
Evaluation B

$C_{17}H_{14}N_2O_2$ (c) 75LEB/ARO
2,2-Bis-(4-cyanatophenyl)propane
Heat Capacity 298.15 K, $C_p = 355.64\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 0 to 420 K.
Entropy 298.15 K, $S = 391.2\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c/liq 355.83 K, $\Delta H = 26694\ J \cdot mol^{-1}$
$\Delta S = 74.89\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 278.3098
Wiswesser Line Notation ONCR DX1&1&R DCNO
Evaluation A

$C_{17}H_{14}N_2O_2$ (c) 77LEB/RAB4
2,2-Bis-(4-cyanatophenyl)propane
Heat Capacity 300 K, $C_p = 360\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 13 to 400 K. Data given graphically. Value estimated from graph.
Phase Changes
c/liq 355.8 K, $\Delta H = 26700\ J \cdot mol^{-1}$
$\Delta S = 74.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 278.3078
Wiswesser Line Notation ONCR DX1&1&R DCNO
Evaluation C(C_p); A(Phase changes)

$(C_{17}H_{14}N_2O_2)_n$ (amorph) 75LEB/ARO
Poly[2,2-bis-(4-phenoxypropane)] 2,4,6-triazine; Polycyanate
Heat Capacity 298.15 K, $C_p = 326.8\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 0 to 420 K.
Entropy 298.15 K, $S = 325.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 278.3098
Wiswesser Line Notation T6N CN ENJ BOR& DX1&1&RO* DOR& DX1&1&RO* EOR& DX1&1&RO*/ 1/3
Evaluation A

$C_{17}H_{20}Cl_2N_2S$ (c) 83CHA/MAS
Chlorpromazine hydrochloride;
2-Chloro-9-(3-dimethylaminopropyl)-10-phenothiazine hydrochloride
Phase Changes
c/liq 467.2 K, $\Delta H = 28420\ J \cdot mol^{-1}$
$\Delta S = 60.8\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 355.3305
Wiswesser Line Notation T C666 BN ISJ B3N1&1 FG &GH
Evaluation C
(Pre-melting began at 461.7 K).

$C_{17}H_{30}$ (liq) 62GOL/BEL
Cyclopentylbicyclohexyl
Heat Capacity 311 K, $C_p = 430.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 100, 200, 300 °F.
Molecular Weight 234.4240
Wiswesser Line Notation L6TJ A- AL6TJ X- AL5TJ
Evaluation C

$C_{17}H_{30}$ (liq) 63GUD/CAM
Cyclopentylbicyclohexyl
Heat Capacity 313 K, $C_p = 433.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 483 K.
Molecular Weight 234.4240
Wiswesser Line Notation L6TJ A- AL6TJ X- AL5TJ
Evaluation C

$C_{17}H_{32}$ (liq) 63GUD/CAM
Bis(ethylcyclohexyl)methane
Heat Capacity 313 K, $C_p = 466.1\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 483 K.
Molecular Weight 236.4398
Wiswesser Line Notation L6TJ A2 X1- AL6TJ X2
Evaluation C

$C_{17}H_{32}$ (liq) 63GUD/CAM
1-Cyclohexyl-1-isopropylcyclohexylethane
Heat Capacity 313 K, $C_p = 439.3\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 583 K.
Molecular Weight 236.4398
Wiswesser Line Notation L6TJ AY1&- AL6TJ XY1&1
Evaluation C

$C_{17}H_{34}O_2$ (c) 36KIN/GAR
Methyl hexadecanoate; Methyl palmitate
Phase Changes
c/liq 302.2 K, $\Delta H = 14971\ J \cdot mol^{-1}$
Molecular Weight 270.4544
Wiswesser Line Notation 15VO1
Evaluation B

$C_{17}H_{34}O_2$ (c) 56WIR/DRO
Methyl hexadecanoate; Methyl palmitate
Heat Capacity 298.15 K, $C_p = 474.47\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 15 to 297 K.
Entropy 298.15 K, $S = 495.09\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 270.4544
Wiswesser Line Notation 15VO1
Evaluation A

$C_{17}H_{34}O_2$ (c) 82SCH/MIL
Heptadecanoic acid
Heat Capacity 298.15 K, C_p=475.74 J·mol^{-1}·K^{-1}
Temperature range 80 to 350 K.
Phase Changes
c,II/c,I 329.2 K, ΔH=7435 J·mol^{-1}
ΔS=22.59 J·mol^{-1}·K^{-1}
c,I/liq 334.25 K, ΔH=51342 J·mol^{-1}
ΔS=153.60 J·mol^{-1}·K^{-1}
Molecular Weight 270.4544
Wiswesser Line Notation QV16
Evaluation A

$C_{17}H_{34}O_4$ (c) 65SIL/DAU
2-Monomyristin
Heat Capacity 298 K, C_p=506.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 302.4532
Wiswesser Line Notation Q1Y1QOV13
Evaluation B

$C_{17}H_{34}O_4$ (c) 65SIL/DAU
1-Monomyristin
Heat Capacity 298 K, C_p=520.1 J·mol^{-1}·K^{-1}
One temperature. β_L form.
Molecular Weight 302.4532
Wiswesser Line Notation Q1YQ1OV13
Evaluation B

$C_{17}H_{36}$ (liq) 55SCH/BUS
n-Heptadecane
Phase Changes
c,II/c,I 283.65 K
c,I/liq 294.85 K
Molecular Weight 240.4714
Wiswesser Line Notation 17H
Evaluation B

$C_{17}H_{36}$ (liq) 67MES/GUT
n-Heptadecane
Heat Capacity 298.15 K, C_p=534.34 J·mol^{-1}·K^{-1}
Temperature range 12 to 380 K.
Entropy 298.15 K, S=652.24 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 284.27 K, ΔH=10942 J·mol^{-1}
ΔS=38.50 J·mol^{-1}·K^{-1}
c,I/liq 295.14 K, ΔH=40164 J·mol^{-1}
ΔS=136.08 J·mol^{-1}·K^{-1}
Molecular Weight 240.4714
Wiswesser Line Notation 17H
Evaluation A

$C_{17}H_{36}O$ (liq) 89KHA/ZYK
1-Heptadecanol; n-Heptadecyl alcohol
Heat Capacity 333.15 K, C_p=649.6 J·mol^{-1}·K^{-1}
Temperature range 333 to 583 K.
Molecular Weight 256.4708
Wiswesser Line Notation Q17
Evaluation B

$C_{17}H_{40}Br_2N_2$ (c,II) 74BUR/VEI
1,5-Bis(triethylammonium)pentane dibromide
Heat Capacity 298 K, C_p=493.7 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
Phase Changes
c,II/c,I 465 K, ΔH=24480 J·mol^{-1}
ΔS=52.6 J·mol^{-1}·K^{-1}
Temperature range 458 to 471 K.
Molecular Weight 432.3244
Wiswesser Line Notation 2K2&2&5K2&2&2 E 2
Evaluation B

$C_{18}D_{14}$ (c,I) 79CAI/DW(
p-Terphenyl-d_{14}
Phase Changes
c,II/c,I 178.8 K, ΔH=193 J·mol^{-1}
ΔS=1.08 J·mol^{-1}·K^{-1}
Molecular Weight 244.3954
Wiswesser Line Notation RR DR &1B-F/2BCEF/5B-F/H-2 14
Evaluation C

$C_{18}D_{14}$ (c,I) 88SAI/ATA
p-Terphenyl-d_{14}
Heat Capacity 298.15 K, C_p=319.66 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S=315.23 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 180.3 K, ΔH=288 J·mol^{-1}
ΔS=1.63 J·mol^{-1}·K^{-1}
Lambda-type transition.
Molecular Weight 244.3954
Wiswesser Line Notation RR DR &1B-F/2BCEF/5B-F/H-2 14
Evaluation A

$C_{18}H_{11}N_3O_7$ (c) 79FAR/SH
Acenaphthene picric acid
Phase Changes
c/liq 436.3 K, ΔH=36000 J·mol^{-1}
ΔS=82.5 J·mol^{-1}·K^{-1}
Molecular Weight 381.3008
Wiswesser Line Notation L566 1A LT&&J &WNR BQ CNW ENW
Evaluation B

$C_{18}H_{12}$ (c) 50UEB/OR
Benzanthrene
Heat Capacity 298.15 K, C_p=273.6 J·mol^{-1}·K^{-1}
Temperature range 293 to 368 K. Equation only.
Molecular Weight 228.2928
Wiswesser Line Notation L C6666 1A Q IHJ
Evaluation C

$C_{18}H_{12}$ (c) 71WON/WE
Triphenylene; 9,10-Benzophenanthrene
Heat Capacity 298.15 K, C_p=259.20 J·mol^{-1}·K^{-1}
Temperature range 5 to 514 K.
Entropy 298.15 K, S=254.68 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 471.01 K, ΔH=24744 J·mol^{-1}
ΔS=52.53 J·mol^{-1}·K^{-1}
Molecular Weight 228.2928
Wiswesser Line Notation L B6 H666J
Evaluation A

$C_{18}H_{12}$ (c) 80WON/WES

Naphthacene

Heat Capacity 298.15 K, C_p=236.6 J·mol^{-1}·K^{-1}

Temperature range 5 to 350 K.

Entropy 298.15 K, S=215.4 J·mol^{-1}·K^{-1}

Molecular Weight 228.2928

Wiswesser Line Notation L C6666J

Evaluation A

$C_{18}H_{12}$ (c) 92SAB/ELW3

Triphenylene; 9,10-Benzophenanthrene

Phase Changes

c/liq 471.06 K, ΔH=24190 J·mol^{-1}

Molecular Weight 228.2928

Wiswesser Line Notation L B6 H666J

Evaluation A

$C_{18}H_{12}N_4O_6$ (c) 80RAD/RAD

Carbazole-1,3,5-trinitrobenzene adduct

Heat Capacity 298.15 K, C_p=404.8 J·mol^{-1}·K^{-1}

Temperature range 180 to 430 K. Data given graphically. C_p calculated from equation.

Phase Changes

c,I/liq 477.5 K, ΔH=43702 J·mol^{-1}

ΔS=91.52 J·mol^{-1}·K^{-1}

Molecular Weight 380.3160

Wiswesser Line Notation T B656 HMJ &WNR CNW ENW

Evaluation B

$C_{18}H_{14}$ (c) 72CHA/BES

o-Terphenyl

Heat Capacity 298.15 K, C_p=274.75 J·mol^{-1}·K^{-1}

Temperature range 2 to 350 K. Also data for annealed and quenched glass.

Entropy 298.15 K, S=298.81 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 329.35 K, ΔH=17192 J·mol^{-1}

ΔS=52.20 J·mol^{-1}·K^{-1}

Molecular Weight 230.3086

Wiswesser Line Notation RR BR

Evaluation A

$C_{18}H_{14}$ (liq) 72CHA/BES

o-Terphenyl

Heat Capacity 298.15 K, C_p=369.05 J·mol^{-1}·K^{-1}

Temperature range 250 to 360 K. Supercooled liquid below Tm 329.35 K.

Entropy 298.15 K, S=337.11 J·mol^{-1}·K^{-1}

Molecular Weight 230.3086

Wiswesser Line Notation RR BR

Evaluation A

$C_{18}H_{14}$ (liq) 58WAL/BRO

m-Terphenyl

Heat Capacity 370 K, C_p=417.1 J·mol^{-1}·K^{-1}

Temperature range 200 to 600 °F.

Molecular Weight 230.3086

Wiswesser Line Notation RR CR

Evaluation B

$C_{18}H_{14}$ (c,I) 79CAI/DWO

p-Terphenyl

Heat Capacity

C_p data not given.

Phase Changes

Temperature range 10 to 300 K.

c,II/c,I 193.3 K, ΔH=95 J·mol^{-1}

ΔS=0.49 J·mol^{-1}·K^{-1}

Obtained T=191.0 K, ΔS=0.45 J·mol^{-1}, from DSC data.

Molecular Weight 230.3086

Wiswesser Line Notation RR DR

Evaluation C

$C_{18}H_{14}$ (c) 79SMI

p-Terphenyl

Phase Changes

c/liq 486.3 K, ΔH=35500 J·mol^{-1}

ΔS=73.0 J·mol^{-1}·K^{-1}

Molecular Weight 230.3086

Wiswesser Line Notation RR DR

Evaluation A

$C_{18}H_{14}$ (c) 82WAS/RAD

p-Terphenyl

Heat Capacity 300 K, C_p=260 J·mol^{-1}·K^{-1}

Temperature range 180 to 500 K. Data given graphically. Value estimated from graph.

Phase Changes

c,II/c,I 400 to 493.1 K

c/liq 493.1 K, ΔH=41600 J·mol^{-1}

ΔS=84.4 J·mol^{-1}·K^{-1}

Molecular Weight 230.3086

Wiswesser Line Notation RR DR

Evaluation D(C_p), B(Phase changes)

$C_{18}H_{14}$ (c) 83CHA

p-Terphenyl

Heat Capacity 298.15 K, C_p=278.68 J·mol^{-1}·K^{-1}

Temperature range 4 to 580 K. C_p=35.12+0.58825T +0.0010062T^2−8.042×10^{-7}T^3 from 80 to 300 K.

Entropy 298.15 K, S=285.62 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 193.55 K

Lambda transition.

c/liq 487.0 K, ΔH=35300 J·mol^{-1}

ΔS=72.5 J·mol^{-1}·K^{-1}

Molecular Weight 230.3086

Wiswesser Line Notation RR DR

Evaluation A

$C_{18}H_{14}$ (c,I) 88SAI/ATA2

p-Terphenyl

Heat Capacity 298.15 K, C_p=278.12 J·mol^{-1}·K^{-1}

Temperature range 5 to 300 K.

Entropy 298.15 K, S=285.23 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 193.5 K, ΔH=304 J·mol^{-1}

ΔS=1.63 J·mol^{-1}·K^{-1}

Lambda-type transition.

Molecular Weight 230.3086

Wiswesser Line Notation RR DR

Evaluation A

$C_{18}H_{15}As$ (c) 31SMI/AND2
Triphenylarsine
Heat Capacity 298.5 K, C_p=321.3 J·mol^{-1}·K^{-1}
Temperature range 102 to 311 K. Value is unsmoothed experimental datum.
Molecular Weight 306.2381
Wiswesser Line Notation R-AS-R&R
Evaluation B

$C_{18}H_{15}Bi$ (c) 31SMI/AND2
Triphenylbismuthine; Bismuth triphenyl
Heat Capacity 298.5 K, C_p=328.4 J·mol^{-1}·K^{-1}
Temperature range 102 to 323 K.
Molecular Weight 440.2969
Wiswesser Line Notation R-BI-R&R
Evaluation B

$C_{18}H_{15}Bi$ (c) 79STE
Triphenylbismuthine; Bismuth triphenyl
Heat Capacity 298.15 K, C_p=330.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 440.2969
Wiswesser Line Notation R-BI-R&R
Evaluation B

$C_{18}H_{15}ClSi$ (c) 68KOS/MOS
Triphenylchlorosilane
Heat Capacity 298.15 K, C_p=337.6 J·mol^{-1}·K^{-1}
Temperature range 12.39 to 386.93 K
Entropy 298.15 K, S=370.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 370.6 K, ΔH=26878 J·mol^{-1}
ΔS=72.53 J·mol^{-1}·K^{-1}
Molecular Weight 294.8550
Wiswesser Line Notation G-SI-R&R&R
Evaluation A

$C_{18}H_{15}N$ (c) 31SMI/AND2
Triphenylamine
Heat Capacity 298.5 K, C_p=297.5 J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 245.3232
Wiswesser Line Notation RNR&R
Evaluation B

$C_{18}H_{15}OP$ (c) 77HAR/HEA
Triphenylphosphine oxide
Heat Capacity 298.15 K, C_p=317 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.14 J·K^{-1}·g^{-1}.
Molecular Weight 278.2897
Wiswesser Line Notation OPR&R&R
Evaluation B

$C_{18}H_{15}OP$ (c) 78JOR/AIR
Triphenylphosphine oxide
Heat Capacity 298 K, C_p=470 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 429 K, ΔH=23800 J·mol^{-1}
ΔS=95.6 J·mol^{-1}·K^{-1}
Molecular Weight 278.2897
Wiswesser Line Notation OPR&R&R
Evaluation C

$C_{18}H_{15}OP$ (c) 88KIR/DOM
Triphenylphosphine oxide
Phase Changes
c/liq 431.9 K, ΔH=24220 J·mol^{-1}
ΔS=56.08 J·mol^{-1}·K^{-1}
Molecular Weight 278.2897
Wiswesser Line Notation OPR&R&R
Evaluation A

$C_{18}H_{15}OP$ (c) 89HUL/VAN
Triphenylphosphine oxide
Heat Capacity 314 K, C_p=339 J·mol^{-1}·K^{-1}
Temperature range 339 to 459 K.
Phase Changes
c/liq 429.6 K, ΔH=23400 J·mol^{-1}
Molecular Weight 278.2897
Wiswesser Line Notation OPR&R&R
Evaluation B

$C_{18}H_{15}O_4P$ (c) 86RAB/PET
Triphenylphosphate
Heat Capacity 300 K, C_p=356.2 J·mol^{-1}·K^{-1}
Temperature range 12 to 340 K.
Entropy 300 K, S=397.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 322.55 K, ΔH=29610 J·mol^{-1}
ΔS=91.84 J·mol^{-1}·K^{-1}
Molecular Weight 326.2879
Wiswesser Line Notation RO 3PO
Evaluation A

$C_{18}H_{15}P$ (c) 31SMI/AND2
Triphenylphosphine
Heat Capacity 298.5 K, C_p=312.5 J·mol^{-1}·K^{-1}
Temperature range 102 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 262.2903
Wiswesser Line Notation RPR&R
Evaluation B

$C_{18}H_{15}P$ (c) 88KIR/DOM
Triphenylphosphine
Phase Changes
c/liq 354.4 K, ΔH=19690 J·mol^{-1}
ΔS=55.56 J·mol^{-1}·K^{-1}
Molecular Weight 262.2903
Wiswesser Line Notation RPR&R
Evaluation A

$C_{18}H_{15}Sb$ (c) 31SMI/AND2
Triphenylstilbene; Antimony triphenyl
Heat Capacity 298.5 K, C_p=325.5 J·mol^{-1}·K^{-1}
Temperature range 102 to 311 K.
Molecular Weight 353.0665
Wiswesser Line Notation R-SB-R&R
Evaluation B

$C_{18}H_{16}$ (liq) 78GOO/SCO
4bβ,4cα,9,9aα,9bβ,10-Hexahydrocyclobuta-[1,2-a:4,3-a′]diindene; syn,trans-Truxane
Heat Capacity 298.15 K, C_p=275.1 J·mol^{-1}·K^{-1}
One temperature. C_p=0.283 cal·g^{-1}.
Molecular Weight 232.3244
Wiswesser Line Notation L D6 C5 B456&TTT&J
Evaluation B

$C_{18}H_{16}$ (liq) 78GOO/SCO
4bα,4cβ,5,9bβ,9cα,10-Hexahydrocyclabuta-[1,2-a:3,4-a′]diindene; anti,trans-Truxane
Heat Capacity 298.15 K, C_p=252.7 J·mol^{-1}·K^{-1}
One temperature. C_p=0.260 cal·g^{-1}.
Molecular Weight 232.3244
Wiswesser Line Notation L E6 C5 B456&TTT&J
Evaluation B

$C_{18}H_{16}N_2O_2$ (c) 83ZAM/KAI
meso-2,3-Dimethoxy-2,3-diphenylsuccinonitrile
Heat Capacity 298.15 K, C_p=305.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 292.3366
Wiswesser Line Notation NCXO1&R&XO1&CN&R
Evaluation B

$C_{18}H_{16}O_2Si$ (c) 75LEB/MIL
Dianisyldiethynylsilane
Heat Capacity 298.15 K, C_p=402.5 J·mol^{-1}·K^{-1}
Temperature range 60 to 315 K. Data deposited in VINITI, No. 1667-75, 11 June 1975.
Entropy 298.15 K, S=446.4 J·mol^{-1}·K^{-1}
Molecular Weight 292.4087
Wiswesser Line Notation 1UU1 2-SI-1R DO1 2
Evaluation B

$C_{18}H_{18}$ (c) 44EIB
1-Methyl-7-isopropylphenanthrene; Retene
Heat Capacity 298.1 K, C_p=294.6 J·mol^{-1}·K^{-1}
Temperature range 25 to 200 °C, equations only, in t °C. C_p(c)=0.2620+0.001584t cal·g^{-1}·C^{-1} (15 to 60 °C); C_p(liq)=0.364+0.000661t cal·g^{-1}·C^{-1} (96 to 200 °C).
Phase Changes
c/liq 369.0 K, ΔH=18030 J·mol^{-1}
ΔS=48.9 J·mol^{-1}·K^{-1}
Molecular Weight 234.3402
Wiswesser Line Notation L B666J EY1&1 K1
Evaluation C

$C_{18}H_{18}$ (liq) 78GOO/SCO
2,2′-Biindanyl
Heat Capacity 298.15 K, C_p=332.4 J·mol^{-1}·K^{-1}
One temperature. C_p=0.339 cal·g^{-1}.
Molecular Weight 234.3402
Wiswesser Line Notation L56T&J C- CL56T&J
Evaluation B

$C_{18}H_{18}$ (c) 83KRA/BEC
2,3-Dimethyl-2,3-diphenylbutane
Heat Capacity 298 K, C_p=321.1 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.322 cal·K^{-1}·g^{-1}.
Molecular Weight 238.3718
Wiswesser Line Notation 1X1&R&X1&1&R
Evaluation B

$C_{18}H_{18}ClNS$ (c) 83CHA/MAS
Chlorprothixene;
2-Chloro-9-(3-dimethylamino-propylidene)-10-thioxanthene
Phase Changes
c/liq 370.3 K, ΔH=27820 J·mol^{-1}
ΔS=75.1 J·mol^{-1}·K^{-1}
Molecular Weight 315.8663
Wiswesser Line Notation T C666 BS IYT EG IU3N1&1
Evaluation C

$C_{18}H_{18}N_2O_5$ (c) 32SPA/THO
Ethyl azoxybenzenedicarboxylate
Heat Capacity 303 K, C_p=451.0 J·mol^{-1}·K^{-1}
Temperature range 30 to 150 °C.
Phase Changes
liq/liq 395.7 K, ΔH=5439 J·mol^{-1}
ΔS=13.7 J·mol^{-1}·K^{-1}
Liquid crystal-isotropic liquid transition.
c/liq 386.9 K, ΔH=20485 J·mol^{-1}
ΔS=52.9 J·mol^{-1}·K^{-1}
Crystal-liquid crystal transition.
Molecular Weight 342.3506
Wiswesser Line Notation 2OVR DNO&UNR DVO2
Evaluation B
Uncertain isomer; para assumed.

$C_{18}H_{18}O_6$·0.460CO (c) 63STE/COU
β-Quinol carbon monoxide clathrate
Heat Capacity 298.15 K, C_p=431.79 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K. Data also given for the 0.626, 0.757 and the 0.810 CO clathrates.
Molecular Weight 343.2214
Wiswesser Line Notation QR DQ 3 &CO 0.46
Evaluation A

$C_{18}H_{20}$ (c) 69SHI/MCN
3,3-Paracyclophane
Heat Capacity 300 K, C_p=324.3 J·mol^{-1}·K^{-1}
Temperatures 300, 318 K.
Molecular Weight 236.3560
Wiswesser Line Notation L G6 C-14-6 A B G- G-&T&J
Evaluation B

$C_{18}H_{20}O_2$ (c) 90WHI/ZAK
4-p-Hydroxyphenyl-2,2,4-trimethylchroman
Heat Capacity 308.19 K, C_p=354.2 J·mol^{-1}·K^{-1}
Temperature range 30 to 330 K. Unsmoothed experimental datum. Data also given for the ethanol and carbon tetrachloride adducts.
Molecular Weight 268.3548
Wiswesser Line Notation T66 BOT&J C1 C1 D1 DR DQ
Evaluation B

$C_{18}H_{21}NO$ (liq) 74SHI/MAE
N-(4-Methoxybenzylidene)-p-n-butylaniline
Heat Capacity 298.15 K, C_p=475.3 J·mol^{-1}·K^{-1}
Temperature range 2 to 330 K. Nematic liquid crystal.
Phase Changes
c,I/liq 294.45 K, ΔH=13148.6 J·mol^{-1}
ΔS=44.65 J·mol^{-1}·K^{-1}
liq=Nematic liquid crystal. c,I=metastable crystal form.
c,III/liq 295.65 K, ΔH=15937.7 J·mol^{-1}
ΔS=53.91 J·mol^{-1}·K^{-1}
liq=Nematic liquid crystal. c,III=stable crystal form.
liq/liq 320.14 K, ΔH=284.1 J·mol^{-1}
ΔS=0.89 J·mol^{-1}·K^{-1}
Nematic-isotropic liquid transition.
Molecular Weight 267.3700
Wiswesser Line Notation 4R DNU1R DO1
Evaluation A

$C_{18}H_{21}NO$ (liq) 75JAN/JAN
N-(4-Methoxybenzylidene)-p-n-butylaniline
Heat Capacity 300 K, C_p=490 J·mol^{-1}·K^{-1}
Temperature range 100 to 340 K. C_p value estimated from graphical data.
Phase Changes
c/liq 295.3 K, ΔH=18033 J·mol^{-1}
ΔS=61.04 J·mol^{-1}·K^{-1}
Data also given for metastable modification
294.0 K, ΔH=14757 J·mol^{-1}
ΔS=50.21 J·mol^{-1}·K^{-1}
Molecular Weight 267.3700
Wiswesser Line Notation 4R DNU1R DO1
Evaluation A(Phase changes), D(C_p)
Phase change data for the metastable modification clearing point also given: T=317.0 K; $\Delta\Delta S$=1.962 J·mol^{-1}·K^{-1}.

$C_{18}H_{21}NO$ (liq) 82SHI/MIZ
N-(4-Methoxybenzylidene)-p-n-butylaniline
Heat Capacity 298.15 K, C_p=477 J·mol^{-1}·K^{-1}
Temperature range 293 to 333 K. Data given graphically. C_p value is a graphical estimate.
Phase Changes
liq/liq 320.137 K
Nematic-isotropic liquid transition.
Molecular Weight 267.3700
Wiswesser Line Notation 4R DNU1R DO1
Evaluation C

$C_{18}H_{21}NO_2$ (c) 71SOR/SEK
N-(2-Hydroxy-4-methoxybenzylidene)-p-butylaniline
Phase Changes
c/liq 317 K
liq/liq 337.5 K
Nematic mesophase to isotropic.
Molecular Weight 283.3694
Wiswesser Line Notation 4R DNU1R BQ DO1
Evaluation A

$C_{18}H_{21}NO_2$ (c) 73SOR/SEK
N-(2-Hydroxy-4-methoxybenzylidene)-p-butylaniline
Heat Capacity 300 K, C_p=451.12 J·mol^{-1}·K^{-1}
Temperature range 12 to 375 K.
Entropy 300 K, S=420.77 J·mol^{-1}·K^{-1}
Phase Changes
liq/liq 335.65 K, ΔH=887.4 J·mol^{-1}
ΔS=2.64 J·mol^{-1}·K^{-1}
Nematic-isotropic liquid transition.
c/liq 314.52 K, ΔH=24405 J·mol^{-1}
ΔS=71.24 J·mol^{-1}·K^{-1}
Molecular Weight 283.3694
Wiswesser Line Notation 4R DNU1R BQ DO1
Evaluation A

$C_{18}H_{22}$ (liq) 56MCE
p,p′-Diisopropylbiphenyl
Heat Capacity 422 K, C_p=520.5 J·mol^{-1}·K^{-1}
Temperature range 300 to 600 °F.
Molecular Weight 238.3718
Wiswesser Line Notation 1Y1&R DR DY1&1
Evaluation C
Quoted in 58WAL/BRO.

$C_{18}H_{22}$ (c) 83KRA/BE
2,3-Dimethyl-2,3-diphenylbutane
Heat Capacity 298 K, C_p=321.1 J·mol^{-1}·K^{-1}
One temperature. C_p given as equal to 0.322 cal·K^{-1}·g^{-1}
Molecular Weight 238.3718
Wiswesser Line Notation 1X1&R&X1&1&R
Evaluation C

$C_{18}H_{22}N_2O$ (liq) 85SHA/ZH
4-Ethoxy-4′-butylazobenzene
Heat Capacity 325.49 K, C_p=535.0 J·mol^{-1}·K^{-1}
Temperature range 325 to 363 K. Unsmoothed experimental datum.
Phase Changes
liq/liq 355.8 K, ΔH=655 J·mol^{-1}
ΔS=1.84 J·mol^{-1}·K^{-1}
Molecular Weight 282.3846
Wiswesser Line Notation 4R DNUNR DO2
Evaluation B

$C_{18}H_{22}O_2$ (c) 57MA
Di-α-cumyl peroxide
Phase Changes
c/liq 312.35 K, ΔH=28137 J·mol^{-1}
Molecular Weight 270.3706
Wiswesser Line Notation 1YR&1&OOYR&1&1
Evaluation A

$C_{18}H_{24}$ (c) 81JEN/OBI
Triamantane
Phase Changes
c,II/c,I 293.65 K, ΔH=1106 J·mol^{-1}
ΔS=3.77 J·mol^{-1}·K^{-1}
Room temperature specific heat anomaly.
Molecular Weight 240.3876
Wiswesser Line Notation L666 B666 E6/B-L/CN/JO/EP/HQ B- (
-11-AAABBCEFFJJ Q JXTJ
Evaluation A

$C_{18}H_{24}Cr$ (c) 72NIK/SA
Bis(diisopropylbenzene)chromium
Heat Capacity 298.15 K, C_p=633.9 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S=569.0 J·mol^{-1}·K^{-1}
Molecular Weight 292.3836
Wiswesser Line Notation L6ϕJ AY1&1 DY1&1 ϕ-CR– ϕL6ϕJ AY1&
DY1&1
Evaluation B

$C_{18}H_{24}CrI$ (c) 72NIK/SA
Bis(mesitylene)chromium iodide
Heat Capacity 298.15 K, C_p=437.2 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S=443.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 260 K, ΔH=105 J·mol^{-1}
ΔS=0.40 J·mol^{-1}·K^{-1}
Molecular Weight 419.2881
Wiswesser Line Notation L6ϕJ A1 C1 D1 -CR– ϕL6ϕJ A1 C1 D1 δ
Evaluation B

$C_{18}H_{24}FeN_6S_6$ (c) 92KUL/IYE
Bis-(2,2′-bi-5-methyl-2-thiazoline)diisothiocyanato iron(II)
Heat Capacity
Temperature range 115 to 300 K. Data given graphically only.
Phase Changes
c,II/c,I 206 K, ΔH=5700 J·mol^{-1}
ΔS=27.5 J·mol^{-1}·K^{-1}
Approximate values.
Molecular Weight 572.6348
Wiswesser Line Notation T5NU CSTJ E1 B- BT5NU CSTJ E1 &-FE-NCS2
Evaluation B

$C_{18}H_{27}FeO_6$ (c) 92RIB/FER3
Tris(3-methylpentane-2,4-dionato)iron(III)
Phase Changes
c/g 422 K, ΔH=164500 J·mol^{-1}
Molecular Weight 395.2547
Wiswesser Line Notation D6O-FE-O ADK D1 E1 F1 B-& BD6O-FE-O ADJ D1 E1 F1 B-& BDO-FE-O ADJ D1 E1 F1
Evaluation A

$C_{18}H_{28}O_4Si_4$ (c) 75MEK/KAR
1,1,3,3,5,5-Hexamethyl-7,7-diphenylcyclotetrasiloxane
Heat Capacity
Temperature range 13 to 320 K.
Entropy 298.15 K, S=758.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 305.09 K, ΔH=42731 J·mol^{-1}
ΔS=140.1 J·mol^{-1}·K^{-1}
Molecular Weight 420.7588
Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI-OTJ A1 A1 C1 C1 E1 E1 GR GR
Evaluation B

$C_{18}H_{28}O_4Si_4$ (c) 81MEK/KAR
1,1,3,3,5,5-Hexamethyl-7,7-diphenylcyclotetrasiloxane
Heat Capacity 298.15 K, C_p=633.0 J·mol^{-1}·K^{-1}
Temperature range 13 to 390 K. Data given graphically.
Entropy 298.15 K, S=758.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 304.96 K, ΔH=42731 J·mol^{-1}
ΔS=140.1 J·mol^{-1}·K^{-1}
Molecular Weight 420.7588
Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI-OTJ A1 A1 C1 C1 E1 E1 GR GR
Evaluation A

$C_{18}H_{30}$ (c) 86CHI/ANN
Hexaethylbenzene
Phase Changes
c/g ΔH=94977 J·mol^{-1}
Molecular Weight 246.4350
Wiswesser Line Notation 2R B2 C2 D2 E2 F2
Evaluation A

$C_{18}H_{30}$ (liq) 62GOL/BEL
3-Ethylperhydropyrene
Heat Capacity 311 K, C_p=459.8 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 246.4350
Wiswesser Line Notation L666 B6 2AB PJ F2
Evaluation C

$C_{18}H_{30}BaCa_2O_{12}$ (c) 55MOM/SEK
Barium dicalcium propionate
Phase Changes
c/liq 268.4 K, ΔH=7284 J·mol^{-1}
ΔS=27.2 J·mol^{-1}·K^{-1}
Molecular Weight 655.9178
Wiswesser Line Notation OV1 6 &-BE-4 O
Evaluation B

$C_{18}H_{30}Ca_2O_{12}Pb$ (c) 65NAK/SUG
Lead dicalcium propionate
Heat Capacity 298.15 K, C_p=740.6 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=983.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 191.5 K, ΔH=4853 J·mol^{-1}
ΔS=24.4 J·mol^{-1}·K^{-1}
Molecular Weight 725.7878
Wiswesser Line Notation OV1 6 &-CA- 2 &-PB-
Evaluation A

$C_{18}H_{30}Ca_2O_{12}Sr$ (c) 65NAK/SUG
Strontium dicalcium propionate
Heat Capacity 298.15 K, C_p=728.4 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S=949.3 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 104.2 K, ΔH=1067 J·mol^{-1}
ΔS=13.4 J·mol^{-1}·K^{-1}
c,II/c,I 282.6 K, ΔH=667.8 J·mol^{-1}
ΔS=2.55 J·mol^{-1}·K^{-1}
Molecular Weight 606.2078
Wiswesser Line Notation OV1 6 &-CA- 2 &-SR-
Evaluation A

$C_{18}H_{30}O_4$ (c) 77KAR/SAP
p-Diacetylbenzene diethyl ketal
Phase Changes
c,II/c,I 168.2 K, ΔH=1305 J·mol^{-1}
ΔS=8.4 J·mol^{-1}·K^{-1}
c,I/liq 326.21 K, ΔH=23502 J·mol^{-1}
$\Delta\Delta Sm$=23502/326.21=72.0 J·mol^{-1}·K^{-1}.
Molecular Weight 310.4326
Wiswesser Line Notation 2OX1&O2&R DX1&O2&O2
Evaluation A
T(glass)=208.0 K.

$C_{18}H_{30}O_4$ (c) 78KAR/RAB
p-Diacetylbenzene diethyl ketal
Heat Capacity 298.15 K, C_p=462.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 340 K.
Entropy 298.15 K, S=493.8 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 168.24 K, ΔH=1307 J·mol^{-1}
ΔS=8.14 J·mol^{-1}·K^{-1}
c,I/liq 326.61 K, ΔH=23500 J·mol^{-1}
ΔS=71.95 J·mol^{-1}·K^{-1}
Molecular Weight 310.4326
Wiswesser Line Notation 2OX1&O2&R DX1&O2&O2
Evaluation A
T(glass)=208 K.

$C_{18}H_{30}O_4$ (c) 78KAR/SAP
p-Diacetylbenzene diethyl ketal
Heat Capacity 300 K, C_p=460 J·mol^{-1}·K^{-1}
Temperature range 5 to 326.1 K. Data given graphically. Value estimated from graph.
Entropy 298.15 K, S=493.8 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 168.2 K, ΔH=1307 J·mol^{-1}
ΔS=8.15 J·mol^{-1}·K^{-1}
c,I/liq 326.21 K, ΔH=23500 J·mol^{-1}
ΔS=72.04 J·mol^{-1}·K^{-1}
Molecular Weight 310.4326
Wiswesser Line Notation 2OX1&O2&R DX1&O2&O2
Evaluation C(C_p), A(S,Phase changes)
T(glass)=208.0 K.

$C_{18}H_{32}$ (liq) 62GOL/BEL
1-Cyclohexyl-1.3.3-trimethylhydroindan
Heat Capacity 311 K, C_p=457.3 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 248.4521
Wiswesser Line Notation L56TJ B1 B1 D1 D- AL6TJ
Evaluation C

$C_{18}H_{32}$ (liq) 63GUD/CAM
1-Cyclohexyl-1,3,3-trimethylhydroindan
Heat Capacity 313 K, C_p=456.9 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 248.4521
Wiswesser Line Notation L56TJ B1 B1 D1 D- AL6TJ
Evaluation C

$C_{18}H_{32}$ (liq) 62GOL/BEL
o-Tercylcohexyl
Heat Capacity 311 K, C_p=424.3 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 248.4521
Wiswesser Line Notation L6TJ AAL6TJ B- AL6TJ
Evaluation C

$C_{18}H_{32}$ (liq) 63GUD/CAM
o-Tercylcohexyl
Heat Capacity 313 K, C_p=427.2 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 248.4521
Wiswesser Line Notation L6TJ AAL6TJ B- AL6TJ
Evaluation C

$C_{18}H_{32}$ (liq) 62GOL/BEL
m-Tercylcohexyl
Heat Capacity 311 K, C_p=457.3 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 248.4521
Wiswesser Line Notation L6TJ AAL6TJ C- AL6TJ
Evaluation C

$C_{18}H_{32}$ (liq) 63GUD/CAM
m-Tercylcohexyl
Heat Capacity 373 K, C_p=502.1 J·mol^{-1}·K^{-1}
Temperature range 373 to 483 K.
Molecular Weight 248.4521
Wiswesser Line Notation L6TJ AAL6TJ C- AL6TJ
Evaluation C

$C_{18}H_{32}$ (liq) 63GUD/CA
p-Tercylcohexyl
Heat Capacity 423 K, C_p=564.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 248.4521
Wiswesser Line Notation L6TJ AAL6TJ D- AL6TJ
Evaluation C

$C_{18}H_{32}O$ (liq) 88BAG/GU
6,10,14-Trimethyl-3,5-pentadecadien-2-one
Heat Capacity 293.95 K, C_p=555.3 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 264.4502
Wiswesser Line Notation 1Y3Y3YU2U1V1
Evaluation B

$C_{18}H_{34}$ (liq) 63GUD/CA
1,1-Bis(dimethylcyclohexyl)ethane
Heat Capacity 313 K, C_p=461.1 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 250.4666
Wiswesser Line Notation L6TJ A1 X1 XY1&- AL6TJ X1 X1
Evaluation C

$C_{18}H_{34}$ (liq) 63GUD/CA
1,1-Bis(ethylcyclohexyl)ethane
Heat Capacity 313 K, C_p=477.8 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 250.4666
Wiswesser Line Notation L6TJ A2 XY1&- AL6TJ X2
Evaluation C

$C_{18}H_{34}O_2$ (c) 90SAT/YU
cis-ω-12,δ-6-Octadecenoic acid; Petroselinic acid
Phase Changes
c/liq 303.65 K, ΔH=47500 J·mol^{-1}
ΔS=156.4 J·mol^{-1}·K^{-1}
High-melting form.
c/liq 301.65 K
Low-melting form.
Molecular Weight 282.4654
Wiswesser Line Notation QV5U12 -C
Evaluation A

$C_{18}H_{34}O_2$ (liq) 90SAT/YU
Oleic acid; cis-9-Octadecenoic acid
Phase Changes
c,α/liq 286.45 K, ΔH=39600 J·mol^{-1}
ΔS=138.4 J·mol^{-1}·K^{-1}
High-melting, α-form.
c,β/liq 289.35 K, ΔH=51900 J·mol^{-1}
ΔS=179.3 J·mol^{-1}·K^{-1}
Low-melting, β-form.
Molecular Weight 282.4654
Wiswesser Line Notation QV8U9 -C
Evaluation A

$C_{18}H_{34}O_3$ (liq) 84URY/MOC

Castor oil; Natural ricinoleic acid

Heat Capacity 300 K, C_p=646 J·mol^{-1}·K^{-1}

Temperature range 80 to 320 K.

Entropy 300 K, S=620 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 205 K

Glass transition; ΔC_p=0.55 J·g^{-1}·K^{-1} for glass to supercooled liquid transition.

c/liq 264.87 K, ΔH=17016 J·mol^{-1}, ΔS=64.2 J·mol^{-1}·K^{-1}

Molecular Weight 298.4648

Wiswesser Line Notation QV8U2YQ6

Evaluation B

General difference in enthalpy of glassy and crystalline phases at T=0 K is 31.7 J·g^{-1} (9397 J·mol^{-1}). Entropy of the glassy phase at T=0 K is 0.097 J·g^{-1}·K^{-1} (28.8 J·mol^{-1}·K^{-1}). Castor oil is about 88% ricinoleic acid.

$C_{18}H_{34}O_4$ (liq) 76PHI/MAT

Di-n-butyl sebacate

Heat Capacity 312 K, C_p=619 J·mol^{-1}·K^{-1}

Temperature range 312 to 412 K.

Molecular Weight 314.4642

Wiswesser Line Notation 4OV8VO4

Evaluation C

$C_{18}H_{34}O_4Pb$ (c,II) 78ADE/SIM

Lead(II) nonanoate; Lead(II) pelargonate

Heat Capacity 310 K, C_p=926 J·mol^{-1}·K^{-1}

Mean value 353 to 363 K. Data only graphically for c,III. Data also for c,I, 370–378 K, and liquid, 413 to 463 K.

Phase Changes

c,III/c,II 348.9 K, ΔH=32200 J·mol^{-1}, ΔS=92 J·mol^{-1}·K^{-1}

c,II and c,I are mesophases.

c,II/c,I 367.4 K, ΔH=16400 J·mol^{-1}, ΔS=45 J·mol^{-1}·K^{-1}

c,I/liq 384.8 K, ΔH=1300 J·mol^{-1}, ΔS=3.4 J·mol^{-1}·K^{-1}

Molecular Weight 521.6642

Wiswesser Line Notation OV8 2 .PB

Evaluation C

$C_{18}H_{35}O_2Tl$ (c) 76MEI/SEY

Thallium octadecanoate

Phase Changes

c,III/c,II 324 K, ΔH=9623 J·mol^{-1}, ΔS=29.3 J·mol^{-1}·K^{-1}

c,II/c,I 380 K, ΔH=12134 J·mol^{-1}, ΔS=12.1 J·mol^{-1}·K^{-1}

c,I/liq 385 K, ΔH=5439 J·mol^{-1}, ΔS=14.2 J·mol^{-1}·K^{-1}

liq/liq 444 K, ΔH=1381 J·mol^{-1}, ΔS=3.05 J·mol^{-1}·K^{-1}

Mesophase-isotropic.

Molecular Weight 487.8433

Wiswesser Line Notation OV17 .TL

Evaluation B

$C_{18}H_{36}$ (liq) 49PAR/MOO

n-Dodecylcyclohexane

Heat Capacity 298.15 K, C_p=615.5 J·mol^{-1}·K^{-1}

Extrapolation below 80 K, 119.3 J·mol^{-1}·K^{-1}.

Phase Changes

Hump in specific heat curve at 229 to 249 K

c/liq 258.8 K, ΔH=45836 J·mol^{-1}, ΔS=160.4 J·mol^{-1}·K^{-1}

Molecular Weight 252.4824

Wiswesser Line Notation L6TJ A12

Evaluation B(C_p),C(S)

$C_{18}H_{36}$ (liq) 63GUD/CAM

Hexaethylcyclohexane

Heat Capacity 313 K, C_p=530.1 J·mol^{-1}·K^{-1}

Temperature range 313 to 483 K.

Molecular Weight 252.4824

Wiswesser Line Notation L6TJ A2 B2 C2 D2 E2 F2

Evaluation C

$C_{18}H_{36}$ (c) 69BOR/DAL

Cyclooctadecane

Phase Changes

c,II/c,I 298 K, ΔH=29288 J·mol^{-1}, ΔS=97.5 J·mol^{-1}·K^{-1}

c/liq 346 K, ΔH=9874 J·mol^{-1}, ΔS=28.4 J·mol^{-1}·K^{-1}

Molecular Weight 252.4824

Wiswesser Line Notation L-18-TJ

Evaluation B

$C_{18}H_{36}N_2O_2$ (c) 53WIL/DOL

N,N′-Di-n-hexyladipamide

Heat Capacity 373 K, C_p=644.7 J·mol^{-1}·K^{-1}

Temperature range 373 to 583 K.

Phase Changes

c/liq 432 K, ΔH=4079.5 J·mol^{-1}, ΔS=94.4 J·mol^{-1}·K^{-1}

Molecular Weight 312.4946

Wiswesser Line Notation 6MV4VM6

Evaluation C

$C_{18}H_{36}O$ (liq) 88BAG/GUR

6,10,14-Trimethyl-2-pentadecanone; Phytone

Heat Capacity 293.85 K, C_p=593.3 J·mol^{-1}·K^{-1}

Temperature range 270 to 340 K. Unsmoothed experimental datum.

Molecular Weight 268.4818

Wiswesser Line Notation 1Y3Y3Y3V1

Evaluation B

$C_{18}H_{36}O_2$ (liq) 34KIN/GAR

Ethyl hexadecanoate; Ethyl palmitate

Phase Changes

c/liq 296.35 K, ΔH=15093 J·mol^{-1}

Molecular Weight 284.4812

Wiswesser Line Notation 15VO2

Evaluation B

Data on the specific heats are given at or near the phase transitions.

$C_{18}H_{36}O_2$ (c) 1889EYK
Octadecanoic acid; Stearic acid
Phase Changes
c/liq 326.1 K, $\Delta H = 64643\ J\cdot mol^{-1}$
$\Delta S = 198\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 284.4812
Wiswesser Line Notation QV17
Evaluation C

$C_{18}H_{36}O_2$ (c) 50SIN/WAR
Octadecanoic acid; Stearic acid
Heat Capacity 298.15 K, $C_p = 561.9\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 154 to 350 K.
Entropy 298.15 K, $S = 435.6\ J\cdot mol^{-1}\cdot K^{-1}$
Extrapolation below 90 K, 64.4 $J\cdot mol^{-1}\cdot K^{-1}$.
Phase Changes
Transition between B & C forms previously reported as 52.90 °C is high. Irreversible and slow change observed as low as 35.2 °C.
c/liq 342.65 K, $\Delta H = 68450\ J\cdot mol^{-1}$
$\Delta S = 1998\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 284.4812
Wiswesser Line Notation QV17
Evaluation C

$C_{18}H_{36}O_2$ (c) 82SCH/MIL2
Octadecanoic acid; Stearic acid
Heat Capacity 298.15 K, $C_p = 501.55\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 80 to 355 K.
Phase Changes
c,I/liq 342.49 K, $\Delta H = 61208\ J\cdot mol^{-1}$
$\Delta S = 178.12\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 284.4812
Wiswesser Line Notation QV17
Evaluation B

$C_{18}H_{36}O_2$ (c) 83BEC/ROU
Octadecanoic acid; Stearic acid
Phase Changes
c/liq 345, 346 K, $\Delta H = 62600\ J\cdot mol^{-1}$
$\Delta S = 181\ J\cdot mol^{-1}\cdot K^{-1}$
First peak due to pre-melting or dissociation.
Molecular Weight 284.4812
Wiswesser Line Notation QV17
Evaluation B

$C_{18}H_{36}O_2$ (c) 90SAT/YOS
Octadecanoic acid; Stearic acid
Phase Changes
c/liq 342.75 K, $\Delta H = 61300\ J\cdot mol^{-1}$
$\Delta S = 178.8\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 284.4812
Wiswesser Line Notation QV17
Evaluation A

$C_{18}H_{37}Cl$ (liq) 75STR/SUN
1-Chlorooctadecane; n-Octadecyl chloride
Heat Capacity 301 K, $C_p = 606.8\ J\cdot mol^{-1}\cdot K^{-1}$
One temperature.
Phase Changes
liq/g 298.15 K, $\Delta H = 98160\ J\cdot mol^{-1}$
$\Delta S = 329.22\ J\cdot mol^{-1}\cdot K^{-1}$
ΔH vaporization from equation using data from 68WAD.
Molecular Weight 288.9433
Wiswesser Line Notation G18
Evaluation B

$C_{18}H_{38}$ (liq) 49PAR/MO
n-Octadecane
Heat Capacity 300 K, $C_p = 564.4\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 80 to 300 K.
Entropy 298.15 K, $S = 696.6\ J\cdot mol^{-1}\cdot K^{-1}$
Supercooled liquid. Extrapolation below 80 K, 127.7 $J\cdot mol^{-1}\cdot K^{-1}$.
Phase Changes
Hump in specific heat curve at 228 to 240 K.
c/liq 301.3 K, $\Delta H = 60484\ J\cdot mol^{-1}$
$\Delta S = 200.7\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 254.4982
Wiswesser Line Notation 18H
Evaluation B(C_p),C(S)

$C_{18}H_{38}$ (c) 55SCH/BU
n-Octadecane
Phase Changes
c,I/liq 301.35 K, $\Delta H = 61379\ J\cdot mol^{-1}$
$\Delta S = 203.6\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 254.4982
Wiswesser Line Notation 18H
Evaluation B

$C_{18}H_{38}$ (c) 67MES/GU
n-Octadecane
Heat Capacity 298.15 K, $C_p = 485.64\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 12 to 380 K.
Entropy 298.15 K, $S = 480.20\ J\cdot mol^{-1}\cdot K^{-1}$
Phase Changes
c/liq 301.33 K, $\Delta H = 61706\ J\cdot mol^{-1}$
$\Delta S = 204.6\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 254.4982
Wiswesser Line Notation 18H
Evaluation A

$C_{18}H_{38}$ (liq) 81HC
n-Octadecane
Heat Capacity 325 K, $C_p = 568\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 300 to 500 K. Cv=2.20 $J\cdot g^{-1}\cdot K^{-1}$.
Molecular Weight 254.4982
Wiswesser Line Notation 18H
Evaluation B

$C_{18}H_{38}$ (c) 85KOL/SY
n-Octadecane
Phase Changes
c/liq 301.0 K, $\Delta H = 60760\ J\cdot mol^{-1}$
$\Delta S = 201.9\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 254.4982
Wiswesser Line Notation 18H
Evaluation A

$C_{18}H_{38}$ (c) 91BAR/SC
n-Octadecane
Phase Changes
c/liq 301.5 K, $\Delta H = 61500\ J\cdot mol^{-1}$
Molecular Weight 254.4982
Wiswesser Line Notation 18H
Evaluation A

$C_{18}H_{38}$ (liq) 91CLA/LET
n-Octadecane
Phase Changes
c,II/c,I $\Delta H = 19850\ J\cdot mol^{-1}$
Transition temperature not measurable.
c,II/liq $\Delta H = 46170\ J\cdot mol^{-1}$
Transition temperature not measureable.
c,I/liq 300.7 K, $\Delta H = 60670\ J\cdot mol^{-1}$
Molecular Weight 254.4982
Wiswesser Line Notation 18H
Evaluation A

$C_{18}H_{38}O$ (liq) 89KHA/ZYK
1-Octadecanol; n-Octadecyl alcohol
Heat Capacity 343.15 K, $C_p = 705.2\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 343 to 583 K.
Molecular Weight 270.4976
Wiswesser Line Notation Q18
Evaluation B

$C_{18}H_{38}O_7$ (liq) 82ZAR
Hexapropylene glycol
Heat Capacity 298 K, $C_p = 807.4\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 298, 323, 363 K.
Molecular Weight 366.4940
Wiswesser Line Notation QYOYOYOYOYOYQ
Evaluation B

$C_{18}H_{38}S$ (liq) 82TUT/GAB
1-Octadecanethiol; n-Octadecyl mercaptan
Heat Capacity 300 K, $C_p = 648.61\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 273 to 373 K. $C_p = 626.52 + 4.423\times10^{-2}T + 9.800\times10^{-5}T^2$.
Molecular Weight 286.5582
Wiswesser Line Notation SH18
Evaluation B

$C_{18}H_{42}Br_2N_2$ (c,II) 74BUR/VER
1,6-Bis(triethylammonium)hexane dibromide
Heat Capacity 298 K, $C_p = 521.3\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 273 to 373 K.
Phase Changes
c,II/c,I 495 K, $\Delta H = 18830\ J\cdot mol^{-1}$
$\Delta S = 38.0\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 482 to 505 K.
Molecular Weight 446.3512
Wiswesser Line Notation 2K2&2&6K2&2&2 E 2
Evaluation B

$C_{18.1}H_{18.6}O_6$ (c) 60PAR/STA
β-Quinol-methane clathrate
Heat Capacity 296.62 K, $C_p = 416.98\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 13 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 332.9836
Wiswesser Line Notation QR DQ 3 &1H 0.165
Evaluation A

$C_{18.4}H_{19.8}O_6$ (c) 60PAR/STA
β-Quinol-methane clathrate
Heat Capacity 297.83 K, $C_p = 428.40\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 13 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 337.6681
Wiswesser Line Notation QR DQ 3 &1H 0.457
Evaluation A

$C_{18.4}H_{44.6}N_2S$ (c,I) 72COP/GAN
Thiourea-2,2-dimethylbutane adduct; 2,2-Dimethylbutane-thiourea adduct
Heat Capacity 298.15 K, $C_p = 154.0\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 12 to 300 K. Values for one mole of thiourea.
Entropy 298.15 K, $S = 191.4\ J\cdot mol^{-1}\cdot K^{-1}$
Does not include possible zero-point entropy.
Phase Changes
c,IV/c,III 69.9 K, $\Delta H = 899\ J\cdot mol^{-1}$
$\Delta S = 12.62\ J\cdot mol^{-1}\cdot K^{-1}$
c,III/c,II 89.5 K, $\Delta H = 3364\ J\cdot mol^{-1}$
$\Delta S = 8.96\ J\cdot mol^{-1}\cdot K^{-1}$
P=37.50 kPa.
c,II/c,I 169.6 K, $\Delta H = 696\ J\cdot mol^{-1}$
$\Delta S = 4.12\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 326.0281
Wiswesser Line Notation 2X1&1&1 2.90 &ZYZUS
Evaluation A

$C_{18.7}H_{21}O_6$ (c) 60PAR/STA
β-Quinol-methane clathrate
Heat Capacity 287.79 K, $C_p = 423.71\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 13 to 298 K. Value is unsmoothed experimental datum.
Molecular Weight 342.4488
Wiswesser Line Notation QR DQ 3 &1H 0.755
Evaluation A

$C_{19}H_{13}N_3O_7$ (c) 79FAR/SHA
Fluorene-picric acid
Phase Changes
c/liq 350.3 K, $\Delta H = 26800\ J\cdot mol^{-1}$
$\Delta S = 76.5\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 395.3276
Wiswesser Line Notation L B656 HHJ &WNR BQ CNW ENW
Evaluation B

$C_{19}H_{14}N_2$ (c) 74KAR/RAB
1,2-Diphenylbenzimidazole
Heat Capacity 298.15 K, $C_p = 318.7\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 10 to 450 K.
Entropy 298.15 K, $S = 306.8\ J\cdot mol^{-1}\cdot K^{-1}$
Molecular Weight 270.3330
Wiswesser Line Notation T56 BN DNJ CR DR
Evaluation A

$C_{19}H_{15}Cl$ (c) 31SMI/AND
Triphenylchloromethane
Heat Capacity 298.5 K, $C_p = 311.7\ J\cdot mol^{-1}\cdot K^{-1}$
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 278.7805
Wiswesser Line Notation GXR&R&R
Evaluation C

$C_{19}H_{15}Cl$ (c) 91NAO/SEK
Triphenylchloromethane
Heat Capacity 298.15 K, C_p=367.27 J·mol^{-1}·K^{-1}
Temperature range 232 to 411 K. C_p value calculated from equation. C_p(c)=−3980+55.15T−0.2726T^2+6.07×10^{-4}T^3−5.0×10^{-7}T^4 J·mol^{-1}·K^{-1} (232.8 to 359.0 K).
Phase Changes
c/gls 250 K
c/liq 376.8 K, ΔH=27900 J·mol^{-1}
ΔS=74.1 J·mol^{-1}·K^{-1}
Molecular Weight 278.7805
Wiswesser Line Notation GXR&R&R
Evaluation B

$C_{19}H_{16}$ (c) 17HIL/DUS
Triphenylmethane
Heat Capacity 298.15 K, C_p=261.1 J·mol^{-1}·K^{-1}
Temperature range 293 to 418 K. From heat content data.
Phase Changes
c/liq 365.5 K, ΔH=18200 J·mol^{-1}
ΔS=49.8 J·mol^{-1}·K^{-1}
Molecular Weight 244.3354
Wiswesser Line Notation RYR&R
Evaluation C

$C_{19}H_{16}$ (c) 30HUF/PAR
Triphenylmethane
Heat Capacity 294.3 K, C_p=294.6 J·mol^{-1}·K^{-1}
Temperature range 89 to 294 K. Value is unsmoothed datum.
Entropy 298.1 K, S=312.1 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 99.75 J·mol^{-1}·K^{-1}.
Molecular Weight 244.3354
Wiswesser Line Notation RYR&R
Evaluation B(C_p),C(S)

$C_{19}H_{16}$ (c) 31SMI/AND
Triphenylmethane
Heat Capacity 298.15 K, C_p=295.4 J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 244.3354
Wiswesser Line Notation RYR&R
Evaluation C

$C_{19}H_{16}$ (c) 32SPA/THO
Triphenylmethane
Heat Capacity 303 K, C_p=308.8 J·mol^{-1}·K^{-1}
Temperature range 30 to 110 °C.
Phase Changes
c/liq 365.3 K, ΔH=21979 J·mol^{-1}
ΔS=60.2 J·mol^{-1}·K^{-1}
Molecular Weight 244.3354
Wiswesser Line Notation RYR&R
Evaluation B

$C_{19}H_{16}$ (c) 44EIB
Triphenylmethane
Heat Capacity 298.1 K, C_p=333.5 J·mol^{-1}·K^{-1}
Temperature range 30 to 200 °C, equations only, in t °C. C_p(c)=0.326 cal·g^{-1}·C^{-1} (30 to 90 °C); C_p(liq)=0.325+0.000889t cal·g^{-1}·C^{-1} (92 to 200 °C).
Phase Changes
c/liq 365.6 K, ΔH=20920 J·mol^{-1}
ΔS=57.2 J·mol^{-1}·K^{-1}
Molecular Weight 244.3354
Wiswesser Line Notation RYR&R
Evaluation C

$C_{19}H_{16}$ (liq) 50KUI
Triphenylmethane
Heat Capacity 373 K, C_p=454.0 J·mol^{-1}·K^{-1}
Temperature range 100 to 343 °C.
Molecular Weight 244.3354
Wiswesser Line Notation RYR&R
Evaluation B

$C_{19}H_{16}$ (c) 79ST
Triphenylmethane
Heat Capacity 298.15 K, C_p=295.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 244.3354
Wiswesser Line Notation RYR&R
Evaluation B

$C_{19}H_{16}N_2O$ (c) 74KAR/RA
N-Benzoyl-o-aminodiphenylamine
Heat Capacity 298.15 K, C_p=356.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S=340.7 J·mol^{-1}·K^{-1}
Molecular Weight 288.3482
Wiswesser Line Notation RVMR BMR
Evaluation A

$C_{19}H_{16}O$ (c) 31SMI/AN
Triphenylcarbinol
Heat Capacity 298.5 K, C_p=318.8 J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experiment datum.
Molecular Weight 260.3348
Wiswesser Line Notation QXR&R&R
Evaluation C

$C_{19}H_{20}F_3N_3O_3$ (c) 89PIN/GO
2-[3-(trifluoromethyl)-phenyl]amino-3-pyridinecarboxylic acid, β-morpholino ethyl ester; Morniflumate
Heat Capacity 298.15 K, C_p=440.78 J·mol^{-1}·K^{-1}
Temperature range 100 to 500 K. C_p(c)=1.2T+83 J·mol^{-1}·K^{-1} (1 to 340 K). C_p(liq)=1.4T+142 J·mol^{-1}·K^{-1} (356 to 439 K). C_p valu calculated from the equation.
Phase Changes
c/liq 350 K, ΔH=34500 J·mol^{-1}
ΔS=101 J·mol^{-1}·K^{-1}
Molecular Weight 395.3805
Wiswesser Line Notation
Evaluation A

$C_{19}H_{20}N_2O_3$ (c) 83FAN/PC
4-Propionyl-4′-n-butanoyloxyazobenzene
Phase Changes
c/liq 366 K, ΔH=15021 J·mol^{-1}
ΔS=41.04 J·mol^{-1}·K^{-1}
Mesophase observed between 366 and 393 K.
Solid-smectic H or G.
Molecular Weight 324.3786
Wiswesser Line Notation 3VOR DNUNR DV2
Evaluation A
Smectic H or G-smectic A; smectic A-nematic; nematic-isotropic liqu phase change data also given: 392.65 K, $\Delta\Delta H$=10920 J·mol^{-1}; 409. K, $\Delta\Delta H$=4100 J·mol Δ; 428.65 K, $\Delta\Delta H$=753 J·mol^{-1}.

$C_{19}H_{20}N_2O_3$ (c) 88FAN/POE
4-n-Pentanoyl-4-n′-ethanoyloxyazobenzene
Phase Changes
c,II/c,I 367.5 K, ΔH=6840 J·mol^{-1}
ΔS=18.61 J·mol^{-1}·K^{-1}
c,I/liq 387.4 K, ΔH=26966 J·mol^{-1}
ΔS=69.609 J·mol^{-1}·K^{-1}
Solid-nematic.
liq/liq 400.1 K, ΔH=665 J·mol^{-1}
ΔS=1.661 J·mol^{-1}·K^{-1}
Nematic-isotropic.
Molecular Weight 324.3786
Wiswesser Line Notation 4VR DNUNR DOV1
Evaluation A

$C_{19}H_{22}ClNO$ (c) 77TSU/SOR
p-n-Hexyloxybenzylideneamino-p′-chlorobenzene
Heat Capacity 300 K, C_p=430 J·mol^{-1}·K^{-1}
Temperature range 300 to 385 K. Data graphically only.
Phase Changes
c/liq 327.70 K, ΔH=10880 J·mol^{-1}
ΔS=33.2 J·mol^{-1}·K^{-1}
Crystal-smectic transition.
liq/liq 333.90 K, ΔH=12350 J·mol^{-1}
ΔS=37.0 J·mol^{-1}·K^{-1}
Smectic-smectic transition.
Molecular Weight 315.8419
Wiswesser Line Notation GR DNU1R DO6
Evaluation C(C_p); B(phase transition)

$C_{19}H_{22}ClNO$ (c) 82TSU/SOR
p-n-Hexyloxybenzylideneamino-p′-chlorobenzene
Heat Capacity 298.15 K, C_p=434.94 J·mol^{-1}·K^{-1}
Temperature range 15 to 385 K.
Entropy 298.15 K, S=447.58 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 327.7 K, ΔH=10880 J·mol^{-1}
ΔS=33.2 J·mol^{-1}·K^{-1}
Crystal to intermediate phase S3.
liq/liq 333.90 K, ΔH=12350 J·mol^{-1}
ΔS=37.0 J·mol^{-1}·K^{-1}
S_3-smectic B liquid transition.
liq/liq 362.98 K, ΔH=3390 J·mol^{-1}
ΔS=9.3 J·mol^{-1}·K^{-1}
Smectic B - smectic A liquid transition.
liq/liq 370.38 K, ΔH=5790 J·mol^{-1}
ΔS=15.6 J·mol^{-1}·K^{-1}
Smectic A - isotropic liquid transition.
Molecular Weight 315.8419
Wiswesser Line Notation GR DNU1R DO6
Evaluation A

$C_{19}H_{22}FNO$ (c) 82TSU/SOR2
p-n-Hexyloxybenzylideneamino-p′-fluorobenzene
Heat Capacity 298.15 K, C_p=442.55 J·mol^{-1}·K^{-1}
Temperature range 15 to 385 K.
Entropy 298.15 K, S=438.76 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 328.07 K, ΔH=23220 J·mol^{-1}
ΔS=70.7 J·mol^{-1}·K^{-1}
Crystal to smectic B.
liq/liq 330.33 K, ΔH=3050 J·mol^{-1}
ΔS=9.2 J·mol^{-1}·K^{-1}
Smectic B - smectic A transition.
liq/liq 334.88 K, ΔH=3410 J·mol^{-1}
ΔS=10.2 J·mol^{-1}·K^{-1}
Smectic A - nematic liquid transition.
liq/liq 336.33 K, ΔH=1170 J·mol^{-1}
ΔS=3.5 J·mol^{-1}·K^{-1}
Nematic - isotropic liquid transition.
Molecular Weight 299.3873
Wiswesser Line Notation FR DNU1R DO6
Evaluation A

$C_{19}H_{22}O_2$ (c) 72YOU/HAL
4-Methoxy-4′-butoxy-trans-stilbene
Phase Changes
liq/liq 435 K, ΔH=757 J·mol^{-1}
ΔS=1.7 J·mol^{-1}·K^{-1}
Nematic-isotropic liquid transition.
c/liq 442 K, ΔH=39665 J·mol^{-1}
ΔS=89.7 J·mol^{-1}·K^{-1}
Crystal-isotropic liquid transition.
Molecular Weight 282.3816
Wiswesser Line Notation 4OR D1U1R DO1 -T
Evaluation B

$C_{19}H_{23}NO$ (c) 73SOR/NAK
N-p-Ethoxybenzylidene-p′-butylaniline
Heat Capacity 300 K, C_p=425 J·mol^{-1}·K^{-1}
Temperature range 14 to 375 K. Data estimated from graph.
Phase Changes
liq/liq 349.08 K, ΔH=1553 J·mol^{-1}
ΔS=4.524 J·mol^{-1}·K^{-1}
Nematic-isotropic.
c/liq 305.62 K, ΔH=27090 J·mol^{-1}
ΔS=88.71 J·mol^{-1}·K^{-1}
Solid-nematic.
Molecular Weight 281.3968
Wiswesser Line Notation 4R DNU1R DO2
Evaluation B

$C_{19}H_{23}NO$ (c) 74SOR/NAK
N-p-Ethoxybenzylidene-p′-butylaniline
Heat Capacity 298.15 K, C_p=429.09 J·mol^{-1}·K^{-1}
Temperature range 14 to 375 K.
Entropy 298.15 K, S=421.788 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 305.62 K, ΔH=27090 J·mol^{-1}
ΔS=88.71 J·mol^{-1}·K^{-1}
Crystal-nematic.
liq/liq 349.08 K, ΔH=1553 J·mol^{-1}
ΔS=4.524 J·mol^{-1}·K^{-1}
Nematic-isotropic.
Molecular Weight 281.3968
Wiswesser Line Notation 4R DNU1R DO2
Evaluation A

$C_{19}H_{23}NO$ (c) 82TSU/SOR3
p-n-Hexyloxybenzylideneaniline
Heat Capacity 298.15 K, C_p=404.52 J·mol^{-1}·K^{-1}
Temperature range 16 to 385 K.
Entropy 298.15 K, S=424.16 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 73.41 K, ΔH=192 J·mol^{-1}
ΔS=2.70 J·mol^{-1}·K^{-1}
c,I/liq 321.63 K, ΔH=30910 J·mol^{-1}
ΔS=96.1 J·mol^{-1}·K^{-1}
Solid-isotropic liquid.
Molecular Weight 281.3968
Wiswesser Line Notation 6OR D1UNR
Evaluation A

$C_{19}H_{30}O_2$ (c) 89MAS/MAU
Androstanolone; 5α-Androstane-3-one-17β-ol
Phase Changes
c,III/liq 453.0 K, ΔH=19790 J·mol^{-1}
Monotropic.
c,II/liq 454.2 K, ΔH=23070 J·mol^{-1}
Monotropic.
c,I/liq 455.5 K, ΔH=27150 J·mol^{-1}
Monotropic.
Molecular Weight 290.4448
Wiswesser Line Notation L E5 B666 OVTJ A1 E1 FQ
Evaluation B

$C_{19}H_{36}$ (liq) 63GUD/CAM
4-n-Heptylbicyclohexyl
Heat Capacity 313 K, C_p=484.9 J·mol^{-1}·K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 264.4934
Wiswesser Line Notation L6TJ A- AL6TJ D7
Evaluation C

$C_{19}H_{36}$ (liq) 63GUD/CAM
Bis(2,4,6-trimethylcyclohexyl)methane
Heat Capacity 373 K, C_p=590.8 J·mol^{-1}·K^{-1}
Temperature range 373 to 483 K.
Molecular Weight 264.4934
Wiswesser Line Notation L6TJ A1 C1 E1 B1- AL6TJ B1 D1 F1
Evaluation C

$C_{19}H_{36}$ (liq) 62GOL/BEL
1,1-Dicyclohexylheptane
Heat Capacity 311 K, C_p=531.4 J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 264.4934
Wiswesser Line Notation L6TJ AY6&- AL6TJ
Evaluation C

$C_{19}H_{36}$ (liq) 63GUD/CAM
1,1-Dicyclohexylheptane
Heat Capacity 313 K, C_p=534.7 J·mol^{-1}·K^{-1}
Temperature range 313 to 583 K.
Molecular Weight 264.4934
Wiswesser Line Notation L6TJ AY6&- AL6TJ
Evaluation C

$C_{19}H_{38}O_2$ (c) 36KIN/GA
Ethyl heptadecanoate; Ethyl margarate
Phase Changes
c,II/c,I 298.3 K, ΔH=4946 J·mol^{-1}
Heat of transition at melting point.
Molecular Weight 298.5080
Wiswesser Line Notation 16VO2
Evaluation B

$C_{19}H_{38}O_2$ (c) 36KIN/GA
Methyl octadecanoate; Methyl stearate
Phase Changes
c/liq 310.93 K, ΔH=19234 J·mol^{-1}
Molecular Weight 298.5080
Wiswesser Line Notation 17VO1
Evaluation B

$C_{19}H_{38}O_2$ (c) 82SCH/M
Nonadecanoic acid
Heat Capacity 298.15 K, C_p=525.35 J·mol^{-1}·K^{-1}
Temperature range 80 to 355 K.
Phase Changes
c,II/c,I 338.0 K, ΔH=9177 J·mol^{-1}
ΔS=27.15 J·mol^{-1}·K^{-1}
c,I/liq 341.23 K, ΔH=57618 J·mol^{-1}
ΔS=168.85 J·mol^{-1}·K^{-1}
Molecular Weight 298.5080
Wiswesser Line Notation QV18
Evaluation B

$C_{19}H_{38}O_4$ (c) 40CLA/S
2-Monopalmitin
Heat Capacity 298 K, C_p=607.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 330.5068
Wiswesser Line Notation Q1Y1QOV15
Evaluation B

$C_{19}H_{38}O_4$ (c) 65SIL/D
2-Monopalmitin
Heat Capacity 298 K, C_p=558.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 330.5068
Wiswesser Line Notation Q1Y1QOV15
Evaluation B

$C_{19}H_{38}O_4$ (c) 40CLA/S
1-Monopalmitin
Heat Capacity 298 K, C_p=602.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 330.5068
Wiswesser Line Notation Q1YQ1OV15
Evaluation B

$C_{19}H_{38}O_4$ (c) 65SIL/D
1-Monopalmitin
Heat Capacity 298 K, C_p=566.9 J·mol^{-1}·K^{-1}
One temperature. β_L form.
Molecular Weight 330.5068
Wiswesser Line Notation Q1YQ1OV15
Evaluation B

$C_{19}H_{40}$ (c) 55SCH/BUS
n-Nonadecane
Phase Changes
c,II/c,I 295.95 K, $\Delta H = 13807\ J \cdot mol^{-1}$
$\Delta S = 46.7\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 305.15 K, $\Delta H = 45815\ J \cdot mol^{-1}$
$\Delta S = 150.1\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 268.5250
Wiswesser Line Notation 19H
Evaluation B

$C_{19}H_{40}$ (liq) 69ATK/LAR
n-Nonadecane
Heat Capacity 353 K, $C_p = 640\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 353 to 453 K. Equation only.
Molecular Weight 268.5250
Wiswesser Line Notation 19H
Evaluation C

$C_{19}H_{40}$ (c) 79CLA/LET
n-Nonadecane
Phase Changes
c,II/c,I 295.95 K, $\Delta H = 13665\ J \cdot mol^{-1}$
$\Delta S = 46.2\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 303.95 K, $\Delta H = 47395\ J \cdot mol^{-1}$
$\Delta S = 155.9\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 268.5250
Wiswesser Line Notation 19H
Evaluation B

$C_{19}H_{40}$ (liq) 84GRI/AND
n-Nonadecane
Heat Capacity 313.15 K, $C_p = 602.6\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 313 to 433 K. Unsmoothed experimental datum given as 2.244 kJ/kg·K.
Molecular Weight 268.5250
Wiswesser Line Notation 19H
Evaluation B

$C_{19}H_{40}$ (c) 91BAR/SCH
n-Nonadecane
Phase Changes
c,II/c,I 296.1 K, $\Delta H = 13750\ J \cdot mol^{-1}$
c,I/liq 305.1 K, $\Delta H = 43750\ J \cdot mol^{-1}$
Molecular Weight 268.5250
Wiswesser Line Notation 19H
Evaluation A

$C_{19}H_{40}$ (liq) 91TRE/COS
2,6,10,14-Tetramethylpentadecane
Heat Capacity 298.15 K, $C_p = 569.76\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 268.5250
Wiswesser Line Notation 1Y1&3Y1&3Y1&3Y1&1
Evaluation B

$C_{20}H_{10}N_4$ (c) 78BOE/WES
Naphthalene-1,2,4,5-tetracyanobenzene
Heat Capacity 298.15 K, $C_p = 370.3\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 300 K.
Entropy 298.15 K, $S = 421.8\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,II/c,I 75 K, $\Delta H = 192\ J \cdot mol^{-1}$
$\Delta S = 2.97\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 306.3258
Wiswesser Line Notation L66J &NCR BCN DCN ECN
Evaluation A

$C_{20}H_{10}O_6$ (c) 80BOE/WES2
Naphthalene-pyromellitic dianhydride adduct
Heat Capacity 298.15 K, $C_p = 392.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 300 K.
Entropy 298.15 K, $S = 411.5\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 346.2954
Wiswesser Line Notation T C565 DVOV JVOJV &L66J
Evaluation A

$C_{20}H_{12}$ (c) 80WON/WES
Perylene
Heat Capacity 298.15 K, $C_p = 274.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 5 to 575 K.
Entropy 298.15 K, $S = 264.6\ J \cdot mol^{-1} \cdot K^{-1}$
Phase Changes
c,I/liq 550.95 K, $\Delta H = 31874\ J \cdot mol^{-1}$
$\Delta S = 57.91\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 252.3148
Wiswesser Line Notation L666 L6 K6 2AL TJ
Evaluation A

$C_{20}H_{12}$ (c) 92SAB/ELW3
Perylene
Phase Changes
c/liq 551.29 K, $\Delta H = 32580\ J \cdot mol^{-1}$
Molecular Weight 252.3148
Wiswesser Line Notation L666 L6 K6 2AL TJ
Evaluation A

$C_{20}H_{13}N_3O_6$ (c) 80RAD/RAD
Anthracene-1,3,5-trinitrobenzene adduct
Heat Capacity 298.15 K, $C_p = 424.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 180 to 420 K. Data given graphically. C_p calculated from equation.
Phase Changes
c,I/liq 438.6 K, $\Delta H = 40401\ J \cdot mol^{-1}$
$\Delta S = 92.11\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 391.3392
Wiswesser Line Notation L C666J &WNR CNW ENW/
Evaluation B

$C_{20}H_{13}N_3O_7$ (c) 79FAR/SHA
Anthracene picric acid
Phase Changes
c,II/c,I 364.0 K, $\Delta H = 10500\ J \cdot mol^{-1}$
$\Delta S = 28.8\ J \cdot mol^{-1} \cdot K^{-1}$
c/liq 417.6 K, $\Delta H = 24300\ J \cdot mol^{-1}$
$\Delta S = 58.2\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 407.3386
Wiswesser Line Notation L C666J &WNR BQ CNW ENW
Evaluation B

$C_{20}H_{14}$ (c) 70AND/WES
Triptycene; 9,10-o-Benzeno-9,10-dihydroanthracene
Heat Capacity 298.15 K, C_p=282.67 J·mol^{-1}·K^{-1}
Temperature range 5 to 550 K.
Entropy 298.15 K, S=273.97 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 527.18 K, ΔH=30275 J·mol^{-1}
ΔS=57.43 J·mol^{-1}·K^{-1}
Molecular Weight 254.3306
Wiswesser Line Notation L6 H66 O66/GT 2AF T GH NHJ
Evaluation A

$C_{20}H_{14}$ (c) 73ROD/WES
Triptycene; 9,10-o-Benzeno-9,10-dihydroanthracene
Heat Capacity 298.15 K, C_p=283.1 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.266 cal·K^{-1}·g^{-1}.
Molecular Weight 254.3306
Wiswesser Line Notation L6 H66 O66/GT 2AF T GH NHJ
Evaluation A

$C_{20}H_{14}$ (c) 79FAR/SHA
β,β'-Binaphthyl
Phase Changes
c/liq 461.2 K, ΔH=38900 J·mol^{-1}
ΔS=84.4 J·mol^{-1}·K^{-1}
Molecular Weight 254.3306
Wiswesser Line Notation L66J A- AL66J
Evaluation B

$C_{20}H_{14}O_4$ (c) 84OZC/ASR
4,4′-Diethanoyloxydiphenyldiacetylene
Phase Changes
c,III/c,II 449 K, ΔH=7110 J·mol^{-1}
ΔS=15.86 J·mol^{-1}·K^{-1}
c,II/c,I 488 K, ΔH=40200 J·mol^{-1}
ΔS=62.38 J·mol^{-1}·K^{-1}
Molecular Weight 318.3282
Wiswesser Line Notation 1VOR DIUU2UU1R DOV1
Evaluation A
First heating, gradual decomposition observed on cycling.

$C_{20}H_{14}O_4$ (c) 84GRA/AVR
Phenolphthalein
Heat Capacity
Temperature range 300 to 550 K. Data given graphically.
Phase Changes
c,II/c,I 411 K, ΔH=22594 J·mol^{-1}
ΔS=55.0 J·mol^{-1}·K^{-1}
Amorphous/crystal.
c/liq 534 K, ΔH=51045 J·mol^{-1}
ΔS=95.6 J·mol^{-1}·K^{-1}
Molecular Weight 318.3282
Wiswesser Line Notation T56 BVOT&J DR DQ DR DQ
Evaluation B

$C_{20}H_{16}$ (c) 31SMI/AND
Triphenylethylene
Heat Capacity 298.5 K, C_p=309.2 J·mol^{-1}·K^{-1}
Temperature range 102 to 322 K. Value is unsmoothed experimental datum.
Molecular Weight 256.3464
Wiswesser Line Notation RYR&U1R
Evaluation C

$C_{20}H_{16}F_6Fe_2I_2Sb$ (c) 92WEB/HAG
1′,1‴-Diiodobiferrocenium hexafluoroantimonate
Heat Capacity
Temperature range 16 to 303 K.
Phase Changes
c,III/c,II 134 K, ΔH=740 J·mol^{-1}
ΔS=6.0 J·mol^{-1}·K^{-1}
c,II/c,I 270 K, ΔH=60 J·mol^{-1}
ΔS=0.3 J·mol^{-1}·K^{-1}
Molecular Weight 857.5958
Wiswesser Line Notation L5ϕJ AE ϕ-FE- ϕL5ϕJ A- AL5ϕJ ϕ-FE-- ϕL5ϕJ AE &-SB-F6
Evaluation A

$C_{20}H_{16}F_{12}O_8Zr$ (c) 92RIB/FER2
Tetrakis(1,1,1-trifluoropentane-2,4-dionato) zirconium (IV); Zirconium α,α,α-trifluoroacetylacetonate
Phase Changes
c/g 390 K, ΔH=118700 J·mol^{-1}
Molecular Weight 703.5424
Wiswesser Line Notation D6O-ZR-O ADJ DXFFF F1 B-& BD6O-ZR-O ADJ DXFFF F1 B-& BD6O-ZR-O ADJ DXFFF F1 B-& BD6O-ZR-O ADJ DXFFF F1
Evaluation A

$C_{20}H_{16}Fe_2I_3$ (c) 87SOR/NIS
Biferrocenium triiodide
Heat Capacity 300 K, C_p=463.72 J·mol^{-1}·K^{-1}
Temperature range 14 to 360 K. Interpolated data.
Phase Changes
c,II/c,I 358.675 K, ΔH=538 J·mol^{-1}
ΔS=1.77 J·mol^{-1}·K^{-1}
Molecular Weight 748.7539
Wiswesser Line Notation L5ϕJ ϕ-FE- ϕL5ϕJ A- AL5ϕJϕ-FE- ϕL5ϕJ &I3
Evaluation A

$C_{20}H_{18}$ (c) 31SMI/AND
1,1,1-Triphenylethane
Heat Capacity 298.5 K, C_p=316.7 J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 258.3622
Wiswesser Line Notation 1XR&R&R
Evaluation C

$C_{20}H_{18}$ (c) 31SMI/AND
1,1,2-Triphenylethane
Heat Capacity 298.5 K, C_p=319.7 J·mol^{-1}·K^{-1}
Temperature range 102 to 311 K. Value is unsmoothed experimental datum.
Molecular Weight 258.3622
Wiswesser Line Notation RYR&1R
Evaluation C

$C_{20}H_{18}Sn$ (c) 85CAR/LAY
Triphenyl vinyl tin
Heat Capacity 298.15 K, C_p=486.4 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.29 J·K^{-1}·g^{-1}.
Molecular Weight 377.0522
Wiswesser Line Notation 1U1-SN-R&R&R
Evaluation B

$C_{20}H_{20}$ (liq) 78GOO/SCO
5,6,6a,6b,7,8,12b,12c-Octahydrodibenzo-[a,i]biphenylene
Heat Capacity 298.15 K, C_p=333.4 J·mol^{-1}·K^{-1}
One temperature. C_p=0.306 cal·g^{-1}.
Molecular Weight 260.3780
Wiswesser Line Notation L D6 C6 B466 &TTT&J
Evaluation B

$C_{20}H_{20}$ (liq) 78GOO/SCO
5,6,6a,6b,11,12,12a,12b-Octahydrodibenzo-[a,g]biphenylene
Heat Capacity 298.15 K, C_p=323.6 J·mol^{-1}·K^{-1}
One temperature. C_p=0.297 cal·g^{-1}.
Molecular Weight 260.3780
Wiswesser Line Notation L F6 C6 B466 &TTT&J
Evaluation B

$C_{20}H_{22}$ (liq) 78GOO/SCO
2,2′-Bitetralin
Heat Capacity 298.15 K, C_p=379.9 J·mol^{-1}·K^{-1}
One temperature. C_p=0.346 cal·g^{-1}.
Molecular Weight 262.3938
Wiswesser Line Notation L66T&J C- CL66TT&J
Evaluation B

$C_{20}H_{22}N_2O$ (c) 79TSU/SOR
p-n-Hexyloxybenzylideneamino-p′-benzonitrile
Heat Capacity 298.15 K, C_p=432.51 J·mol^{-1}·K^{-1}
Temperature range 15 to 385 K.
Entropy 298.15 K, S=450.56 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 306.98 K. ΔH=5110 J·mol^{-1}
ΔS=16.7 J·mol^{-1}·K^{-1}
c,I/liq 334.05 K, ΔH=23770 J·mol^{-1}
ΔS=71.2 J·mol^{-1}·K^{-1}
Solid nematic.
liq/liq 375.10 K, ΔH=1750 J·mol^{-1}
ΔS=3.2 J·mol^{-1}·K^{-1}
Nematic-isotropic liquid transition (Note: 1750/375.10=4.67 J·mol^{-1}·K^{-1}).
Molecular Weight 306.4066
Wiswesser Line Notation NCR DNU1R DO6
Evaluation A

$C_{20}H_{22}N_2O_3$ (c) 88FAN/POE
4-n-Pentanoyl-4-n′-propanoyloxyazobenzene
Phase Changes
c,II/c,I 345.1 K, ΔH=2632 J·mol^{-1}
ΔS=7.627 J·mol^{-1}·K^{-1}
c,I/liq 391.5 K, ΔH=24167 J·mol^{-1}
ΔS=61.731 J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 394.1 K, ΔH=3272 J·mol^{-1}
ΔS=8.301 J·mol^{-1}·K^{-1}
Smectic A-nematic.
liq/liq 406.1 K, ΔH=690 J·mol^{-1}
ΔS=1.699 J·mol^{-1}·K^{-1}
Nematic-isotropic.
Molecular Weight 338.4054
Wiswesser Line Notation 4VR DNUNR DOV2
Evaluation A

$C_{20}H_{22}O_6$ (c) 91KRI
Butyl p-(p-ethoxyphenoxycarbonyl)phenylcarbonate
Phase Changes
c,II/liq 328.3 K, ΔH=23400 J·mol^{-1}
Radial spherulite/nematic.
c,I/liq 337.6 K, ΔH=31800 J·mol^{-1}
Tangential spherulite/nematic.
liq/liq 358.1 K
Nematic/isotropic.
Molecular Weight 358.3902
Wiswesser Line Notation 4OVOR DVOR DO2
Evaluation A

$C_{20}H_{24}N_2O_3$ (liq) 85SHA/ZHU
4-Methyoxy-4′-heptanoylazobenzene
Heat Capacity 351.84 K, C_p=685.9 J·mol^{-1}·K^{-1}
Temperature range 351 to 374 K. Unsmoothed experimental datum.
Phase Changes
liq/liq 371.6 K, ΔH=573 J·mol^{-1}
ΔS=1.54 J·mol^{-1}·K^{-1}
Molecular Weight 340.4212
Wiswesser Line Notation 6VOR DNUNR DO1
Evaluation B

$C_{20}H_{24}O_2$ (c) 72YOU/HAL
2-Methoxy-4′-pentoxy-trans-stilbene
Phase Changes
c/liq 435 K, ΔH=41170 J·mol^{-1}
ΔS=94.6 J·mol^{-1}·K^{-1}
Crystal-isotropic liquid transition.
liq/liq 427 K, ΔH=782 J·mol^{-1}
ΔS=1.8 J·mol^{-1}·K^{-1}
Nematic-isotropic liquid transition.
Molecular Weight 296.4084
Wiswesser Line Notation 5OR D1U1R DO1 -T
Evaluation B

$C_{20}H_{25}NO$ (c) 82TSU/SOR4
p-n-Hexyloxybenzylidene-p′-toluidine
Heat Capacity 298.15 K, C_p=441.40 J·mol^{-1}·K^{-1}
Temperature range 17 to 385 K.
Entropy 298.15 K, S=448.95 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 317.5 K, ΔH=5040 J·mol^{-1}
ΔS=15.89 J·mol^{-1}·K^{-1}
Superheating phenomenon occurs at 324 K.
c,I/liq 334.26 K. ΔH=25040 J·mol^{-1}
ΔS=74.90 J·mol^{-1}·K^{-1}
Solid-nematic.
liq/liq 346.90 K, ΔH=1370 J·mol^{-1}
ΔS=3.0 J·mol^{-1}·K^{-1}
Nematic-isotropic liquid transition.
Molecular Weight 295.4236
Wiswesser Line Notation 60R D1UNR D1
Evaluation A

$C_{20}H_{26}N_2O_3$ (c) 90BAM/GOD
4,4′-Di-n-butyloxyazoxybenzene
Phase Changes

c,IV/c,III	315.5 K,	$\Delta H = 10440\ J \cdot mol^{-1}$
		$\Delta S = 33.09\ J \cdot mol^{-1} \cdot K^{-1}$
c,III/c,II	323.4 K,	$\Delta H = 930\ J \cdot mol^{-1}$
		$\Delta S = 2.88\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I	360.5 K,	$\Delta H = 1570\ J \cdot mol^{-1}$
		$\Delta S = 4.36\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq	376.7 K,	$\Delta H = 20960\ J \cdot mol^{-1}$
		$\Delta S = 55.64\ J \cdot mol^{-1} \cdot K^{-1}$

c,I to nematic liquid.
Molecular Weight 326.4376
Wiswesser Line Notation 4OR DNUNO&R DO4
Evaluation A

$C_{20}H_{26}O$ (c) 79LEW/ENE
Norethindrone
Phase Changes

c/liq	479 K,	$\Delta H = 39600\ J \cdot mol^{-1}$
		$\Delta S = 82.7\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 282.4248
Wiswesser Line Notation L E5 B666 OV MUTJ E1 FQ F1UU1
Evaluation A

$C_{20}H_{28}O_8Zr$ (c) 86GRI/LAZ
Zirconium acetylacetonate; Tetrakis(pentane-2,4-dionato)zirconium (IV)
Phase Changes

c/liq	470.8 K,	$\Delta H = 50100\ J \cdot mol^{-1}$
		$\Delta S = 106.3\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 487.6564
Wiswesser Line Notation D60-ZR-O ADJ D1 F1 B-& BD6O-ZR-O ADJ D1 F1 B-& BD60-ZR-O ADJ D1 F1 B-& BD6O-ZR-O ADJ D1 F1
Evaluation A

$C_{20}H_{28}O_8Zr$ (c) 91JAS
Zirconium acetylacetonate; Tetrakis(pentane-2,4-dionato)zirconium (IV)
Phase Changes

c/liq	472 K,	$\Delta H = 22597\ J \cdot mol^{-1}$

Molecular Weight 487.6564
Wiswesser Line Notation D60-ZR-O ADJ D1 F1 B-& BD6O-ZR-O ADJ D1 F1 B-& BD60-ZR-O ADJ D1 F1 B-& BD6O-ZR-O ADJ D1 F1
Evaluation D

$C_{20}H_{28}O_8Zr$ (c) 92RIB/FER2
Zirconium acetylacetonate; Tetrakis(pentane-2.4-dionato)zirconium (IV)
Phase Changes

c/g	406 K,	$\Delta H = 125800\ J \cdot mol^{-1}$

Molecular Weight 487.6564
Wiswesser Line Notation D6O-ZR-O ADJ D1 F1 B-& BD6O-ZR-O ADJ D1 F1 B-& BD6O-ZR-O ADJ D1 F1 B-& BD6O-ZR-O ADJ D1 F1
Evaluation A

$C_{20}H_{30}$ (c) 84BER/BEC
Hexacyclopropylethane

Heat Capacity	298.15 K,	$C_p = 396.1\ J \cdot mol^{-1} \cdot K^{-1}$

One temperature.
Molecular Weight 270.4570
Wiswesser Line Notation
Evaluation B

$C_{20}H_{30}Cl_2FeN_6O$ (c) 85KAJ/SOR
Tris(2-picolylamine)iron chloride ethanolate

Heat Capacity	300 K,	$C_p = 590\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 13 to 315 K. Data graphically only. Value estimated from graph.
Phase Changes

c,III/c,II	114.04 K	
c,II/c,I	122.21 K,	$\Delta H = 6140\ J \cdot mol^{-1}$
		$\Delta S = 50.59\ J \cdot mol^{-1} \cdot K^{-1}$

Total transition enthalpy and entropy.
Molecular Weight 500.2734
Wiswesser Line Notation T6NJ B1ZH 3 .FE G2 &G2
Evaluation C_p(C), transitions(A)

$C_{20}H_{30}O_3Si_3$ (liq) 87DZH/KUL
1,1,3,3-Tetraethyl-5,5-diphenylcylotrisiloxane

Heat Capacity	298.15 K,	$C_p = 629.6\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 5 to 315 K.

Entropy	298.15 K,	$S = 711.4\ J \cdot mol^{-1} \cdot K^{-1}$

Phase Changes

c/liq	279.082 K,	$\Delta H = 18374\ J \cdot mol^{-1}$
		$\Delta S = 66.01\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 402.7117
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 ER ER
Evaluation A

$C_{20}H_{34}$ (liq) 63GUD/CAN
Diethylhydropyrene

Heat Capacity	313 K,	$C_p = 510.9\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 313 to 583 K.
Molecular Weight 274.4886
Wiswesser Line Notation L666 B6 2AB PTJ X2 X2
Evaluation C

$C_{20}H_{34}O_5Si_5$ (liq) 77KUL/DZH
Octamethyldiphenylcyclopentasiloxane
Heat Capacity
No C_p data given. Data in paper, deposited in VINITI, No. 986-77, 1-March, 1977.
Molecular Weight 494.9131
Wiswesser Line Notation
T-10-O-SI-O-SI-O-SI-O-SI-O-SITJ A1 B1 C1 D1 E1 X1 X1 X1 XR& XR
Evaluation B

$C_{20}H_{36}$ (liq) 63GUD/CAN
Bis(cyclohexylmethyl)cyclohexane

Heat Capacity	373 K,	$C_p = 603.8\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 373 to 583 K.
Molecular Weight 276.5044
Wiswesser Line Notation L6TJ A1AL6TJ X1- AL6TJ
Evaluation C

$C_{20}H_{38}HgO_4$ (liq) 78AD
Mercuric decanoate; Mercuric caprate

Heat Capacity	410 K,	$C_p = 817.0\ J \cdot mol^{-1} \cdot K^{-1}$

Mean value 403 to 420 K. Data only graphically for solid.
Phase Changes

c,II/c,I	380.8 K,	$\Delta H = 5300\ J \cdot mol^{-1}$
		$\Delta S = 13.9\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq	389.3 K,	$\Delta H = 70200\ J \cdot mol^{-1}$
		$\Delta S = 180.3\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 543.1078
Wiswesser Line Notation OV9 2 .HG
Evaluation C

$C_{20}H_{38}O$ (liq) 88BAG/GUR
3,7,11,15-Tetramethyl-1-hexadecyn-3-ol
Heat Capacity 293.85 K, C_p=712.7 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 294.5196
Wiswesser Line Notation 1Y3Y3Y3XQ1UU1
Evaluation B

$C_{20}H_{38}O$ (liq) 88BAG/GUR
3,7,11,15-Tetramethyl-1-hexadecen-3-ol; Isophytol
Heat Capacity 293.75 K, C_p=729.5 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K. Unsmoothed experimental datum.
Molecular Weight 294.5196
Wiswesser Line Notation 1Y3Y3Y3XQ1U1
Evaluation B

$C_{20}H_{38}O_4Pb$ (c) 76ADE/SIM
Lead(II) decanoate
Phase Changes
c/liq 354.9 K, ΔH=32700 J·mol^{-1}
ΔS=92.0 J·mol^{-1}·K^{-1}
Crystal-smectic.
liq/liq 367.4 K, ΔH=20000 J·mol^{-1}
ΔS=54.4 J·mol^{-1}·K^{-1}
Smectic-isomorphous.
liq/liq 385.2 K, ΔH=1000 J·mol^{-1}
ΔS=2.7 J·mol^{-1}·K^{-1}
Isomorphous-liquid.
Molecular Weight 549.7178
Wiswesser Line Notation OV9 2 .PB
Evaluation B

$C_{20}H_{38}O_4Zn$ (c) 78KON/RUF
Zinc(II) n-decanoate
Phase Changes
c,III/c,II 372 K, ΔH=2100 J·mol^{-1}
c,II/c,I 378 K, ΔH=3800 J·mol^{-1}
c,I/liq 407 K, ΔH=49000 J·mol^{-1}
ΔS=120 J·mol^{-1}·K^{-1}
Molecular Weight 407.8978
Wiswesser Line Notation OV9 2 .ZN
Evaluation B

$C_{20}H_{40}Br_2N_2$ (c) 74BUR/VER
1,2-Bis(triallylammonium)ethane dibromide
Heat Capacity 298 K, C_p=520.5 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
Molecular Weight 468.3574
Wiswesser Line Notation 1U2K2U1&2U1&2K2U1&2U1&2U1 E 2
Evaluation B

$C_{20}H_{40}O_2$ (c) 34KIN/GAR
Ethyl octadecanoate; Ethyl stearate
Phase Changes
c,II/c,I 300.15 K, ΔH=6373 J·mol^{-1}
β-α transition.
c,I/liq 304.2 K, ΔH=12339 J·mol^{-1}
α-liq transition.
Molecular Weight 312.5348
Wiswesser Line Notation 17VO2
Evaluation B
Data on the specific heats are given at or near the phase transitions.

$C_{20}H_{40}O_2$ (c) 36KIN/GAR
Methyl nonadecanoate
Phase Changes
c,II/c,I 311.79 K, ΔH=6054 J·mol^{-1}
Heat of transition at melting point.
Molecular Weight 312.5348
Wiswesser Line Notation 18VO1
Evaluation B

$C_{20}H_{40}O_2$ (c) 82SCH/MIL2
Eicosanoic acid
Heat Capacity 298.15 K, C_p=545.14 J·mol^{-1}·K^{-1}
Temperature range 80 to 355 K.
Phase Changes
c,I/liq 348.23 K, ΔH=69204 J·mol^{-1}
ΔS=198.7 J·mol^{-1}·K^{-1}
Molecular Weight 312.5348
Wiswesser Line Notation QV19
Evaluation B

$C_{20}H_{42}$ (c) 30PAR/HUF
n-Eicosane
Heat Capacity 279.1 K, C_p=602.5 J·mol^{-1}·K^{-1}
Temperature range 94 to 280 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, S=558.6 J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 64.68 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 309.7 K, ΔH=61476 J·mol^{-1}
ΔS=198.50 J·mol^{-1}·K^{-1}
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation B(C_p),C(S)

$C_{20}H_{42}$ (c) 55SCH/BUS
n-Eicosane
Phase Changes
c,II/c,I 309.35 K
c,I/liq 309.75 K, ΔH=69873 J·mol^{-1}
ΔS=225.6 J·mol^{-1}·K^{-1}
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation B

$C_{20}H_{42}$ (c) 73COM
n-Eicosane
Phase Changes
c/liq 309.75 K, ΔH=69873 J·mol^{-1}
ΔS=225.6 J·mol^{-1}·K^{-1}
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation B

$C_{20}H_{42}$ (liq) 81HOE
n-Eicosane
Heat Capacity 325 K, C_p=664 J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K. Cv=2.32 J·g^{-1}·K^{-1}.
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation B

$C_{20}H_{42}$ (c) 84SYU/TUM
n-Eicosane
Phase Changes
c/liq 308.5 K, $\Delta H = 70900\ J \cdot mol^{-1}$
$\Delta S = 229.8\ J \cdot mol^{-1} \cdot K^{-1}$
Relative error in determination ±5%.
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation C

$C_{20}H_{42}$ (c) 85KOL/SYU
n-Eicosane
Phase Changes
c/liq 308.8 K, $\Delta H = 67800\ J \cdot mol^{-1}$
$\Delta S = 219.6\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation A

$C_{20}H_{42}$ (liq) 89KSI
n-Eicosane
Phase Changes
c,α/liq 309.63 K
c,β/liq 309.32 K
c,α/c,β 309.24 K
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation A

$C_{20}H_{42}$ (c) 91BAR/SCH
n-Eicosane
Phase Changes
c/liq 309.6 K, $\Delta H = 69000\ J \cdot mol^{-1}$
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation A

$C_{20}H_{42}$ (liq) 91CLA/LET
n-Eicosane
Phase Changes
c,II/c,I $\Delta H = 18395\ J \cdot mol^{-1}$
Transition temperature not measurable.
c,II/liq 309.2 K, $\Delta H = -46170\ J \cdot mol^{-1}$
c,I/liq 310.0 K, $\Delta H = 66935\ J \cdot mol^{-1}$
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation A

$C_{20}H_{42}S$ (liq) 82TUT/GAB
1-Eicosanethiol; n-Eicosanyl mercaptan
Heat Capacity 300 K, $C_p = 725.84\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 273 to 373 K. $C_p = 702.70 + 4.703 \times 10^{-2} T + 10.040 \times 10^{-5} T^2$.
Molecular Weight 314.6118
Wiswesser Line Notation SH20
Evaluation B

$C_{20}H_{44}ClN$ (c) 88VAN/WHI
Di-n-decylammonium chloride
Heat Capacity 297.93 K, $C_p = 631.9\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 25 to 350 K. Unsmoothed experimental datum.
Phase Changes
c,III/c,II 320.13 K
c,II/c,I 321.50 K, $\Delta H = 50590\ J \cdot mol^{-1}$
$\Delta S = 158.97\ J \cdot mol^{-1} \cdot K^{-1}$
$\Delta\Delta H$, $\Delta\Delta S$ combined data.
Molecular Weight 334.0273
Wiswesser Line Notation 10M10 &GH
Evaluation A

$C_{20}H_{44}Sn$ (liq) 72MAS/RAB
Tetraamylstannane; Tin tetraamyl
Heat Capacity 298.15 K, $C_p = 652.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 60 to 300 K.
Phase Changes
c,II/c,I 181.4 K, $\Delta H = -9920\ J \cdot mol^{-1}$
Metastable transition.
Molecular Weight 403.2576
Wiswesser Line Notation 5-SN-5&5&5
Evaluation B

$C_{20}H_{46}Br_2N_2$ (c,II) 74BUR/VEF
1,8-Bis(triethylammonium)octane dibromide
Heat Capacity 298 K, $C_p = 574.5\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 273 to 373 K.
Phase Changes
c,II/c,I 438 K, $\Delta H = 12130\ J \cdot mol^{-1}$
$\Delta S = 27.7\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 430 to 446 K.
Molecular Weight 474.4048
Wiswesser Line Notation 2K2&2&8K2&2&2 E 2
Evaluation B

$C_{20}H_{48}CdCl_4N_2$ (c) 85RIC/CAV
Bis-decylammonium tetrachlorocadmium
Phase Changes
c,III/c,II 308 K, $\Delta H = 8000\ J \cdot mol^{-1}$
$\Delta S = 25\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I 313 K, $\Delta H = 29500\ J \cdot mol^{-1}$
$\Delta S = 95\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 570.8346
Wiswesser Line Notation -10-ZH 2 .CD G4
Evaluation B

$C_{20}H_{48}Cl_4MnN_2$ (c) 75BOC/ARI
Tetrachlorobis-(decylammonium) manganese II
Phase Changes
c,III/c,II 309 K, $\Delta H = 1937\ J \cdot mol^{-1}$
$\Delta S = 6.3\ J \cdot mol^{-1} \cdot K^{-1}$
c,II/c,I 437 K, $\Delta H = 16.8\ J \cdot mol^{-1}$
$\Delta S = 0.038\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 513.3626
Wiswesser Line Notation MN Z10&Z10 -G4
Evaluation A

$C_{20}H_{48}CrI_2P_4$ (c) 93SOR/YUM
trans-Bis[1,2-bis(diethylphosphino)ethane] diiodochromium(II)
Heat Capacity 300 K, C_p=740.96 J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 171.15 K, ΔH=6686 J·mol^{-1}
ΔS=39.45 J·mol^{-1}·K^{-1}
Molecular Weight 718.2992
Wiswesser Line Notation
Evaluation A

$C_{20.84}H_{16.66}O_{0.62}$ (c) 78KAR/SAP
Polyphenylene PP-1 (linear)
Heat Capacity 300 K, C_p=280 J·mol^{-1}·K^{-1}
Temperature range 100 to 600 K. Data given graphically. Value estimated from graph.
Entropy 298.15 K, S=253.0 J·mol^{-1}·K^{-1}
Molecular Weight 277.0205
Wiswesser Line Notation /*R DR C* ER/
Evaluation C
WLN excludes ketal end groups and uses the repeating unit: $(C_{18}H_{12})_n$.

$C_{20.84}H_{16.66}O_{0.62}$ (c) 79KAR/SAP
Polyphenylene PP-2 (crosslinked)
Heat Capacity 300 K, C_p=230 J·mol^{-1}·K^{-1}
Temperature range 100 to 600 K. Data given graphically. Value estimated from graph.
Entropy 298.15 K, S=222.5 J·mol^{-1}·K^{-1}
Molecular Weight 277.0205
Wiswesser Line Notation /R A* D- ARC* ER/
Evaluation C
WLN excludes ketal end groups and uses the repeating unit: $(C_{18}H_{12})_n$. PP-2 is the product of thermal crosslinking of PP-1.

$(C_{21}H_{12}N_2O_2)_n$ (c) 73KAR/MOC2
Poly-2,2′-(m-phenylene)-5,5′-dibenzoxazole methane
Heat Capacity 300 K, C_p = 324.6 J· mol^{-1}· K^{-1}
Temperature range 100 to 490 K.
Entropy 300 K, S=330.3 J·mol^{-1}·K^{-1}
Molecular Weight 324.3381
Wiswesser Line Notation /T56 BN DOJ C* H1H- HT56 BN DOJ CR& C*/
Evaluation B
Anomaly in the C_p vs. T curve at 450 to 520 K.

$(C_{21}H_{12}N_2O_2)_n$ (c) 75KAR/RAB
Poly-2,2′-(m-phenylene)-5,5′-dibenzoxazole methane
Heat Capacity
Temperature range 60 to 350 K. Data given graphically.
Entropy 300 K, S=330.3 J·mol^{-1}·K^{-1}
Molecular Weight 324.3381
Wiswesser Line Notation /T56 BN DOJ C* H1H- HT56 BN DOJ CR& C*/
Evaluation A

$C_{21}H_{14}N_2O_4$ (c) 78MAR/CIO
Bis-(4-(N-maleicimido)phenyl)methane
Heat Capacity 298 K, C_p=118.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 571 K. Values for solid seem odd; increase from 118 to 345 J·mol^{-1}·K^{-1} at 420 K.
Phase Changes
c/liq 430.9 K, ΔH=18220 J· mol^{-1}
ΔS=42.3 J· mol^{-1}· K^{-1}
Molecular Weight 358.3526
Wiswesser Line Notation T5VNVJ BR D1R D- BT5VNVJ
Evaluation D

$C_{21}H_{15}N_3$ (c) 84LEB/BYK2
Triphenyl-s-triazine
Heat Capacity 298.15 K, C_p = 345.1 J· mol^{-1}· K^{-1}
Temperature range 18 to 330 K.
Entropy 298.15 K, S = 349.6 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 506.65 K
Molecular Weight 309.3696
Wiswesser Line Notation T6N CN ENJ BR DR FR
Evaluation A

$C_{21}H_{15}N_{11}O_{20}$ (c) 24TAY/RIN
Tetryl-bis(trinitrotoluene) complex
Heat Capacity 293 K, C_p = 955.6 J· mol^{-1}· K^{-1}
Temperature range 90 to 333 K.
Molecular Weight 741.4112
Wiswesser Line Notation WNN1&R DNW DNW FNW &WNR BCNW ENW 2
Evaluation C

$C_{21}H_{16}$ (c) 77FIN/MES
1,2′-Dinaphthylmethane
Heat Capacity 298.15 K, C_p=314.51 J· mol^{-1}· K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, S=310.75 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 369.55 K, ΔH=30557.0 J· mol^{-1}
ΔS = 82.69 J· mol^{-1}· K^{-1}
Molecular Weight 268.3574
Wiswesser Line Notation L66J B1- CL66J
Evaluation A

$(C_{21}H_{16}N_2O_4)_n$ (c) 73KAR/MOC2
Poly-4,4′-dihydroxy-3,3′-isophthalamidodiphenylmethane
Heat Capacity 300 K, C_p=476.1 J· mol^{-1}· K^{-1}
Temperature range 100 to 490 K.
Entropy 300 K, S=448.1 J· mol^{-1}· K^{-1}
Molecular Weight 360.3685
Wiswesser Line Notation /*VMR BQ EIR DQ CMVR C*/
Evaluation B
Anomalies in C_p vs. T curve at 360 to 440 K and 450 to 520 K.

$(C_{21}H_{16}N_2O_4)_n$ (c) 75KAR/RAB
Poly-4,4′-dihydroxy-3,3′-isophthalamidodiphenylmethane
Heat Capacity
Temperature range 60 to 350 K. Data given graphically.
Entropy 300 K, S = 448.1 J· mol^{-1}· K^{-1}
Molecular Weight 360.3685
Wiswesser Line Notation /*VMR BQ EIR DQ CMVR C*/
Evaluation A

$C_{21}H_{21}O_4P$ (gls) 86OVC/POD
Tricresyl phosphate
Heat Capacity 298.15 K, C_p = 578 J· mol^{-1}· K^{-1}
Temperature range 6 to 320 K.
Entropy 298.15 K, S = 570 J· mol^{-1}· K^{-1}
Molecular Weight 368.3683
Wiswesser Line Notation OPOR D1 &OR D1 &OR D1
Evaluation A
Glass transition, T(glass) = 207.0 K.

$C_{21}H_{24}N_2O_3$ (c) 88FAN/POE
4-*n*-Pentanoyl-4-*n*′-butanoyloxyazobenzene
Phase Changes
c/liq 373.3 K, ΔH=14234 J·mol^{-1}
ΔS=38.12 J· mol^{-1}· K^{-1}
Solid-smectic 2.
liq/liq 378.1 K, ΔH=14242 J· mol^{-1}
ΔS= 37.67 J· mol^{-1}· K^{-1}
Smectic 2-smectic A.
liq/liq 398.4 K, ΔH=3406 J· mol^{-1}
ΔS=8.548 J· mol^{-1}· K^{-1}
Smectic A-nematic.
liq/liq 404.7 K, ΔH=766 J· mol^{-1}
ΔS=1.891 J· mol^{-1}· K^{-1}
Nematic-isotropic.
Molecular Weight 352.4322
Wiswesser Line Notation 4VR DNUNR DOV3
Evaluation A

$C_{21}H_{24}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-hexanoyloxyazobenzene
Phase Changes
liq/liq 361.65 K, ΔH=2720 J·mol^{-1}
Smectic A—smectic B (monotropic phase) liquid transition.
c/liq 372.15 K, ΔH=29790 J· mol^{-1}
Solid–smectic A.
liq/liq 411.65 K, ΔH=3933 J· mol^{-1}
Smectic A–nematic liquid transition.
liq/liq 420.65 K, ΔH=879 J· mol^{-1}
Nematic–isotropic liquid transition.
Molecular Weight 352.4322
Wiswesser Line Notation 5VOR DNUNR DV2
Evaluation A

$C_{21}H_{24}O_3Si_3$ (c) 75MEK/KAR3
cis-1,3,5-Trimethyl-1,3,5-triphenylcyclotrisiloxane
Heat Capacity 298.15 K, C_p=538.5 J· mol^{-1}· K^{-1}
Temperature range 13 to 390 K.
Entropy 298.15 K, S=571.1 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 374.4 K, ΔH=43070 J· mol^{-1}
ΔS=115.5 J· mol^{-1}· K^{-1}
Molecular Weight 408.6753
Wiswesser Line Notation T6-SI O-SI-O-SI-OTJ A1 AR C1 CR E1 ER -C
Evaluation

$C_{21}H_{24}O_3Si_3$ (c) 75MEK/KAR3
trans-1,3,5-Trimethyl-1,3,5-triphenylcyclotrisiloxane
Heat Capacity 298.15 K, C_p=506.7 J· mol^{-1}· K^{-1}
Temperature range 13 to 390 K.
Entropy 298.15 K, S=565.3 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 321.2 K, ΔH=43769 J· mol^{-1}
ΔS=136.4 J· mol^{-1}· K^{-1}
Molecular Weight 408.6753
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A1 AR C1 CR E1 ER-T
Evaluation A

$C_{21}H_{24}Si_3O_3$ (c) 81MEK/KAR
cis-Tri(methylphenyl)trisiloxane
Heat Capacity 298.15 K, C_p = 538.5 J· mol^{-1}· K^{-1}
Temperature range 13 to 390 K. Data given graphically.
Entropy 298.15 K, S=571.1 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 373.2 K, ΔH= 47254 J· mol^{-1}
ΔS=115.5 J· mol^{-1}· K^{-1}
Molecular Weight 408.6753
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A1 AR C1 CR E1 ER -C
Evaluation A

$C_{21}H_{24}Si_3O_3$ (c) 81MEK/KAR
trans-Tri(methylphenyl)trisiloxane
Heat Capacity 298.15 K, C_p=506.7 J· mol^{-1}· K^{-1}
Temperature range 13 to 390 K. Data given graphically.
Entropy 298.15 K, S=564 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 320.9 K, ΔH=43769 J· mol^{-1}
ΔS=136.4 J· mol^{-1}· K^{-1}
Molecular Weight 408.6753
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A1 AR C1 CR E1 ER -T
Evaluation A

$C_{21}H_{24}O_4$ (c) 87LES/LIC
2,2-*Bis*(phenyl-4-glycidoxy)propane
Heat Capacity 298 K, C_p=485.9 J· mol^{-1}· K^{-1}
Temperature range 250 to 300 K.
Phase Changes
c/liq 313 K
Molecular Weight 340.4182
Wiswesser Line Notation T3OTJ B1OR DXR DO1- -BT3OTJ
Evaluation B

$C_{21}H_{25}N$ (liq) 82THO/MAR
4-Octyl-4′-cyanobiphenyl
Phase Changes
c/liq 294.45 K, ΔH=25700 J· mol^{-1}
ΔS= 87.3 J· mol^{-1}· K^{-1}
Solid-smectic A.
liq/liq 306.921 K
Smectic A-nematic. Continuous transition with an upper limit of 0.4 J·mol^{-1}.
liq/liq 313.91 K, ΔH=612 J· mol^{-1}
ΔS=1.95 J· mol^{-1}· K^{-1}
Nematic-isotropic.
Molecular Weight 291.4352
Wiswesser Line Notation NCR DR D8
Evaluation B

$C_{21}H_{25}N$ (c) 83MAR/THC
4-Octyl-4′-cyanobiphenyl
Phase Changes
c/liq 294.45 K, ΔH=25700 J· mol^{-1}
Solid-smectic A.
liq/liq 306.921 K, ΔH=0.4 J· mol^{-1}
Smectic A-nematic.
liq/liq 313.91 K, ΔH=612 J· mol^{-1}
Nematic-isotropic.
Molecular Weight 291.4352
Wiswesser Line Notation NCR DR D8
Evaluation D

$C_{21}H_{25}NO$ (c) 78JOH/HAY
Octyloxycyanobiphenyl
Heat Capacity
C_p data given graphically only. Temperature range 334 to 348 K.
Smectic A-nematic transition at 340 K.
Molecular Weight 307.4346
Wiswesser Line Notation NCR DR DO8
Evaluation D

$C_{21}H_{25}NO_5$ (c) 79BAT/BUK
4-Nitrophenyl-4′-*n*-octyloxybenzoate
Phase Changes

c,II/c,I	323 K	
c,II/liq	323.2 K,	ΔH=34720 J· mol^{-1}
		ΔS=108 J· mol^{-1}· K^{-1}
liq/liq	334 K,	ΔH=90 J· mol^{-1}
		ΔS=0.30 J· mol^{-1}· K^{-1}

Smectic A nematic.

liq/liq	341 K,	ΔH=290 J· mol^{-1}
		ΔS=0.88 J· mol^{-1}· K^{-1}

Nematic-isotropic.
Molecular Weight 371.4322
Wiswesser Line Notation WNR DOVR DO8
Evaluation B

$C_{21}H_{25}NO_5$ (c) 82RAC/MAS
4-Nitrophenyl-4′-*n*-octyloxybenzoate
Heat Capacity 300 K, C_p=510 J· mol^{-1}· K^{-1}
Temperature range 100 to 356 K. Data given graphically. Value given is an estimate from the graph.
Phase Changes

c/liq	323.70 K,	ΔH=34426 J· mol^{-1}
		ΔS=106.4 J· mol^{-1}· K^{-1}

Solid-smectic.

liq/liq	334.9 K,	ΔH=213 J· mol^{-1}
		ΔS=0.59 J· mol^{-1}· K^{-1}

Smectic-nematic.

liq/liq	341.2 K,	ΔH=448 J· mol^{-1}
		ΔS=1.3 J· mol^{-1}· K^{-1}

Nematic-isotropic.
Molecular Weight 371.4322
Wiswesser Line Notation WNR DOVR DO8
Evaluation B

$C_{21}H_{26}O_2$ (c) 72YOU/HAL
4-Methoxy-4′-hexoxy-trans-stilbene
Phase Changes

c/liq	430 K,	ΔH=41380 J· mol^{-1}
		ΔS=96.2 J· mol^{-1}· K^{-1}

Crystal-isotropic liquid transition.

liq/liq	426 K,	ΔH=791 J· mol^{-1}
		ΔS=1.9 J· mol^{-1}· K^{-1}

Nematic-isotropic liquid transition.
Molecular Weight 310.4352
Wiswesser Line Notation 6OR D1U1R CO1 -T
Evaluation B

$C_{21}H_{27}N_7O_{14}P_2\cdot 3H_2O$ (c) 79YAN/RUP
Nicotinamide adenine dinucleotide trihydrate; NAD
Heat Capacity 298 K, C_p=773 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 717.4760
Wiswesser Line Notation T56 BN DN FN HNJ IZ D- BT5OTJ CQ DQ E1OPQOPOP1OPO1- BT5OTJ CQ DQ E-AT6NJ CVZ &QH 3
Evaluation C

$C_{21}H_{30}O$ (c) 92ABB/JIM
1,1′-Diadamantyl ketone
Heat Capacity 298.15 K, C_p=355.2 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 298.4674
Wiswesser Line Notation L66 B6/B-H/DI A B- C 1B ITJ BV- BL66 B6/B-H/DI A B- C 1B ITJ
Evaluation B

$C_{21}H_{38}$ (liq) 63GUD/CAM
9-(2′-Ethylhexyl)perhydrofluorene
Heat Capacity 313 K, C_p=610.4 J· mol^{-1}· K^{-1}
Temperature range 313 to 583 K.
Molecular Weight 290.5312
Wiswesser Line Notation L B656TJ H1Y4&2
Evaluation C

$C_{21}H_{38}$ (liq) 63GUD/CAM
1,1,3-Tricyclohexylpropane
Heat Capacity 373 K, C_p=638.1 J· mol^{-1}· K^{-1}
Temperature range 373 to 583 K.
Molecular Weight 290.5312
Wiswesser Line Notation L6TJ AY2AL6TJ&- AL6TJ
Evaluation C

$C_{21}H_{38}O_6$ (liq) 76PHI/MAT
Tricaproin; Glyceryl tricaproate
Heat Capacity 313 K, C_p = 753 J· mol^{-1}· K^{-1}
Temperature range 313 to 413 K.
Molecular Weight 386.5276
Wiswesser Line Notation 5VO1YOV5&1OV5
Evaluation C

$C_{21}H_{40}$ (liq) 63GUD/CAM
4-*n*-Nonylbicyclohexyl
Heat Capacity 313 K, C_p=578.8 J· mol^{-1}· K^{-1}
Temperature range 313 to 483 K.
Molecular Weight 292.5470
Wiswesser Line Notation L6TJ A -AL6TJ D9
Evaluation C

$C_{21}H_{42}Br_2N_2$ (c) 74BUR/VER
1,3-*Bis*(triallylammonium)propane dibromide
Heat Capacity 298 K, C_p = 538.1 J· mol^{-1}· K^{-1}
Temperature range 273 to 373 K.
Molecular Weight 482.3842
Wiswesser Line Notation 1U2K2U1&2U1&3K2U1&2U1&2U1 2
Evaluation B

$C_{21}H_{42}O_2$ (c) 36KIN/GAR
Ethyl nonadecanoate
Phase Changes

c,II/c,I	309.2 K,	ΔH=6631 J· mol^{-1}

Heat of transition at melting point.
Molecular Weight 358.5604
Wiswesser Line Notation 18VO2
Evaluation B

$C_{21}H_{42}O_2$ (c) 36KIN/GAR
Methyl eicosanoate
Phase Changes
c/liq 318.56 K, ΔH=26434 J· mol^{-1}
Molecular Weight 358.5604
Wiswesser Line Notation 19VO1
Evaluation B

$C_{21}H_{42}O_4$ (c) 65SIL/DAU
2-Monostearin
Heat Capacity 298 K, C_p=610.4 J· mol^{-1}· K^{-1}
One temperature.
Molecular Weight 358.5604
Wiswesser Line Notation Q1Y1QOV17
Evaluation B

$C_{21}H_{42}O_4$ (c,α) 55WAR/VIC
1-Monostearin
Heat Capacity 298.2 K, C_p=866.0 J· mol^{-1}· K^{-1}
Temperature range −74 to 114 °C. Give experimental points and equations for solid and liquid states. Sub-alpha form, C_p=0.4977+ 0.00318t cal·g^{-1}·C^{-1}, −13 to 40 °C; liquid, C_p = 0.5118 + 0.00182t cal·g^{-1}· C^{-1}, 87 to 100 °C.
Phase Changes
c,α/liq 347.2 K, ΔH=59095 J· mol^{-1}
ΔS= 170.2 J· mol^{-1}· K^{-1}
Molecular Weight 358.5604
Wiswesser Line Notation Q1YQ1OV17
Evaluation C

$C_{21}H_{42}O_4$ (c) 65SIL/DAU
1-Monostearin
Heat Capacity 298 K, C_p = 610.4 J· mol^{-1}· K^{-1}
One temperature. B_L-form.
Molecular Weight 358.5604
Wiswesser Line Notation Q1YQ1OV17
Evaluation B

$C_{21}H_{44}$ (c) 55SCH/BUS
n-Heneicosane
Phase Changes
c,II/c,I 305.65 K, ΔH=15481 J· mol^{-1}
ΔS= 50.6 J· mol^{-1}· K^{-1}
c,I/liq 313.35 K, ΔH=47698 J· mol^{-1}
ΔS= 152.2 J· mol^{-1}· K^{-1}
Molecular Weight 296.5786
Wiswesser Line Notation 21H
Evaluation B

$C_{21}H_{44}$ (liq) 84GRI/AND
n-Heneicosane
Heat Capacity 315.93 K, C_p = 666.4 J· mol^{-1}· K^{-1}
Temperature range 316 to 433 K. Unsmoothed experimental datum given as 2.247 kJ/kg· K.
Molecular Weight 296.5786
Wiswesser Line Notation 21H
Evaluation B

$C_{21}H_{44}$ (c) 91BAR/SCH
n-Heneicosane
Phase Changes
c,II/c,I 305.1 K, ΔH=16500 J·mol^{-1}
c,I/liq 313.4 K, ΔH = 46000 J· mol^{-1}
Molecular Weight 296.5786
Wiswesser Line Notation 21H
Evaluation A

$C_{22}H_{13}N_3O_7$ (c) 79FAR/SHA
Fluoranthene-picric acid
Phase Changes
c,II/c,I 365.6 K, ΔH=13800 J· mol^{-1}
ΔS= 37.7 J· mol^{-1}· K^{-1}
c/liq 462.4 K, ΔH=24700 J· mol^{-1}
ΔS = 53.4 J· mol^{-1}· K^{-1}
Molecular Weight 431.3606
Wiswesser Line Notation L C6566 1A PJ &WNR BQ CNW ENW
Evaluation B

$C_{22}H_{13}N_3O_7$ (c) 79FAR/SHA
Pyrene-picric acid
Phase Changes
c,III/c,II 443.2 K, ΔH=2900 J· mol^{-1}
ΔS=6.5 J· mol^{-1}· K^{-1}
c,II/c,I 456.6 K, ΔH=1200 J· mol^{-1}
ΔS=2.6 J· mol^{-1}· K^{-1}
c/liq 506.6 K, ΔH=32600 J· mol^{-1}
ΔS = 64.4 J· mol^{-1}· K^{-1}
Molecular Weight 431.3606
Wiswesser Line Notation L666 B6 2AB PJ &WNR BQ CNW ENW
Evaluation B

$(C_{22}H_{14}N_2O_7)_n$ (c) 77KAR/BAZ
Poly-(*p*,*p*′-diphenylene oxide)pyromellitimide
Heat Capacity 300 K, C_p = 592.4 J· mol^{-1}· K^{-1}
Temperature range 60 to 400 K.
Entropy 300 K, S = 543.9 J· mol^{-1}· K^{-1}
Molecular Weight 418.3619
Wiswesser Line Notation /*ZVR BVQ DVQ EVMR DOR*/
Evaluation B

$C_{22}H_{14}O_4$ (c) 77KAR/RAB
1,4-Bis(phenylglyoxaloyl)benzene
Heat Capacity 300 K, C_p = 435 J· mol^{-1}· K^{-1}
Temperature range 100 to 700 K. Data given graphically. Value estimated from graph.
Entropy 300 K, S = 381.0 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 425.1 K, ΔH=32300 J· mol^{-1}
ΔS=76.0 J· mol^{-1}· K^{-1}
Molecular Weight 342.3502
Wiswesser Line Notation RVVR DVVR
Evaluation C(C_p), A(S, Phase changes)

$C_{22}H_{18}N_4O_4$ (c) 79KAR/SAI
4′,4″-Diphenylenephthalidodicarboxylic acid dihydrazide
Heat Capacity 298.15 K, C_p = 460.7 J· mol^{-1}· K^{-1}
Temperature range 60 to 298 K.
Entropy 298.15 K, S = 441.4 J· mol^{-1}· K^{-1}
Molecular Weight 402.4086
Wiswesser Line Notation ZMVR DX& BT56 BHOVJ&R& DVMZ
Evaluation A

$C_{22}H_{18}O_4$ (c) 84OZC/ASR

4,4′-Dipropanoyloxydiphenyldiacetylene

Phase Changes

c,III/c,II	351 K,	ΔH=586 J· mol^{-1}
		ΔS=1.674 J· mol^{-1}· K^{-1}
c,II/c,I	359 K.	ΔH=7530 J· mol^{-1}
		ΔS= 20.96 J· mol^{-1}· K^{-1}
c,I/liq	430 K,	ΔH=19400 J· mol^{-1}
		ΔS=45.35 J· mol^{-1}· K^{-1}

Solid–nematic.

liq/liq	470 K,	ΔH=1380 J· mol^{-1}
		ΔS= 2.929 J· mol^{-1}· K^{-1}

Nematic–isotropic liquid transition.

Molecular Weight 346.3818

Wiswesser Line Notation 2VOR D1UU2UU1R DOV2

Evaluation A

$C_{22}H_{20}AuN_2S_8Se_4$ (c) 89SAI/KAM

Bis[dimethyl(ethylenedithio)diselenadithiafulvalene} dicyanoaurate(I)

Heat Capacity

Temperature range 150 to 250 K. Data given graphically.

Phase Changes

c,II/c,I	180 K,	ΔH = 100 J· mol^{-1}
		ΔS=0.5 J· mol^{-1}· K^{-1}

Hump between 160 and 190 K.

Molecular Weight 1081.6999

Wiswesser Line Notation

Evaluation A

$C_{22}H_{20}N_2O_2$ (c) 87BYK/KIP

3-Phenyl-5-phenoxymethyl-2-N-phenyliminooxazolidine

Heat Capacity 298.15 K, C_p=400.2 J· mol^{-1}· K^{-1}

Temperature range 0 to 330 K.

Entropy 298.15 K, S=426.2 J· mol^{-1}· K^{-1}

Molecular Weight 344.4122

Wiswesser Line Notation T5NYOTJ AR BUNR D1OR

Evaluation A

$C_{22}H_{20}N_2O_4$ (c) 73HAM/MIT

N,N′-Bis(*m*-methoxyphenyl)terephthalamide

Heat Capacity 298.15 K, C_p=458.1 J· mol^{-1}· K^{-1}

One temperature.

Molecular Weight 376.4110

Wiswesser Line Notation 1OR CMVR DVMR CO1

Evaluation C

$C_{22}H_{20}N_2O_4$ (c) 73HAM/MIT

N,N′-Bis(*p*-methoxyphenyl)terephthalamide

Heat Capacity 298.15 K, C_p=467.8 J· mol^{-1}· K^{-1}

One temperature.

Molecular Weight 376.4110

Wiswesser Line Notation 1OR DMVR DVMR DO1

Evaluation C

$C_{22}H_{24}O_6$ (c) 74AND/BAC

Di(*p*-methoxyphenyl)-*trans*-cyclohexane-1,4-dicarboxylate

Heat Capacity 297.0 K, C_p = 478.5 J· mol^{-1}· K^{-1}

Temperature range 297 to 550 K. Value is unsmoothed experimental datum.

Phase Changes

c,II/c,I	411.58 K,	ΔH = 4806 J· mol^{-1}
		ΔS = 11.69 J· mol^{-1}· K^{-1}
c,I/liq	416.16 K,	ΔH = 31481 J· mol^{-1}
		ΔS = 76.51 J· mol^{-1}· K^{-1}

Crystal I - nematic liquid transition.

liq/liq	516.0 K,	ΔH = 2865 J· mol^{-1}
		ΔS = 5.7 J· mol^{-1}· K^{-1}

Nematic - isotropic liquid transition.

Molecular Weight 384.4280

Wiswesser Line Notation L6TJ AVOR BO1& DVOR DO1

Evaluation A

$C_{22}H_{26}$ (c) 83KRA/BEC

1,1′-Diphenyl-1,1′-bicyclopentane

Heat Capacity 298 K, C_p=375.5 J· mol^{-1}· K^{-1}

One temperature. C_p given as 0.309 cal.K^{-1}.g^{-1}.

Molecular Weight 290.4474

Wiswesser Line Notation L5TJ AR A- AL5TJ AR

Evaluation B

$C_{22}H_{26}F_6FeN_4O_2P$ (c) 90SOR/MAE

Bis-[N-(1-acetyl-2-propylidene)(2-pyridylmethyl) amine]iron(III) phosphorus hexafluoride

Heat Capacity 298.15 K, C_p = 623.479 J· mol^{-1}· K^{-1}

Temperature range 5 to 310 K.

Entropy 298.15 K, S = 731.869 J· mol^{-1}· K^{-1}

Phase Changes

c,II/c,I	190 K,	ΔH=7025 J· mol^{-1}
		ΔS= 36.19 J· mol^{-1}· K^{-1}

Spin-crossover, 120 to 280 K.

Molecular Weight 579.2842

Wiswesser Line Notation T6NJ B1NY1&U1V1 2 .FE P F 6

Evaluation A

$C_{22}H_{26}N_2O_3$ (c) 88FAN/POE

4-*n*-Pentanoyl-4-*n*′-pentanoyloxyazobenzene

Phase Changes

c/liq	355.1 K,	ΔH=7100 J· mol^{-1}
		ΔS=20.00 J· mol^{-1}· K^{-1}

Solid-smectic 2.

liq/liq	377.1 K,	ΔH=4690 J· mol^{-1}
		ΔS= 12.44 J· mol^{-1}· K^{-1}

Smectic 2-smectic 1.

liq/liq	377.5 K,	ΔH=7682 J· mol^{-1}
		ΔS= 20.34 J· mol^{-1}· K^{-1}

Smectic 1-smectic A.

liq/liq	399.5 K,	ΔH=6088 J· mol^{-1}
		ΔS= 15.24 J· mol^{-1}· K^{-1}

Smectic A-isotropic.

Molecular Weight 366.4590

Wiswesser Line Notation 4VR DNUNR DOV4

Evaluation A

$C_{22}H_{26}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-heptanoyloxyazobenzene
Phase Changes
liq/liq 358.55 K, ΔH=84 J·mol^{-1}
Hexatic - monotropic smectic B liquid transition.
liq/liq 362.85 K, ΔH=1590 J· mol^{-1}
Smectic A - monotropic hexatic liquid transition.
c/liq 365.15 K, ΔH = 24811 J· mol^{-1}
ΔS = 67.95 J· mol^{-1}· K^{-1}
Solid - smectic A.
liq/liq 414.65 K, ΔH=5314 J· mol^{-1}
Smectic A - nematic liquid transition.
liq/liq 416.65 K, ΔH = 920 J· mol^{-1}
Nematic - isotropic liquid transition.
Molecular Weight 366.4590
Wiswesser Line Notation 6VOR DNUNR DV2
Evaluation A

$C_{22}H_{27}N$ (c) 83MAR/THO
4-Nonyl-4′-cyanobiphenyl
Phase Changes
liq/liq 320.8 K, ΔH=5 J· mol^{-1}
ΔS=0.02 J· mol^{-1}· K^{-1}
Smectic A - nematic.
liq/liq 322.7 K, ΔH=1200 J· mol^{-1}
ΔS=3.7 J· mol^{-1}· K^{-1}
Nematic–isotropic.
c/liq ΔH=34500 J· mol^{-1}
Solid - smectic A.
Molecular Weight 305.4620
Wiswesser Line Notation NCR DR D9
Evaluation D

$C_{22}H_{28}N_2NiO_4$ (c) 72ARA/SOR
Bis[N-(3-methoxysalicylidene)isopropylamine] nickel(II)
Heat Capacity 299.010 K, C_p=741.87 J· mol^{-1}· K^{-1}
Temperature range 230 to 343 K. Unsmoothed experimental datum.
Molecular Weight 443.1742
Wiswesser Line Notation T6 C6-NI- BO JNJ DO1 JY1&1 A-& AT6 C6-NI- BO JNJ DO1 JY1&1
Evaluation B
T(glass)= 297.5 K, ΔC_p = 172 J· mol^{-1}· K^{-1}.

$C_{22}H_{28}O_2$ (c) 72YOU/HAL
4-Methoxy-4′-heptoxy-trans-stilbene
Phase Changes
liq/liq 421 K, ΔH = 665 J· mol^{-1}
ΔS = 1.6 J· mol^{-1}· K^{-1}
Nematic-isotropic liquid transition.
c/liq 423 K, ΔH=42760 J· mol^{-1}
ΔS=101.1 J· mol^{-1}· K^{-1}
Crystal-isotropic liquid transition.
Molecular Weight 324.4620
Wiswesser Line Notation 7OR D1U1R DO1 -T
Evaluation B

$C_{22}H_{28}O_2$ (c) 79LEW/ENE
Norethindrone acetate
Phase Changes
c/liq 480 K, ΔH=27300 J· mol^{-1}
ΔS=56.9 J· mol^{-1}· K^{-1}
Molecular Weight 324.4620
Wiswesser Line Notation L E5 B666 OV MUTJ E1 FV1 F1UU1
Evaluation A

$C_{22}H_{29}NO$ (c) 83SOR/TAN
N-*p*-*n*-Pentyloxybenzylidene-*p*′-*n*-butylaniline
Heat Capacity 298.15 K, C_p = 512.71 J· mol^{-1}· K^{-1}
Temperature range 11 to 393 K. C_p = 2.3491T −187.67 J· mol^{-1}· K^{-1} (11 to 299.69 K). C_p value is calculated from equation.
Entropy 280 K, S = 478.16 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 299.69 K, ΔH=22680 J· mol^{-1}
ΔS=75.70 J· mol^{-1}· K^{-1}
Solid-smectic G liquid transition.
liq/liq 325.72 K, ΔH=7110 J· mol^{-1}
ΔS= 21.79 J· mol^{-1}· K^{-1}
Smectic G - nematic liquid transition.
liq/liq 342.48 K, ΔH=1780 J· mol^{-1}
ΔS=5.22 J· mol^{-1}· K^{-1}
Nematic - isotropic liquid transition.
Molecular Weight 323.4772
Wiswesser Line Notation 5OR D1UNR D4
Evaluation A

$C_{22}H_{29}NO$ (gls) 83SOR/TAN
N-*p*-*n*-Pentyloxybenzylidene-*p*′-*n*-butylaniline
Heat Capacity 300 K, C_p = 561.46 J· mol^{-1}· K^{-1}
Temperature range 10 to 320 K.
Entropy 300 K, S = 588.03 J· mol^{-1}· K^{-1}
Molecular Weight 323.4772
Wiswesser Line Notation 5OR D1UNR D4
Evaluation A
Glassy and undercooled S_G phase.

$C_{22}H_{36}Br_2N_2$ (c,II) 74BUR/VER
1,4-Bis(triallylammonium)butene-2-dibromide
Heat Capacity 298 K, C_p = 582.4 J· mol^{-1}· K^{-1}
Temperature range 273 to 373 K.
Phase Changes
c,II/c,I 430 K, ΔH=9200 J· mol^{-1}
ΔS=21.4 J· mol^{-1}· K^{-1}
Temperature range 425 to 436 K.
Molecular Weight 494.3951
Wiswesser Line Notation 1U2K2U1&2U1&2U2K2U1&2U1&2U1&E &E
Evaluation B

$C_{22}H_{36}N_2O_4$ (c) 89LEB/KIP
1,4-Bis-(2,2,6,6-tetramethyl-4-oxy-1-oxylpiperidyl) butadiyne
Heat Capacity 298.15 K, C_p = 562.2 J· mol^{-1}· K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 579.1 J· mol^{-1}· K^{-1}
Molecular Weight 392.5374
Wiswesser Line Notation T6NTJ B1 B1 DQ F1 F1 AO1UU2UU1O-AT6NTJ B1 B1 DQ F1 F1
Evaluation B
Empirical formula in 89LEB/KIP is given as $C_{22}H_{34}N_2O_4$.

$(C_{22}H_{36}N_2O_4)_n$ (c) 89LEB/KIP
Poly-1,4-bis-(2,2,6,6-tetramethyl-4-oxy-1-oxylpiperidyl)butadiyne
Heat Capacity 298.15 K, C_p = 531.3 J· mol^{-1}· K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 572.5 J· mol^{-1}· K^{-1}
Molecular Weight 392.5374
Wiswesser Line Notation /T6NTJ B1 B1 DQ F1 F1 AO *YU1U1UY-* AT6NTJ B1 B1 DQ F1 F1/
Evaluation B
Empirical formula in 89LEB/KIP is given as $C_{22}H_{34}N_2O_4$.

$C_{22}H_{42}O_4$ (liq) 85OVC/MOS
Di(2-ethylhexyl)adipate
Heat Capacity 300 K, C_p = 701.5 J· mol^{-1}· K^{-1}
Temperature range 6 to 300 K.
Entropy 300 K, S = 865 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 161.5 K
Glass transition.
Molecular Weight 370.5714
Wiswesser Line Notation 4Y1&1OV4VO1Y1&4
Evaluation A

$C_{22}H_{42}O_4$ (liq) 75PHI/WAL
Di-*n*-hexyl sebacate
Heat Capacity 303.15 K, C_p = 711 J· mol^{-1}· K^{-1}
Temperature range 303 to 393 K.
Phase Changes
c/liq 274 K
Molecular Weight 370.5714
Wiswesser Line Notation 60V8VO6
Evaluation B

$C_{22}H_{42}O_4$ (liq) 76PHI/MAT
Di-*n*-hexyl sebacate
Heat Capacity 315 K, C_p = 732 J· mol^{-1}· K^{-1}
Temperature range 315 to 414 K.
Molecular Weight 370.5714
Wiswesser Line Notation 60V8VO6
Evaluation C

$C_{22}H_{42}O_4Pb$ (c,II) 78ADE/SIM
Lead(II) undecanoate
Heat Capacity 365 K, C_p = 894 J· mol^{-1}· K^{-1}
Temperature range 363 to 371 K. Data only graphically for c,III. Data also for c,I, and liquid.
Phase Changes
c,III/c,II 360.9 K, ΔH=50700 J· mol^{-1}
ΔS=140 J· mol^{-1}· K^{-1}
c,II and c,I, are mesophases.
c,II/c,I 377.0 K, ΔH=27500 J· mol^{-1}
ΔS=73 J· mol^{-1}· K^{-1}
c,I/liq 383.7 K, ΔH=1100 J· mol^{-1}
ΔS=2.9 J· mol^{-1}· K^{-1}
Molecular Weight 577.7714
Wiswesser Line Notation OV10 2 .PB
Evaluation C

$C_{22}H_{44}$ (c) 69BOR/DAL
1.1.10.10-Tetramethylcyclooctadecane
Phase Changes
c/liq 359 K. ΔH=39581 J· mol^{-1}
ΔS=110 J· mol^{-1}· K^{-1}
Molecular Weight 308.5896
Wiswesser Line Notation L-18-TJ A1 A1 J1 J1
Evaluation B

$C_{22}H_{44}N_2O_2$ (c) 53WIL/DOL
N,N′-Di-*n*-hexylsebacamide
Heat Capacity 333-483 K. C_p = 1064.1 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 415 K. ΔH=53680 J· mol^{-1}
ΔS= 129.3 J· mol^{-1}· K^{-1}
Molecular Weight 368.6018
Wiswesser Line Notation 6MV8VM6
Evaluation C

$C_{22}H_{44}O_2$ (c) 34KIN/GAR
Ethyl eicosanoate
Phase Changes
c,II/c,I 396.65 K, ΔH=7781 J· mol^{-1}
β-α transition.
c,I/liq 313.51 K, ΔH = 15575 J· mol^{-1}
α-liq transition.
Molecular Weight 340.5884
Wiswesser Line Notation 19VO2
Evaluation B
Data on the specific heats are given at or near the phase transitions.

$C_{22}H_{44}O_2$ (c,II) 86KAL/JAC
Butyl octadecanoate
Phase Changes
c,II/c,I 288.4 K, ΔH=2220 J·mol^{-1}
ΔS=7.70 J· mol^{-1}· K^{-1}
c,I/liq 299.72 K, ΔH=37480 J· mol^{-1}
299.72 K, ΔS=121.5 J· mol^{-1}· K^{-1}
Molecular Weight 340.5884
Wiswesser Line Notation 17VO4
Evaluation A

$C_{22}H_{46}$ (c,II) 31GAR/VAN
n-Docosane
Heat Capacity 299 K, C_p = 563.6 J· mol^{-1}· K^{-1}
Temperature range 280 to 347 K. Mean value 17 to 35 °C, β-form.
Phase Changes
c,II/c,I 313.4 K, ΔH=8950 J· mol^{-1}
ΔS=28.6 J· mol^{-1}· K^{-1}
β-α transition.
c,I/liq 317.0 K, ΔH=15210 J· mol^{-1}
ΔS= 48.0 J· mol^{-1}· K^{-1}
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation B

$C_{22}H_{46}$ (c) 55SCH/BUS
n-Docosane
Phase Changes
c,II/c,I 316.15 K, ΔH=28870 J· mol^{-1}
ΔS= 92.12 J· mol^{-1}· K^{-1}
c,I/liq 317.15 K, ΔH=48953 J· mol^{-1}
ΔS= 154.4 J· mol^{-1}· K^{-1}
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation B

$C_{22}H_{46}$ (liq) 69ATK/LAR
n-Docosane
Heat Capacity 353 K, C_p = 739 J· mol^{-1}· K^{-1}
Temperature range 353 to 453 K. Equation only.
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation C

$C_{22}H_{46}$ (c) 73COM
n-Docosane
Phase Changes
c,II/c,I 316.25 K, ΔH=28200 J· mol^{-1}
ΔS= 89.2 J· mol^{-1}· K^{-1}
c,I/liq 317.25 K, ΔH=48952 J· mol^{-1}
ΔS= 154.3 J· mol^{-1}· K^{-1}
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation B

$C_{22}H_{46}$ (c) 79CLA/LET
n-Docosane
Phase Changes
c,II/c,I 315.15 K, ΔH=29505 J· mol^{-1}
ΔS= 93.6 J· mol^{-1}· K^{-1}
c,I/liq 316.05 K, ΔH=47837 J· mol^{-1}
ΔS= 151.4 J· mol^{-1}· K^{-1}
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation B

$C_{22}H_{46}$ (c) 81HOE
n-Docosane
Heat Capacity 300 K, C_p = 468 J· mol^{-1}· K^{-1}
Temperature range 300 to 500 K. C_v = 1.48 J· g^{-1}· K^{-1}.
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation B

$C_{22}H_{46}$ (c) 91BAR/SCH
n-Docosane
Phase Changes
c/liq 316.9 K, ΔH=78500 J· mol^{-1}
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation A

$C_{22}H_{46}$ (liq) 91CLA/LET
n-Docosane
Phase Changes
c,II/c,I 315.5 K, ΔH=28605 J· mol^{-1}
c,I/liq 316.8 K, ΔH=47801 J· mol^{-1}
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation A

$C_{22}H_{46}$ (c) 91DOM/WYR
n-Docosane
Phase Changes
c,II/c,I 314.45 K, ΔH=36350 J· mol^{-1}
c,I/liq 315.20 K, ΔH=39760 J· mol^{-1}
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation A

$C_{22}H_{48}$ (liq) 58SEL/AST
Bis(cyclopentane)-2,2-dimethylbutane adduct
Heat Capacity 298.15 K, C_p = 148.66 J· mol^{-1}· K^{-1}
Temperature range 14 to 300 K.
Entropy 298.15 K, S = 689.61 J· mol^{-1}· K^{-1}
Does not include zero point entropy.
Phase Changes
c,II/c,I 83.2 K, ΔH=4128.4 J· mol^{-1}
ΔS= 49.62 J· mol^{-1}· K^{-1}
c,I/liq 137.71 K, ΔH=2513.7 J· mol^{-1}
ΔS= 18.25 J· mol^{-1}· K^{-1}
Molecular Weight 312.6212
Wiswesser Line Notation L5TJ 2 &2X1&1&1
Evaluation A

$C_{22}H_{50}Br_2N_2$ (c,II) 74BUR/VER
1,10-Bis(triethylammonium)decane dibromide
Heat Capacity 298 K, C_p = 640.2 J· mol^{-1}· K^{-1}
Temperature range 273 to 373 K.
Phase Changes
c,II/c,I 444 K, ΔH=840 J· mol^{-1}
ΔS=1.9 J· mol^{-1}· K^{-1}
Temperature range 437 to 452 K.
Molecular Weight 502.4584
Wiswesser Line Notation 2K2&2&10K2&2&2 E 2
Evaluation B

$C_{23}H_{15}N_3O_7$ (c) 79FAR/SHA
1,2-Benzfluorene picric acid
Phase Changes
c/liq 402.7 K, ΔH=45600 J· mol^{-1}
ΔS= 113.2 J· mol^{-1}· K^{-1}
Molecular Weight 445.3874
Wiswesser Line Notation L D6 B566 CHJ &WNR BQ CNW ENW
Evaluation B

$C_{23}H_{15}N_3O_7$ (c) 79FAR/SHA
2,3-Benzfluorene picric acid
Phase Changes
c/liq 392.8 K, ΔH=33500 J· mol^{-1}
ΔS= 85.3 J· mol^{-1}· K^{-1}
Molecular Weight 445.3874
Wiswesser Line Notation L D6 B656 LHJ &WNR BQ CNW ENW
Evaluation B

$C_{23}H_{17}N$ (c) 84BYK/KIP
2,4,6-Triphenylpyridine
Heat Capacity 298.15 K, C_p = 358.6 J· mol^{-1}· K^{-1}
Temperature range 14 to 330 K.
Entropy 298.15 K, S=371.6 J· mol^{-1}· K^{-1}
Molecular Weight 307.3940
Wiswesser Line Notation T6NJ BR DR FR
Evaluation A

$C_{23}H_{17}N$ (c) 85LEB/BYK
2,4,6-Triphenylpyridine
Heat Capacity 298.15 K, C_p = 358.6 J· mol^{-1}· K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 371.6 J· mol^{-1}· K^{-1}
Molecular Weight 307.3940
Wiswesser Line Notation T6NJ BR DR FR
Evaluation A

$C_{23}H_{28}N_2O_3$ (c) 88FAN/POE
4-*n*-Pentanoyl-4-*n*′-hexanoyloxyazobenzene
Phase Changes
c,II/c,I 323.8 K, ΔH=4665 J· mol^{-1}
ΔS= 14.41 J· mol^{-1}· K^{-1}
c,I/liq 365.1 K, ΔH=7117 J· mol^{-1}
ΔS= 19.49 J· mol^{-1}· K^{-1}
Solid-smectic 3.
liq/liq 375.2 K, ΔH=3360 J· mol^{-1}
ΔS= 8.954 J· mol^{-1}· K^{-1}
Smectic 3-smectic 1.
liq/liq 377.5 K, ΔH=9569 J· mol^{-1}
ΔS= 25.35 J· mol^{-1}· K^{-1}
Smectic 1-smectic A.
liq/liq 401.2 K, ΔH=5812 J· mol^{-1}
ΔS= 14.49 J· mol^{-1}· K^{-1}
Smectic A-isotropic.
Molecular Weight 380.4858
Wiswesser Line Notation 5VOR DNUNR DV4
Evaluation A

$C_{23}H_{28}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-octanoyloxyazobenzene
Phase Changes
liq/liq 353.75 K, ΔH=42 J· mol^{-1}
Smectic A-nematic.
liq/liq 359.85 K, ΔH = 1423 J· mol^{-1}
Nematic-isotropic.
c/liq 369.65 K, ΔH=27489 J· mol^{-1}
ΔS= 74.36 J· mol^{-1}· K^{-1}
Solid-smectic A.
liq/liq 416.15 K, ΔH = 5314 J· mol^{-1}
Smectic A-monotropic hexatic.
liq/liq 416.65 K, ΔH = 1004 J· mol^{-1}
Hexatic-monotropic Smectic B.
Molecular Weight 380.4858
Wiswesser Line Notation 7VOR DNUNR DV2
Evaluation A

$C_{23}H_{29}N$ (c) 83MAR/THO
Decylcyanobiphenyl
Phase Changes
liq/liq ΔH=2830 J·mol^{-1}
Smectic A - isotropic.
c/liq ΔH=36000 J·mol^{-1}
Solid - smectic A.
Molecular Weight 319.4888
Wiswesser Line Notation NCR DR D10
Evaluation D

$C_{23}H_{30}O_2$ (c) 72YOU/HAL
4-Methoxy-4′-octoxy-*trans*-stilbene
Phase Changes
liq/liq 419 K, ΔH=971 J· mol^{-1}
ΔS=2.3 J·mol^{-1}· K^{-1}
Nematic-isotropic liquid transition.
c/liq 424 K, ΔH=41925 J· mol^{-1}
ΔS=98.9 J· mol^{-1}· K^{-1}
Crystal-isotropic liquid transition.
Molecular Weight 338.4888
Wiswesser Line Notation 8OR D1U1R DO1 -T
Evaluation B

$C_{23}H_{31}NO$ (c) 83YOS/SOR3
N-*p*-*n*-Hexyloxybenzylidene-*p*′-*n*-butylaniline
Heat Capacity 298.15 K, C_p = 512.02 J· mol^{-1}· K^{-1}
Temperature range 11 to 393 K.
Entropy 298.15 K, S = 537.57 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 306.60 K, ΔH=23290 J· mol^{-1}
ΔS= 75.98 J· mol^{-1}· K^{-1}
Solid-smectic G.
liq/liq 331.56 K, ΔH=804 J· mol^{-1}
ΔS=2.53 J· mol^{-1}· K^{-1}
Smectic G-smectic B.
liq/liq 332.86 K, ΔH=3370 J· mol^{-1}
ΔS= 10.14 J· mol^{-1}· K^{-1}
Smectic B-smectic A.
liq/liq 343.24 K, ΔH=3200 J· mol^{-1}
ΔS=9.37 J· mol^{-1}· K^{-1}
Smectic A nematic.
liq/liq 350.92 K, ΔH=1890 J· mol^{-1}
ΔS=5.37 J· mol^{-1}· K^{-1}
Nematic-isotropic.
Molecular Weight 337.5040
Wiswesser Line Notation 60R D1UNR D4
Evaluation A

$C_{23}H_{31}NO$ (gls) 83YOS/SOR3
N-*p*-*n*-Hexyloxybenzylidene-*p*′-*n*-butylaniline
Heat Capacity 300 K, C_p = 595.14 J· mol^{-1}· K^{-1}
Temperature range 10 to 310 K.
Entropy 300 K, S=615.04 J· mol^{-1}· K^{-1}
Residual entropy of the glassy state at 0 K was estimated to be 7.51 ±0.63 J· mol^{-1}· K^{-1}.
Molecular Weight 337.5040
Wiswesser Line Notation 6OR D1UNR D4
Evaluation A

$C_{23}H_{44}O_5$ (c,α) 55WAR/VIC
1-Aceto-3-stearin
Heat Capacity 298.2 K, C_p = 938.5 J· mol^{-1}· K^{-1}
Temperature range −71 to 72 °C. Give experimental points and equations for 2 solid and liquid states. Sub-alpha form, C_p=0.4471+0.00133t cal·g^{-1}· C^{-1} (−73 to −1 °C); alpha form, C_p =0.4513+0.00434t cal· g^{-1}· C^{-1}, (−1 to 27 °C); liquid, C_p=0.2290+0.0068t cal· g^{-1}· C^{-1} (57 to 87 °C).
Phase Changes
c,α/liq 319.9 K, ΔH=41685 J· mol^{-1}
ΔS= 130.3 J· mol^{-1}· K^{-1}
Molecular Weight 400.5976
Wiswesser Line Notation 17VO1YQ1OV1
Evaluation C

$C_{23}H_{46}O_2$ (c) 36KIN/GAR
Methyl behenate
Phase Changes
c/liq 324.99 K, ΔH=29199 J· mol^{-1}
Molecular Weight 354.6152
Wiswesser Line Notation 21VO1
Evaluation B

$C_{23}H_{48}$ (c) 55SCH/BUS
n-Tricosane
Phase Changes
c,II/c,I 313.65 K, ΔH=21757 J· mol^{-1}
ΔS= 69.4 J· mol^{-1}· K^{-1}
c,I/liq 320.65 K, ΔH=53974 J· mol^{-1}
ΔS= 168.3 J· mol^{-1}· K^{-1}
Molecular Weight 324.6322
Wiswesser Line Notation 23H
Evaluation B

$C_{23}H_{48}$ (liq) 69ATK/LAR
n-Tricosane
Heat Capacity 353 K, C_p = 772 J· mol^{-1}· K^{-1}
Temperature range 353 to 453 K.
Molecular Weight 324.6322
Wiswesser Line Notation 23H
Evaluation C

$C_{23}H_{48}$ (c) 84SYU/TUM
n-Tricosane
Phase Changes
c/liq 319.7 K, ΔH=76700 J· mol^{-1}
ΔS= 239.9 J· mol^{-1}· K^{-1}
Relative error in determination ± 5%.
Molecular Weight 324.6322
Wiswesser Line Notation 23H
Evaluation C

$C_{23}H_{48}$ (c) 91BAR/SCH
n-Tricosane
Phase Changes
c,II/c,I 313.5 K, ΔH = 21500 J· mol^{-1}
c,I/liq 320.8 K, ΔH = 52250 J· mol^{-1}
Molecular Weight 324.6322
Wiswesser Line Notation 23H
Evaluation A

$C_{24}H_{12}$ (c) 80WON/WES
Coronene
Heat Capacity 298.15 K, C_p = 313.8 J· mol^{-1}· K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S = 280.9 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 225 K, ΔH=444 J· mol^{-1}
ΔS=1.84 J· mol^{-1}· K^{-1}
Molecular Weight 300.3588
Wiswesser Line Notation L666 B6 C6 D6 E6 6ABCDEF A&J
Evaluation A

$C_{24}H_{12}N_4$ (c) 87ECO/BER
Anthracene TCNB; Anthracene-1,2,4,5-tetracyanobenzene
Heat Capacity
Temperature range 140 to 240 K. Data given graphically.
Phase Changes
c,III/c,II 208.5 K
c,II/c,I 211.5 K, ΔH=151 J· mol^{-1}
ΔS=0.71 J· mol^{-1}· K^{-1}
Total enthalpy and entropy between 180 and 215 K.
Molecular Weight 356.3856
Wiswesser Line Notation NCR BCN DCN ECN &L C666J
Evaluation B

$(C_{24}H_{12}N_6)_n$ (c) 88LEB/BYK
Polytriazine
Heat Capacity 298.15 K, C_p = 395.3 J· mol^{-1}· K^{-1}
Temperature range 0 to 330 K.
Entropy 298.15 K, S = 451.6 J· mol^{-1}· K^{-1}
Molecular Weight 384.3990
Wiswesser Line Notation /T6N CN ENJ BR DYUN*&* DR DYUN*&* FR DYUN*&*/ 1/3
Evaluation A

$C_{24}H_{15}N_3O_7$ (c) 79FAR/SHA
Triphenylene picric acid
Phase Changes
c/liq 501.4 K, ΔH=46900 J· mol^{-1}
ΔS= 93.6 J· mol^{-1}· K^{-1}
Molecular Weight 457.3984
Wiswesser Line Notation L B6 H666J &WNR BQ CNW ENW
Evaluation B

$C_{24}H_{15}N_3O_7$ (c) 79FAR/SHA
1,2-Benzanthracene picric acid
Phase Changes
c/liq 414.3 K, ΔH=32200 J· mol^{-1}
ΔS= 77.7 J· mol^{-1}· K^{-1}
Molecular Weight 457.3984
Wiswesser Line Notation L D6 C666J &WNR BQ CNW ENW
Evaluation B

$C_{24}H_{18}$ (liq) 58WAL/BRO
m-Quaterphenyl
Heat Capacity 370 K, C_p = 553.5 J· mol^{-1}· K^{-1}
Temperature range 200 to 600 °F.
Molecular Weight 306.4062
Wiswesser Line Notation RR CR CR
Evaluation C

$C_{24}H_{18}$ (c) 36PAR/TOD
1,3,5-Triphenylbenzene
Heat Capacity 298.1 K, C_p = 358.32 J· mol^{-1}· K^{-1}
Temperature range 90 to 300 K.
Entropy 298.1 K, S = 367.4 J· mol^{-1}· K^{-1}
Extrapolation below 90 K, 114.64 J· mol^{-1}· K^{-1}.
Molecular Weight 306.4063
Wiswesser Line Notation RR CR ER
Evaluation B(C_p),C(S)

$C_{24}H_{18}$ (c) 82LEB/BYK
1,3,5-Triphenylbenzene
Heat Capacity 298.15 K, C_p = 361.0 J· mol^{-1}· K^{-1}
Temperature range 13.8 to 480 K.
Entropy 298.15 K, S = 375.5 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 446 K, ΔH=33400 J· mol^{-1}
ΔS= 75.1 J· mol^{-1}· K^{-1}
Molecular Weight 306.4063
Wiswesser Line Notation RR CR ER
Evaluation A

$C_{24}H_{18}$ (c) 79SMI
p-Quaterphenyl
Phase Changes
c/liq 587.2 K, ΔH=37800 J· mol^{-1}
ΔS= 64.4 J· mol^{-1}· K^{-1}
Molecular Weight 306.4062
Wiswesser Line Notation RR DR DR
Evaluation A

$C_{24}H_{18}$ (c) 82WAS/RAD
p-Quaterphenyl
Heat Capacity 300 K, C_p = 340 J· mol^{-1}· K^{-1}
Temperature range 180 to 600 K. Data given graphically. Value estimated from graph.
Phase Changes
c,III/c,II 190–260 K, ΔH=1100 J· mol^{-1}
c,II/c,I 450–540 K, ΔH=1000 J· mol^{-1}
c/liq 586.7 K, ΔH=57600 J· mol^{-1}
ΔS= 98.2 J· mol^{-1}· K^{-1}
Molecular Weight 306.4062
Wiswesser Line Notation RR DR DR
Evaluation C(C_p), B(Phase changes)

$C_{24}H_{18}$ (c) 85SAI/ATA
p-Quaterphenyl
Heat Capacity 298.15 K, C_p = 362.52 J· mol^{-1}· K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, S = 363.64 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 233.0 K, ΔH=414 J· mol^{-1}
ΔS=1.82 J· mol^{-1}· K^{-1}
Transition region 180 to 270 K.
Molecular Weight 306.4062
Wiswesser Line Notation RR DR DR
Evaluation A

$C_{24}H_{18}FeO_2$ (c) 81TOM/CUR
1,1′-Dibenzoylferrocene
Heat Capacity 298 K, C_p = 466.1 J· mol^{-1}· K^{-1}
Temperature range 293 to 353 K. Equation given.
Phase Changes
c/liq 379.7 K
Molecular Weight 394.2520
Wiswesser Line Notation L5ϕJ AVR ϕ-FE- -ϕL5ϕJ AVR
Evaluation B

$C_{24}H_{20}BK$ (c) 57DAV/STA
Potassium tetraphenyl boron
Heat Capacity 298.15 K, C_p = 418.23 J· mol^{-1}· K^{-1}
Temperature range 20 to 298 K.
Entropy 298.15 K, S = 440.16 J· mol^{-1}· K^{-1}
Molecular Weight 358.3303
Wiswesser Line Notation RBR&R&R &-K-
Evaluation B

$C_{24}H_{20}RBb$ (c) 57DAV/STA
Rubidium tetraphenyl boron
Heat Capacity 298.15 K, C_p = 412.96 J· mol^{-1}· K^{-1}
Temperature range 20 to 298 K.
Entropy 298.15 K, S = 444.76 J· mol^{-1}· K^{-1}
Molecular Weight 404.6998
Wiswesser Line Notation RBR&R&R &-RB-
Evaluation B

$C_{24}H_{20}CrI$ (c) 72NIK/SAF
Bis(biphenyl)chromium iodide
Heat Capacity 298.15 K, C_p = 437.2 J· mol^{-1}· K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S = 424.7 J· mol^{-1}· K^{-1}
Molecular Weight 487.3225
Wiswesser Line Notation L6ϕJA- AL6ϕJ ϕ-CR-ϕL6ϕJA- AL6ϕJ &I
Evaluation B

$C_{24}H_{20}Si$ (c) 31SMI/AND2
Tetraphenylsilane
Heat Capacity 298.5 K, C_p = 395.8 J· mol^{-1}· K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 336.5075
Wiswesser Line Notation R-SI-R&R&R
Evaluation B

$C_{24}H_{20}Sn$ (c) 31SMI/AND2
Tetraphenylstannane; Tetraphenyl tin
Heat Capacity 298.5 K, C_p = 426.3 J· mol^{-1}· K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 427.1120
Wiswesser Line Notation R-SN-R&R&R
Evaluation B

$(C_{24}H_{22}N_2O_2)_n$ (c) 89CHE/JAN
Poly(azomethine)
Heat Capacity 300 K, C_p = 453.1 J· mol^{-1}· K^{-1}
Temperature range 230 to 620 K. C_p(c)=0.000701787^2+1.0658T+ 70.174 J/mol· K (230 to 270 K). C_p(liq) = 0.8419T + 371.82 J/mol · K (350 to 600 K).
Phase Changes
liq/liq 534.7 K, ΔH=20200 J· mol^{-1}
Disordering transition. 50% crystallinity.
Molecular Weight 370.4500
Wiswesser Line Notation /*NR B1 DO2OR C1 DNU1R D1*/
Evaluation B
Poly(azomethine) with one ethylene glycol spacer. T(glass) = 350 K.

$C_{24}H_{22}N_4O$ (c) 73KAR/SAP
4,4′-Dianilino-3,3′-diaminodiphenyl oxide; 4,4′- Dianilino-3,3′-diaminodiphenyl ether
Heat Capacity 300 K, C_p = 458.1 J· mol^{-1}· K^{-1}
Temperature range 20 to 300 K.
Entropy 300 K, S = 431.8 J· mol^{-1}· K^{-1}
Molecular Weight 382.4640
Wiswesser Line Notation RMR CZ DOR CZ DMR
Evaluation B

$C_{24}H_{22}O_4$ (c) 84OZC/ASR
4,4′-Dibutanoyloxydiphenyldiacetylene
Phase Changes
c,V/c,IV 319 K, ΔH=10400 J· mol^{-1}
ΔS= 32.51 J· mol^{-1}· K^{-1}
c,IV/ c,III 368 K, ΔH=1510 J· mol^{-1}
ΔS= 4.100 J· mol^{-1}· K^{-1}
c,II/c,I 408 K, ΔH=12.5 J· mol^{-1}
ΔS= 0.2929 J· mol^{-1}· K^{-1}
c,II/c,II,c,II/c,I transitions combined.
c,I/liq 416 K, ΔH=20100 J· mol^{-1}
ΔS = 48.28 J· mol^{-1}· K^{-1}
Solid-nematic.
Molecular Weight 374.4354
Wiswesser Line Notation 3VOR D1UU2UU1R DOV3
Evaluation A
Nematic-isotropic liquid phase change data also given: 453 K, ΔH=1250 J· mol^{-1}, ΔS=2.76 J· mol^{-1}· K^{-1}.

$C_{24}H_{24}BN$ (c) 57DAV/STA
Ammonium tetraphenyl boron
Heat Capacity 298.15 K, C_p = 434.93 J· mol^{-1}· K^{-1}
Temperature range 20 to 298 K.
Entropy 298.15 K, S = 457.31 J· mol^{-1}· K^{-1}
Molecular Weight 337.2703
Wiswesser Line Notation RBR&R&R &ZH
Evaluation B

$C_{24}H_{26}I_3Fe_2$ (c) 91NAK/NIS
1′,1‴-Diethylbiferrocenium triiodide
Heat Capacity 298.15 K, C_p = 559.24 J· mol^{-1}· K^{-1}
Temperature range 5 to 310 K.
Entropy 298.15 K, S = 680.21 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 67.2 K, ΔS = 2.9 J· mol^{-1}· K^{-1}
Molecular Weight 806.8769
Wiswesser Line Notation
Evaluation A

$C_{24}H_{28}O_2Si_3$ (liq) 81SHA/DZH
1,1,1,5,5,5-Hexamethyl-3,3-diphenyltrisiloxane
Heat Capacity 298 K, C_p = 648 J· mol^{-1}· K^{-1}
Temperature range 12 to 300 K.
Entropy 298 K, S = 769 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 270.49 K, ΔH=22753 J· mol^{-1}
ΔS= 84.12 J· mol^{-1}· K^{-1}
Molecular Weight 432.7405
Wiswesser Line Notation 1-SI-1&1&O-SI-R&R&O- SI-1&1&1
Evaluation A
T(glass) = 178 K.

$C_{24}H_{30}$ (c) 83KRA/BEC
1,1′-Diphenyl-1,1′-bicyclohexane
Heat Capacity 298 K, C_p = 403.8 J· mol^{-1}· K^{-1}
One temperature. C_p given as 0.303 Cal.K^{-1}.g^{-1}.
Molecular Weight 318.5010
Wiswesser Line Notation L6TJ AR A- AL6TJ AR
Evaluation B

$C_{24}H_{30}N_2O_3$ (c) 88FAN/POE
4-*n*-Pentanoyl-4-*n*′-heptanoyloxyazobenzene
Phase Changes
c,II/c,I 347.1 K, ΔH=7510 J· mol^{-1}
ΔS= 21.64 J· mol^{-1}· K^{-1}
c,I/liq 371.4 K, ΔH=13272 J· mol^{-1}
ΔS = 35.74 J· mol^{-1}· K^{-1}
Solid-smectic 1.
liq/liq 375.6 K, ΔH=8707 J· mol^{-1}
ΔS= 23.18 J· mol^{-1}· K^{-1}
Smectic 1-smectic A.
liq/liq 401.7 K, ΔH=6832 J· mol^{-1}
ΔS= 17.01 J· mol^{-1}· K^{-1}
Smectic A-isotropic.
liq/liq 371.1 K, ΔH=4623 J· mol^{-1}
ΔS= 12.46 J· mol^{-1}· K^{-1}
Smectic 1-smectic monotropic.
Molecular Weight 394.5126
Wiswesser Line Notation 6VOR DNUNR DV4
Evaluation A

$C_{24}H_{30}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4'-*n*-nonanoyloxyazobenzene
Phase Changes
liq/liq 353.25 K, ΔH=42 J· mol^{-1}
Hexatic-monotropic smectic B.
c/liq 367.15 K, ΔH = 3017 J· mol^{-1}
ΔS=8.22 J· mol^{-1}· K^{-1}
Solid smectic A.
liq/liq 361.05 K, ΔH = 1757 J· mol^{-1}
Smectic A-monotropic hexatic.
liq/liq 417.15 K. ΔH = 7029 J· mol^{-1}
Smectic A-isotropic.
Molecular Weight 394.5126
Wiswesser Line Notation 8VOR DNUNR DV2
Evaluation A

$C_{24}H_{31}N$ (c) 83MAR/THO
Undecylcyanobiphenyl
Phase Changes
liq/liq ΔH=3800 J· mol^{-1}
Smectic A - isotropic.
c/liq ΔH = 43200 J· mol^{-1}
Solid - smectic A.
Molecular Weight 333.5156
Wiswesser Line Notation NCR NR D11
Evaluation D

$C_{24}H_{32}O_3$ (liq) 85SHA/ZH
4-*n*-Heptoxyphenyl-4′-*n*-butylbenzoate
Heat Capacity 312.14 K, C_p = 793.4 J· mol^{-1}· K^{-1}
Temperature range 312 to 354 K. Unsmoothed experimental datum.
Phase Changes
liq/liq 317.3 K, ΔH = 490 J· mol^{-1}
ΔS = 1.54 J· mol^{-1}· K^{-1}
Molecular Weight 368.5150
Wiswesser Line Notation 7OR DOVR D4
Evaluation B

$C_{24}H_{34}$ (liq) 60KAR/STR
1,1-Diphenyldodecane
Heat Capacity 298.15 K, C_p = 593.7 J· mol^{-1}· K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S = 684.9 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 191 K, ΔH = 1929 J· mol^{-1}
ΔS = 10.1 J· mol^{-1}· K^{-1}
c,I/liq 281.4 K, ΔH = 38844 J· mol^{-1}
ΔS = 138.0 J· mol^{-1}· K^{-1}
Molecular Weight 322.5326
Wiswesser Line Notation 11YR&R
Evaluation B

$C_{24}H_{34}$ (liq) 60KAR/STR
1,1-Diphenyldodecane
Heat Capacity 298.15 K, C_p = 593.9 J· mol^{-1}· K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S = 684.9 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 191 K, ΔH = 1928 J· mol^{-1}
ΔS = 10.1 J· mol^{-1}· K^{-1}
c,I/liq 281.40 K, ΔH = 38844 J· mol^{-1}
ΔS = 138.1 J· mol^{-1}· K^{-1}
Molecular Weight 322.5326
Wiswesser Line Notation 11YR&R
Evaluation A

$C_{24}H_{38}O_4$ (liq) 69RAB/MA
Bis(2-ethylhexyl)phthalate
Heat Capacity 300 K, C_p = 669.4 J· mol^{-1}· K^{-1}
Temperature range 80 to 360 K.
Entropy 300 K, S = 755.2 J· mol^{-1}· K^{-1}
Phase Changes
c,II/c,I 182.5 K, ΔH = 1038 J· mol^{-1}
ΔS = 5.82 J· mol^{-1}· K^{-1}
Glass phase transition.
Molecular Weight 390.5618
Wiswesser Line Notation 4Y2&1OVR BVO1&Y4&2
Evaluation C

$C_{24}H_{38}O_4$ (c) 70MAR/R.
Di-(2-ethylhexyl) *o*-phthalate
Molecular Weight 390.5618
Wiswesser Line Notation 4Y2&1OVR BVO1Y2&4
Evaluation A
T(glass) = 182.5 K.

$C_{24}H_{38}O_4$ (liq) 85RAB/NO
Di-(2-ethylhexyl) *o*-phthalate
Heat Capacity 298.15 K, C_p = 704.7 J· mol^{-1}· K^{-1}
Temperature range 14 to 300 K.
Entropy 298.15 K, S = 807.7 J· mol^{-1}· K^{-1}
Molecular Weight 390.5618
Wiswesser Line Notation 4Y2&1OVR BVO1Y2&4
Evaluation A
Data given for glassy state from 10 to 180 K. Glass transitio temperature. T(glass) = 182.5 K.

$C_{24}H_{38}O_4$ (c) 70MAR/RAB
Dioctyl *o*-phthalate
Heat Capacity 300 K, C_p = 707.1 J· mol^{-1}· K^{-1}
Temperature range 60 to 360 K.
Entropy 300 K, S = 755.2 J· mol^{-1}· K^{-1}
Molecular Weight 390.5618
Wiswesser Line Notation 80VR BVO8
Evaluation B

$C_{24}H_{40}$ (liq) 60KAR/STR
1-Phenyl-1-cyclohexyldodecane
Heat Capacity 298.15 K, C_p = 611.3 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 275.8 K, ΔH=35171 J· mol^{-1}
ΔS = 127.5 J· mol^{-1}· K^{-1}
Molecular Weight 328.5800
Wiswesser Line Notation L6TJ AY11&R
Evaluation B

$C_{24}H_{40}$ (liq) 60KAR/STR4
1-Phenyl-1-cyclohexyldodecane
Heat Capacity 298.15 K, C_p = 611.1 J· mol^{-1}· K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S = 695.9 J· mol^{-1}· K^{-1}
Phase Changes
c,I/liq 275.84 K, ΔH = 35171 J· mol^{-1}
ΔS = 127.7 J· mol^{-1}· K^{-1}
Molecular Weight 328.5800
Wiswesser Line Notation L6TJ AY11&R
Evaluation A

$C_{24}H_{46}$ (c) 60KAR/STR
2,11-Dicyclohexyldodecane
Heat Capacity 298.1 K, C_p=557.3 Jmol^{-1}·K^{-1}
Temperature range 13 to 298 K. Values above 260 K show extensive premelting effects. Value given is corrected for premelting. Experimental value at 298.09 K is 3566 J·mol^{-1}·K^{-1}.
Entropy 298.15 K, S=545.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 300.58 K, ΔH=44271 J·mol^{-1}
ΔS=147.3 J·mol^{-1}·K^{-1}
Molecular Weight 334.6274
Wiswesser Line Notation L6TJ AY1&8Y1&- AL6TJ
Evaluation B

$C_{24}H_{46}$ (c) 60KAR/STR
1,1-Dicyclohexyldodecane
Heat Capacity 298.15 K C_p = 562.7 J· mol^{-1}· K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S = 546.6 J· mol^{-1}· K^{-1}
Phase Changes
c/liq 300.6 K, ΔH = 44267 J· mol^{-1}
ΔS = 147.3 J· mol^{-1}· K^{-1}
Molecular Weight 334.6274
Wiswesser Line Notation L6TJ AY11&- AL6TJ
Evaluation B

$C_{24}H_{46}$ (c) 60KAR/STR4
1,1-Dicyclohexyldodecane
Heat Capacity 298.15 K, C_p=562.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S=545.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 300.58 K, ΔH=44267 J·mol^{-1}
ΔS=147.3 J·mol^{-1}·K^{-1}
Molecular Weight 334.6274
Wiswesser Line Notation L6TJ AY11&- AL6TJ
Evaluation A

$C_{24}H_{46}O_4Cd$ (c) 78KON/RUF
Cadmium(II) *n*-dodecanoate
Phase Changes
c/liq 367.7 K, ΔH= 13000 J·mol^{-1}
ΔS=35 J·mol^{-1}·K^{-1}
Crystal-mesophase.
liq/liq 370.5 K, ΔH=8600 J·mol^{-1}
ΔS=23 J·mol^{-1}·K^{-1}
Mesophase-liquid.
Molecular Weight 511.0350
Wiswesser Line Notation OV11 2 .CD
Evaluation B

$C_{24}H_{46}HgO_4$ (liq) 78ADE
Mercuric dodecanoate; Mercuric laurate
Heat Capacity 420 K, C_p=1089.2 J·mol^{-1}·K^{-1}
Mean value, 413 to 430 K. Data for solid only graphically.
Phase Changes
c/liq 394.2 K, ΔH=94800 J·mol^{-1}
ΔS=240.5 J·mol^{-1}·K^{-1}
Molecular Weight 599.2150
Wiswesser Line Notation OV11 2 .HG
Evaluation C

$C_{24}H_{46}O_4Pb$ (c) 76ADE/SIM
Lead(II) *n*-dodecanoate
Phase Changes
c/liq 365.2 K, ΔH=48300 J·mol^{-1}
ΔS=132 J·mol^{-1}·K^{-1}
Crystal-smectic.
liq/liq 377.2 K, ΔH=29800 J·mol^{-1}
ΔS=79.1 J·mol^{-1}·K^{-1}
Smectic-isomorphous.
liq/liq 381.2 K, ΔH=900 J·mol^{-1}
ΔS=2.5 J·mol^{-1}·K^{-1}
Isomorphous liquid.
Molecular Weight 605.8250
Wiswesser Line Notation OV11 2 .PB
Evaluation B

$C_{24}H_{46}O_4Zn$ (c) 78KON/RUF
Zinc(II) *n*-dodecanoate
Phase Changes
c,II/c,I 372 K, ΔH=1000 J·mol^{-1}
c,I/liq 407 K, ΔH=64000 J·mol^{-1}
ΔS=157 J·mol^{-1}·K^{-1}
Molecular Weight 464.0050
Wiswesser Line Notation OV11 2 .ZN
Evaluation B

$C_{24}H_{48}O_2$ (c) 34KIN/GAR
Ethyl docosanate; Ethyl behenate
Phase Changes
c,II/c,I 312.15 K, $\Delta H = 9578$ J·mol^{-1}
β-α transition.
c,I/liq 320.95 K, $\Delta H = 19157$ J·mol^{-1}
α-liq transition.
Molecular Weight 368.6420
Wiswesser Line Notation 21VO2
Evaluation B
Data on the specific heats are given at or near the phase transitions.

$C_{24}H_{50}$ (c) 49PAR/MOO
n-Tetracosane
Heat Capacity 298.15 K, $C_p = 730.9$ J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K. Specific heat at 290 to 300 K rapidly increasing; possible premelting effects. Value may be high.
Entropy 298.15 K, $S = 651.0$ J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 160.5 J·mol^{-1}·K^{-1}.
Phase Changes
Hump in specific heat curve at 250 to 265 K.
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation B(C_p), C(S)

$C_{24}H_{50}$ (c) 55SCH/BUS
n-Tetracosane
Phase Changes
c,II/c,I 321.25 K, $\Delta H = 31296$ J·mol^{-1}
$\Delta S = 97.4$ J·mol^{-1}·K^{-1}
c,I/liq 323.75 K, $\Delta H = 54894$ J·mol^{-1}
$\Delta S = 169.5$ J·mol^{-1}·K^{-1}
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation B

$C_{24}H_{50}$ (liq) 69ATK/LAR
n-Tetracosane
Heat Capacity 353 K, $C_p = 805$ J·mol^{-1}·K^{-1}
Temperature range 353 to 453 K. Equation only.
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation C

$C_{24}H_{50}$ (c) 73COM
n-Tetracosane
Phase Changes
c,II/c,I 321.35 K, $\Delta H = 31296$ J·mol^{-1}
$\Delta S = 97.4$ J·mol^{-1}·K^{-1}
c,I/liq 323.85 K, $\Delta H = 54894$ J·mol^{-1}
$\Delta S = 169.6$ J·mol^{-1}·K^{-1}
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation B

$C_{24}H_{50}$ (c) 81HOE
n-Tetracosane
Heat Capacity 300 K, $C_p = 601$ J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K. $C_v = 1.75$ J·g^{-1}·K^{-1}.
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation B

$C_{24}H_{50}$ (liq) 84GRI/ANI
n-Tetracosane
Heat Capacity 330.63 K, $C_p = 772.5$ J·mol^{-1}·K^{-1}
Temperature range 331 to 433 K. Unsmoothed experimental datum given as 2.281 kJ/kg·K.
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation B

$C_{24}H_{50}$ (c) 84SYU/TUM
n-Tetracosane
Phase Changes
c/liq 322.0 K, $\Delta H = 81750$ J·mol^{-1}
$\Delta S = 253.9$ J·mol^{-1}·K^{-1}
Relative error in determination ±5%.
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation C

$C_{24}H_{50}$ (c) 91BAR/SCH
n-Tetracosane
Phase Changes
c,II/c,I 321.1 K, $\Delta H = 31500$ J·mol^{-1}
c,I/liq 323.5 K, $\Delta H = 54000$ J·mol^{-1}
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation A

$C_{24}H_{50}$ (liq) 91CLA/LET
n-Tetracosane
Phase Changes
c,II/c,I 321.0 K, $\Delta H = 29155$ J·mol^{-1}
c,I/liq 323.8 K, $\Delta H = 54370$ J·mol^{-1}
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation A

$C_{24}H_{50}$ (c) 91DOM/WYF
n-Tetracosane
Phase Changes
c,II/c,I 318.90 K, $\Delta H = 27680$ J·mol^{-1}
c,I/liq 323.65 K, $\Delta H = 57310$ J·mol^{-1}
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation A

$C_{24}H_{51}N$ (liq) 93STE/CHI
Tri-*n*-octylamine
Heat Capacity 298.15 K, $C_p = 750.8$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 353.6736
Wiswesser Line Notation 8N8&8
Evaluation A

$C_{24}H_{52}ClNO_4$ (c,IV) 73AND/GOR

Tetra-*n*-hexylammonium perchlorate

Heat Capacity 298.15 K, $C_p = 744$ J·mol^{-1}·K^{-1}

Temperature range 300 to 382 K.

Phase Changes

c,IV/c,III	333.57 K,	$\Delta H = 22990$ J·mol^{-1}
		$\Delta S = 68.9$ J·mol^{-1}·K^{-1}
c,III/c,II	355.91 K,	$\Delta H = 5839$ J·mol^{-1}
		$\Delta S = 16.4$ J·mol^{-1}·K^{-1}
c,II/c,I	367.51 K,	$\Delta H = 2658$ J·mol^{-1}
		$\Delta S = 7.2$ J·mol^{-1}·K^{-1}
c,I/liq	379.18 K,	$\Delta H = 16350$ J·mol^{-1}
		$\Delta S = 43.1$ J·mol^{-1}·K^{-1}

Molecular Weight 454.1321

Wiswesser Line Notation 6K6&6&6 G-O4

Evaluation B

$C_{24}H_{56}CdCl_4$ (c) 89ZHA/YAN2

Bis(dodecylammonium)tetrachlorocadmate (II)

Heat Capacity 298.15 K, $C_p = 979.4$ J·mol^{-1}·K^{-1}

Temperature range 280 to 500 K.

Phase Changes

c,II/c,I	332.4 K,	$\Delta H = 48350$ J·mol^{-1}
		$\Delta S = 145.5$ J·mol^{-1}·K^{-1}

Molecular Weight 598.9284

Wiswesser Line Notation 12 ZH 2 .CD G4

Evaluation A

$C_{24}H_{56}CdCl_4N_2$ (c) 85RIC/CAV

Bis(dodecylammonium)tetrachlorocadmate (II)

Phase Changes

c,III/c,II	327 K,	$\Delta H = 40000$ J·mol^{-1}
		$\Delta S = 123$ J·mol^{-1}·K^{-1}
c,II/c,I	331 K,	$\Delta H = 6500$ J·mol^{-1}
		$\Delta S = 21$ J·mol^{-1}·K^{-1}

Molecular Weight 626.9418

Wiswesser Line Notation -12-ZH 2 .CD G4

Evaluation B

$C_{24}H_{56}Cl_4MnN_2$ (c) 87ZHA

Bis(dodecylammonium)tetrachloromanganate (II)

Heat Capacity 298.15 K, $C_p = 869.8$ J·mol^{-1}·K^{-1}

Temperature range 280 to 500 K.

Phase Changes

c,III/c,II	330.6 K,	$\Delta H = 47780$ J·mol^{-1}
		$\Delta S = 144.5$ J·mol^{-1}·K^{-1}
c,II/c,I	334.5 K,	$\Delta H = 5960$ J·mol^{-1}
		$\Delta S = 17.82$ J·mol^{-1}·K^{-1}

Molecular Weight 569.4698

Wiswesser Line Notation -12-ZH 2 .MN G4

Evaluation A

$C_{24}H_{56}Cl_4MnN_2$ (c) 88ZHA/YAN

Bis(dodecylammonium)tetrachloromanganate (II)

Heat Capacity 298.15 K, $C_p = 869.8$ J·mol^{-1}·K^{-1}

Temperature range 280 to 500 K.

Phase Changes

c,III/c,II	330.6 K,	$\Delta H = 47780$ J·mol^{-1}
		$\Delta S = 144.5$ J·mol^{-1}·K^{-1}
c,II/c,I	334.5 K,	$\Delta H = 5960$ J·mol^{-1}
		$\Delta S = 17.82$ J·mol^{-1}·K^{-1}

Molecular Weight 569.4698

Wiswesser Line Notation -12-ZH 2 .MN G4

Evaluation A

$C_{24}H_{56}Cl_4N_2Zn$ (c) 88ZHA/YAN

Bis(dodecylammonium)tetrachlorozincate (II)

Heat Capacity 298.15 K, $C_p = 851.7$ J·mol^{-1}·K^{-1}

Temperature range 280 to 500 K.

Phase Changes

c,II/c,I	364.3 K,	$\Delta H = 66790$ J·mol^{-1}
		$\Delta S = 183.3$ J·mol^{-1}·K^{-1}
c,I/liq	435.1 K,	$\Delta H = 9120$ J·mol^{-1}
		$\Delta S = 20.96$ J·mol^{-1}·K^{-1}

Molecular Weight 579.9118

Wiswesser Line Notation -12-ZH 2 .ZN G4

Evaluation A

$(C_{25}H_{18}O_3S)_n$ (c) 92VAR/JIN

Poly[oxy-1,4-phenylene-sulfonyl-1,4-phenylene-oxy-1,4-phenylene-(1-methylidene)-1,4-phenylene]

Heat Capacity 300 K, $C_p = 501.5$ J·mol^{-1}·K^{-1}

Temperature range 150 to 620 K. $C_p(c) = \exp[-19.7795 + 15.3476(\ln T) - 3.17773(\ln T)^2 + 0.225473(\ln T)^3]$ (150 to 360 K); $C_p(\text{liq}) = 591.81 + 0.57224T$ (500 to 620 K).

Molecular Weight 398.4754

Wiswesser Line Notation /*OR DSWR DOR D1R D*/

Evaluation A

T(glass) = 458.2 K.

$C_{25}H_{20}$ (c) 31SMI/AND

Tetraphenylmethane

Heat Capacity 298.5 K, $C_p = 368.2$ J·mol^{-1}·K^{-1}

Temperature range 102 to 346 K. Value is unsmoothed experimental datum.

Molecular Weight 320.4330

Wiswesser Line Notation RXR&R&R

Evaluation C

$C_{25}H_{20}$ (c) 31SMI/AND2

Tetraphenylmethane

Heat Capacity 298.5 K, $C_p = 368.2$ J·mol^{-1}·K^{-1}

Temperature range 102 to 346 K. Value is unsmoothed experimental datum.

Molecular Weight 320.4330

Wiswesser Line Notation RXR&R&R

Evaluation C

$C_{25}H_{32}N_2O_3$ (c) 8FAN/POE

4-*n*-Pentanoyl-4-*n*′-octanoyloxyazobenzene

Phase Changes

c,II/c,I	333 K,	$\Delta H = 5230$ J·mol^{-1}
		$\Delta S = 15.71$ J·mol^{-1}·K^{-1}
	Estimated values.	
c,I/liq	366.2 K,	$\Delta H = 16309$ J·mol^{-1}
		$\Delta S = 44.53$ J·mol^{-1}·K^{-1}
	Solid-smectic 1.	
liq/liq	370.1 K,	$\Delta H = 7263$ J·mol^{-1}
		$\Delta S = 19.63$ J·mol^{-1}·K^{-1}
	Smectic 1-smectic A.	
liq/liq	403.8 K,	$\Delta H = 6941$ J·mol^{-1}
		$\Delta S = 17.19$ J·mol^{-1}·K^{-1}
	Smectic A-isotropic.	
liq/liq	359.4 K,	$\Delta H = 4682$ J·mol^{-1}
		$\Delta S = 13.03$ J·mol^{-1}·K^{-1}
	Smectic 1-smectic monotropic.	

Molecular Weight 408.5394

Wiswesser Line Notation 7VOR DNUNR DV4

Evaluation A

$C_{25}H_{32}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-decanoyloxyazobenzene
Phase Changes
c/liq 371.15 K, $\Delta H = 32928$ J·mol^{-1}
$\Delta S = 88.72$ J·mol^{-1}·K^{-1}
Solid-smectic A.
Molecular Weight 408.5394
Wiswesser Line Notation 9VOR DNUNR DV2
Evaluation A
Smectic A-esotropic; smectic A-monotropic hexatic liquid phase change data also given: 417.65 K, $\Delta H = 7196$ J·mol^{-1}; 359.95 K, $\Delta H = 1088$ J·mol^{-1}.

$C_{25}H_{34}O_2$ (c) 79LEW/ENE
Norethindrone dimethylpropionate
Phase Changes
c/liq 500 K, $\Delta H = 37800$ J·mol^{-1}
$\Delta S = 75.6$ J·mol^{-1}·K^{-1}
Molecular Weight 366.5424
Wiswesser Line Notation L E5 B666 OV MUTJ E1 FVX F1UU1
Evaluation A

$C_{25}H_{34}O_2S$ (c) 81CHR/RIC
4-*n*-Pentylphenyl-4′-heptyloxythiobenzoate
Heat Capacity
C_p data given graphically only. Temperature range 90 to 370 K.
Phase Changes
c,III/c,II 183.53 K, $\Delta H = 1167$ J·mol^{-1}
$\Delta S = 6.03$ J·mol^{-1}·K^{-1}
c,II/c,I 272 K, $\Delta H = 228$ J·mol^{-1}
$\Delta S = 0.88$ J·mol^{-1}·K^{-1}
c,I/nematic liq 325.87 K, $\Delta H = 28514$ J·mol^{-1}
$\Delta S = 88.45$ J·mol^{-1}·K^{-1}
Nematic—isotropic liquid.
352.2 K, $\Delta H = 2552$ J·mol^{-1}
$\Delta S = 5.36$ J·mol^{-1}·K^{-1}
Molecular Weight 398.6024
Wiswesser Line Notation 7OR DVSR D5
Evaluation A

$C_{25}H_{40}O_2Si_2$ (c) 79LEW/ENE
Norethindrone pentamethyldisiloxyl ether
Phase Changes
c/liq 355 K, $\Delta H = 22900$ J·mol^{-1}
$\Delta S = 64.5$ J·mol^{-1}·K^{-1}
Molecular Weight 428.7608
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1 FSI1&1&O-SI-1&1&1
Evaluation A

$C_{25}H_{41}DO_3$ (c,I) 77IKE/HAT
p-*n*-Octadecyloxybenzoic acid-*d*
Heat Capacity 302 K, $C_p = 137$ J·mol^{-1}·K^{-1}
Temperature range 302 to 420 K. Value is unsmoothed experimental datum for c,I phase.
Phase Changes
c,I/liq 374.2 K, $\Delta H = 65700$ J·mol^{-1}
$\Delta S = 176$ J·mol^{-1}·K^{-1}
c,I-smectic transition.
c,II/liq 365.7 K, $\Delta H = 36500$ J·mol^{-1}
$\Delta S = 101$ J·mol^{-1}·K^{-1}
c,II-smectic transition.
c,III/liq 340.2 K
c,III-smectic transition temperature.
liq/liq 402.5 K, $\Delta H = 14400$ J·mol^{-1}
$\Delta S = 36$ J·mol^{-1}·K^{-1}
Smectic-isotropic liquid transition.
Molecular Weight 392.6112
Wiswesser Line Notation QVR DO18 &1/H-2
Evaluation B

$C_{25}H_{42}O_3$ (c) 76IKE/HAT
p-*n*-Octadecyloxybenzoic acid
Heat Capacity 320 K, $C_p = 145$ J·mol^{-1}·K^{-1}
Temperature range 320 to 420 K. Value is unsmoothed experimental datum for c,I phase.
Phase Changes
c,I/liq 379.5 K, $\Delta H = 67300$ J·mol^{-1}
$\Delta S = 177$ J·mol^{-1}·K^{-1}
c,I-smectic transition.
c,II/liq 371.0 K, $\Delta H = 38900$ J·mol^{-1}
$\Delta S = 105$ J·mol^{-1}·K^{-1}
c,II-smectic transition.
c,III/liq 342.5 K
c,III-smectic transition temperature.
liq/liq 408.5 K, $\Delta H = 13300$ J·mol^{-1}
$\Delta S = 33$ J·mol^{-1}·K^{-1}
Smectic-isotropic liquid transition.
Molecular Weight 390.6050
Wiswesser Line Notation QVR DO18
Evaluation B

$C_{25}H_{46}$ (liq) 62GOL/BEI
4′-*n*-Heptyl-*m*-tercyclohexyl
Heat Capacity 311 K, $C_p = 668.6$ J·mol^{-1}·K^{-1}
Temperatures 100, 200, 300 °F.
Molecular Weight 346.6384
Wiswesser Line Notation L6TJ AAL6TJ C- AL6TJ D7
Evaluation C

$C_{25}H_{46}$ (liq) 63GUD/CAM
4-*n*-Heptyltercyclohexyl
Heat Capacity 373 K, $C_p = 752.7$ J·mol^{-1}·K^{-1}
Temperature range 373 to 483 K.
Molecular Weight 346.6384
Wiswesser Line Notation L6TJ AAL6TJ X- AL6TJ D7
Evaluation C

$C_{25}H_{46}O_6$ (c,α) 55WAR/VIC
1,2-Diaceto-3-stearin
Heat Capacity 298.2 K, $C_p = 904.2$ J·mol^{-1}·K^{-1}
Temperature range −69 to 97 °C. Give experimental points and equations for 2 solid and liquid forms. Sub-alpha form $C_p = 0.4315 + 0.00104t$ cal·g^{-1}·C^{-1} (−73 to −1 °C); alpha form $C_p = 0.4349 + 0.00213t$ cal·g^{-1}·C^{-1} (−3 to 33 °C); liquid $C_p = 0.3790 + 0.00195t$ cal·g^{-1}·C^{-1} (77 to 97 °C).
Phase Changes
c,α/liq 208.3 K, $\Delta H = 45560$ J·mol^{-1}
$\Delta S = 218.7$ J·mol^{-1}·K^{-1}
Molecular Weight 442.6348
Wiswesser Line Notation 17VO1YOV1&1OV1
Evaluation C

$C_{25}H_{48}O_4$ (liq) 83BAB/RAE
Bis(2-ethylhexyl)azalate; Bis(2-ethylhexyl)-nonadioate
Heat Capacity 298.15 K, $C_p = 799.7$ J·mol^{-1}·K^{-1}
Temperature range 13 to 335 K.
Entropy 298.15 K, $S = 899.5$ J·mol^{-1}·K^{-1}
Phase Changes
c,gls/liq 160.0 K
Molecular Weight 412.6518
Wiswesser Line Notation 4Y2&1OV7VO1Y2&4
Evaluation A

$C_{25}H_{52}$ (c) 30PAR/HUF

n-Pentacosane

Heat Capacity 294.5 K, $C_p = 769.0$ J·mol^{-1}·K^{-1}

Temperature range 91 to 295 K. Value is unsmoothed experimental datum.

Entropy 298.15 K, $S = 671.1$ J·mol^{-1}·K^{-1}

Extrapolation below 90 K, 205.9 J·mol^{-1}·K^{-1}.

Molecular Weight 352.6858

Wiswesser Line Notation 25H

Evaluation B(C_p),C(S)

$C_{25}H_{52}$ (liq) 32SPA/THO

n-Pentacosane

Heat Capacity 333 K, $C_p = 815.9$ J·mol^{-1}·K^{-1}

Temperature range 60 to 100 °C.

Phase Changes

c/liq 326.6 K, $\Delta H = 79391$ J·mol^{-1}

$\Delta S = 243.1$ J·mol^{-1}·K^{-1}

Molecular Weight 352.6858

Wiswesser Line Notation 25H

Evaluation B

$C_{25}H_{52}$ (c) 55SCH/BUS

n-Pentacosane

Phase Changes

c,II/c,I 320.15 K, $\Delta H = 26066$ J·mol^{-1}

$\Delta S = 81.4$ J·mol^{-1}·K^{-1}

c,I/liq 326.65 K, $\Delta H = 57739$ J·mol^{-1}

$\Delta S = 176.8$ J·mol^{-1}·K^{-1}

Molecular Weight 352.6858

Wiswesser Line Notation 25H

Evaluation B

$C_{25}H_{52}$ (c) 79CLA/LET

n-Pentacosane

Phase Changes

c,II/c,I 319.85 K, $\Delta H = 25235$ J·mol^{-1}

$\Delta S = 78.9$ J·mol^{-1}·K^{-1}

c,I/liq 326.25 K, $\Delta H = 56605$ J·mol^{-1}

$\Delta S = 173.5$ J·mol^{-1}·K^{-1}

Molecular Weight 352.6858

Wiswesser Line Notation 25H

Evaluation B

$C_{25}H_{52}$ (c) 91BAR/SCH

n-Pentacosane

Phase Changes

c,II/c,I 320.0 K, $\Delta H = 26500$ J·mol^{-1}

c,I/liq 326.7 K, $\Delta H = 56750$ J·mol^{-1}

Molecular Weight 352.6858

Wiswesser Line Notation 25H

Evaluation A

$C_{26}H_{12}N_4$ (c) 76CLA/WOR

1,2,4,5-Tetracyanobenzene-pyrene complex

Heat Capacity 298.15 K, $C_p = 432.0$ J·mol^{-1}·K^{-1}

Temperature range 13 to 295 K.

Entropy 298.15 K, $S = 466.1$ J·mol^{-1}·K^{-1}

Phase Changes

Broad transition in 220 to 250 K. ΔH estimated as 2150 J·mol^{-1}·K^{-1}, $\Delta S = 9.2$ J·mol^{-1}·K^{-1}.

Molecular Weight 380.4076

Wiswesser Line Notation L666 B6 2AB PJ &NCR BCN DCN ECN

Evaluation A

$C_{26}H_{12}O_6$ (c) 78DUN/RAH

Pyrene-pyromellitic dianhydride charge transfer complex

Heat Capacity 298.15 K, $C_p = 435.9$ J·mol^{-1}·K^{-1}

Temperature range 5 to 300 K.

Entropy 298.15 K, $S = 464.6$ J·mol^{-1}·K^{-1}

Molecular Weight 420.3772

Wiswesser Line Notation T C565 DVOV JVOVJ &L666 B6 2AB PJ

Evaluation A

$C_{26}H_{12}O_6$ (c) 80BOE/WES2

Pyrene-pyromellitic dianhydride charge transfer complex

Heat Capacity 298.15 K, $C_p = 446.4$ J·mol^{-1}·K^{-1}

Temperature range 5 to 300 K.

Entropy 298.15 K, $S = 464.8$ J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 155 K, $\Delta H = 213.4$ J·mol^{-1}

$\Delta S = 1.34$ J·mol^{-1}·K^{-1}

Molecular Weight 420.3772

Wiswesser Line Notation T C565 DVOV JVOVJ &L666 B6 2AB PJ

Evaluation A

$C_{26}H_{15}N_3O_7$ (c) 79FAR/SHA

Perylene picric acid

Phase Changes

c/liq 495.0 K, $\Delta H = 42300$ J·mol^{-1}

$\Delta S = 85.5$ J·mol^{-1}·K^{-1}

Molecular Weight 481.4204

Wiswesser Line Notation L666 L6 K6 2AL TJ &WNR BQ CNW ENW

Evaluation B

$C_{26}H_{15}N_3O_7$ (c) 79FAR/SHA

Benzo[a]pyrene picric acid

Phase Changes

c/liq 475.5 K, $\Delta H = 39300$ J·mol^{-1}

$\Delta S = 82.7$ J·mol^{-1}·K^{-1}

Molecular Weight 481.4204

Wiswesser Line Notation L D6 B6666 2AB TJ &WNR BQ CNW ENW

Evaluation B

$C_{26}H_{17}N_3O_7$ (c) 79FAR/SHA

β,β'-Binaphthyl picric acid

Phase Changes

c/liq 464.2 K, $\Delta H = 41400$ J·mol^{-1}

$\Delta S = 89.2$ J·mol^{-1}·K^{-1}

Molecular Weight 483.4362

Wiswesser Line Notation L66J A- AL66J & WNR BQ CNW ENW

Evaluation B

$C_{26}H_{20}$ (c) 31SMI/AND

Tetraphenylethylene

Heat Capacity 298.5 K, $C_p = 387.6$ J·mol^{-1}·K^{-1}

Temperature range 102 to 346 K. Value is unsmoothed experimental datum.

Molecular Weight 332.4448

Wiswesser Line Notation RYR&UYR&R

Evaluation C

$C_{26}H_{20}N_6O$ (c) 84KAR/SHV

Bis-(*o*-aminophenyl)-2,2′-dibenzimidazole oxide

Heat Capacity 298.15 K, $C_p = 471.1$ J·mol^{-1}·K^{-1}

Temperature range 60 to 298 K.

Entropy 298.15 K, $S = 426.3$ J·mol^{-1}·K^{-1}

Molecular Weight 432.4838

Wiswesser Line Notation ZR B- CT56 BM DNJ H- 2 O

Evaluation B

$C_{26}H_{20}Sn$ (c) 85CAR/LAY
Triphenyl phenylethynyl tin
Heat Capacity 298.15 K, C_p=447.5 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.992 J·K^{-1}·g^{-1}.
Molecular Weight 451.1340
Wiswesser Line Notation R-SN-R&R&1UU1R
Evaluation B

$C_{26}H_{22}$ (c) 31SMI/AND
1,1,1,2-Tetraphenylethane
Heat Capacity 298.5 K, C_p=395.4 J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 334.4607
Wiswesser Line Notation RXR&R&1R
Evaluation C

$C_{26}H_{22}$ (c) 31SMI/AND
1,1,2,2-Tetraphenylethane
Heat Capacity 298.5 K, C_p=399.6 J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 334.4607
Wiswesser Line Notation RYR&YR&R
Evaluation C

$(C_{26}H_{26}N_2O_3)_n$ (c) 89CHE/JAN
Poly(azomethine)
Heat Capacity 300 K, C_p=521.8 J·mol^{-1}·K^{-1}
Temperature range 230 to 620 K. $C_p(c)=0.0015529T^2+0.87083T+120.76$ J/mol·K (230 to 250 K). C_p(liq) $=0.9086T+439.73$ J/mol·K (318 to 620 K).
Phase Changes
liq/liq 439.8 K, ΔH=13000 J·mol^{-1}
Disordering transition. 26.9% crystallinity.
liq/liq 566.4 K, ΔH=2000 J·mol^{-1}
ΔS=3.5 J·mol^{-1}·K^{-1}
Isotropic transition.
Molecular Weight 414.5030
Wiswesser Line Notation /*NR B1 DO2O2OR C1 DNU1R D1*/
Evaluation B
Poly(azomethine) with two ethylene glycol spacers. T(glass)=318 K.

$C_{26}H_{26}OSi_2$ (c) 86DZH/KUL
1,3-Dimethyl-1,1,3,3-tetraphenyldisiloxane
Heat Capacity 298.15 K, C_p=503.2 J·mol^{-1}·K^{-1}
Temperature range 4 to 300 K. $C_p(c)=125.6+0.394T+3.94\times10^{-3}T^2$ (80 to 150 K); $C_p(c)=133.78+0.6826T+2.0758\times10^{-3}T^2$ (170 to 290 K).
Entropy 298.15 K, S=570.2 J mol^{-1} K^{-1}
Phase Changes
c/liq 321.95 K, ΔH=26577 J·mol^{-1}
Molecular Weight 410.6618
Wiswesser Line Notation 1-SI-R&R&O-SI-1&R&R
Evaluation A

$C_{26}H_{26}O_3Si_3$ (c) 82KUL/DZH
Dimethyltetraphenylcyclotrisiloxane
Heat Capacity 298.15 K, C_p=571.5 J·mol^{-1}·K^{-1}
Temperature range 4.7 to 300 K. Data given graphically except for data at 298.15 K.
Entropy 298.15 K, S=630.1 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 361.06 K, ΔH=28200 J·mol^{-1}
ΔS=78.2 J·mol^{-1}·K^{-1}
Molecular Weight 470.7461
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A1 A1 CR CR ER ER
Evaluation B

$C_{26}H_{26}O_4$ (c) 84OZC/ASF
4,4′-Dipentanoyloxydiphenyldiacetylene
Phase Changes
c,III/c,II 272 K
c,II/c,I 290 K, ΔH=1240 J·mol^{-1}
ΔS=4.309 J·mol^{-1}·K^{-1}
c,II/c,II, c,II/c,I transitions combined.
c,I/liq 405 K, ΔH=24700 J·mol^{-1}
ΔS=61.04 J·mol^{-1}·K^{-1}
Solid-nematic.
liq/liq 434 K, ΔH=2300 J·mol^{-1}
ΔS=3.390 J·mol^{-1}·K^{-1}
Nematic—isotropic liquid transition.
Molecular Weight 402.4891
Wiswesser Line Notation 4VOR D1UU2UU1R DOV4
Evaluation A

$C_{26}H_{34}$ (c) 83KRA/DE
1,1′-Diphenyl-1,1′-bicyclooctane
Heat Capacity 298 K, C_p=453.8 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.313 cal.K^{-1}.g^{-1}.
Molecular Weight 346.5546
Wiswesser Line Notation L8TJ AR A- AL8TJ AR
Evaluation B

$C_{26}H_{34}N_2O_3$ (c) 88FAN/PO
4-Pentanoyl-4-*n*′-nanoyloxyazobenzene
Phase Changes
c,II/c,I 352.2 K, ΔH=4330 J·mol^{-1}
ΔS=12.30 J·mol^{-1}·K^{-1}
c,I/liq 367.2 K, ΔH=24807 J·mol^{-1}
ΔS=67.559 J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 404.3 K, ΔH=7569 J·mol^{-1}
ΔS=18.72 J·mol^{-1}·K^{-1}
Smectic A-isotropic.
liq/liq 366.8 K, ΔH=6117 J·mol^{-1}
ΔS=16.68 J·mol^{-1}·K^{-1}
Smectic A-Smectic monotropic 1.
Molecular Weight 422.5662
Wiswesser Line Notation 8VOR DNUNR DV4
Evaluation A

$C_{26}H_{34}N_2O_3$ (c) 83FAN/PO
4-Propionyl-4′-*n*-undecanoyloxyazobenzene
Phase Changes
c/liq 370.65 K, ΔH=37489 J·mol^{-1}
ΔS=101.1 J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 416.65 K, ΔH=7573 J·mol^{-1}
Smectic A-isotropic liquid transition.
Molecular Weight 422.5662
Wiswesser Line Notation 10VOR DNUNR DV2
Evaluation A

$C_{26}H_{38}$ (c) 83KRA/BE
2,3-Dimethyl-2,3-bis(4-*tert*-butylphenyl)butane
Heat Capacity 298 K, C_p=529.5 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.361 cal.K^{-1}.g^{-1}.
Molecular Weight 350.5862
Wiswesser Line Notation 1XR&R DX1&1&1 &X1&1&R DX1&1&1
Evaluation B

$C_{26}H_{38}N_2O_3$ (c,I) 79RAC/NGU

4,4′-Bis(*n*-heptyloxy)azoxybenzene

Heat Capacity 300 K, $C_p = 480$ J·mol^{-1}·K^{-1}

Temperature range 90 to 420 K. Data graphically only.

Phase Changes

c,I/liq 347.75 K, $\Delta H = 27450$ J·mol^{-1}; $\Delta S = 78.9$ J·mol^{-1}·K^{-1}

Melting of stable crystal phase.

liq/liq 368.2 K, $\Delta H = 545$ J·mol^{-1}; $\Delta S = 1.5$ J·mol^{-1}·K^{-1}

Smectic-nematic transition.

liq/liq 397.25 K, $\Delta H = 830$ J·mol^{-1}; $\Delta S = 2.1$ J·mol^{-1}·K^{-1}

Nematic-isotropic transition.

Molecular Weight 426.5978

Wiswesser Line Notation 7OR DNUNO&R DO7

Evaluation B

$C_{26}H_{50}O_4$ (liq) 76PHI/MAT

Di-*n*-octyl sebacate

Heat Capacity 318 K, $C_p = 849$ J·mol^{-1}·K^{-1}

Temperature range 318 to 393 K.

Molecular Weight 426.6786

Wiswesser Line Notation 8OV8VO8

Evaluation C

$C_{26}H_{50}O_4Pb$ (c,II) 78ADE/SIM

Lead (II) tridecanoate

Heat Capacity 375 K, $C_p = 1230$ J·mol^{-1}·K^{-1}

Temperature range 371 to 377 K. Data only graphically for c,III. Also data for liquid.

Phase Changes

c,III/c,II 368.7 K, $\Delta H = 58400$ J·mol^{-1}; $\Delta S = 158$ J·mol^{-1}·K^{-1}

c,II and c,I are mesophases.

c,II/c,I 381.5 K, $\Delta H = 38800$ J·mol^{-1}; $\Delta S = 102$ J·mol^{-1}·K^{-1}

Molecular Weight 633.8786

Wiswesser Line Notation OV12 2 .PB

Evaluation C

$C_{26}H_{52}$ (c) 69BOR/DAL

1,1,4,4,10,10,13,13-Octamethyl-cyclooctadecane

Phase Changes

c,II/c,I 427 K, $\Delta H = 6736$ J·mol^{-1}; $\Delta S = 15.9$ J·mol^{-1}·K^{-1}

c/liq 438 K, $\Delta H = 20167$ J·mol^{-1}; $\Delta S = 46.4$ J·mol^{-1}·K^{-1}

Molecular Weight 364.6968

Wiswesser Line Notation L-18-TJ A1 A1 D1 D1 J1 J1 M1 M1

Evaluation B

$C_{26}H_{52}O_2$ (c) 34KIN/GAR

Ethyl tetracosanate

Phase Changes

c,II/c,I 317.65 K, $\Delta H = 11203$ J·mol^{-1}

β-α transition.

c,I/liq 327.35 K, $\Delta H = 22938$ J·mol^{-1}

α-liq transition.

Molecular Weight 396.6956

Wiswesser Line Notation 23VO2

Evaluation B

Data on the specific heats are given at or near the phase transitions.

$C_{26}H_{54}$ (c,II) 31GAR/VAN

n-Hexacosane

Heat Capacity 304 K, $C_p = 677.8$ J·mol^{-1}·K^{-1}

Temperature range 295 to 358 K. Mean value 22–40 °C, β-form.

Phase Changes

c,II/c,I 323.3 K, $\Delta H = 35020$ J·mol^{-1}; $\Delta S = 108.3$ J·mol^{-1}·K^{-1}

β-α transition.

c,I/liq 329.3 K, $\Delta H = 58743$ J·mol^{-1}; $\Delta S = 178.4$ J·mol^{-1}·K^{-1}

Molecular Weight 366.7126

Wiswesser Line Notation 26H

Evaluation B

$C_{26}H_{54}$ (c) 55SCH/BUS

n-Hexacosane

Phase Changes

c,II/c,I 326.45 K, $\Delta H = 32217$ J·mol^{-1}; $\Delta S = 98.7$ J·mol^{-1}·K^{-1}

c,I/liq 329.45 K, $\Delta H = 59496$ J·mol^{-1}; $\Delta S = 180.6$ J·mol^{-1}·K^{-1}

Molecular Weight 366.7126

Wiswesser Line Notation 26H

Evaluation B

$C_{26}H_{54}$ (liq) 69ATK/LAR

n-Hexacosane

Heat Capacity 353 K, $C_p = 870$ J·mol^{-1}·K^{-1}

Temperature range 353 to 453 K. Equation only.

Molecular Weight 366.7126

Wiswesser Line Notation 26H

Evaluation C

$C_{26}H_{54}$ (c) 73COM

n-Hexacosane

Phase Changes

c,II/c,I 326.55 K, $\Delta H = 34225$ J·mol^{-1}; $\Delta S = 104.8$ J·mol^{-1}·K^{-1}

c,I/liq 329.55 K, $\Delta H = 59496$ J·mol^{-1}; $\Delta S = 180.5$ J·mol^{-1}·K^{-1}

Molecular Weight 366.7126

Wiswesser Line Notation 26H

Evaluation B

$C_{26}H_{54}$ (c,II) 76AND/MAR

n-Hexacosane

Heat Capacity 298.15 K, $C_p = 661.2$ J·mol^{-1}·K^{-1}

Temperature range 10 to 360 K.

Entropy 298.15 K, $S = 667.0$ J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 325.5 K, $\Delta H = 33420$ J·mol^{-1}; $\Delta S = 102.7$ J·mol^{-1}·K^{-1}

c,I/liq 329.25 K, $\Delta H = 60700$ J·mol^{-1}; $\Delta S = 184.4$ J·mol^{-1}·K^{-1}

Molecular Weight 366.7126

Wiswesser Line Notation 26H

Evaluation A

$C_{26}H_{54}$ (c) 91BAR/SCH
n-Hexacosane
Phase Changes
c,II/c,I 325.6 K, $\Delta H = 33500$ J·mol^{-1}
c,I/liq 329.2 K, $\Delta H = 60000$ J·mol^{-1}
Molecular Weight 366.7126
Wiswesser Line Notation 26H
Evaluation A

$C_{26}H_{54}$ (liq) 91CLA/LET
n-Hexacosane
Phase Changes
c,II/c,I 325.8 K, $\Delta H = 32820$ J·mol^{-1}
c,I/liq 329.6 K, $\Delta H = 59790$ J·mol^{-1}
Molecular Weight 366.7126
Wiswesser Line Notation 26H
Evaluation A

$C_{26}H_{54}$ (c) 91DOM/WYR
n-Hexacosane
Phase Changes
c,II/c,I 324.40 K, $\Delta H = 30360$ J·mol^{-1}
c,I/liq 329.18 K, $\Delta H = 63920$ J·mol^{-1}
Molecular Weight 366.7126
Wiswesser Line Notation 26H
Evaluation A

$C_{27}H_{30}O_2$ (c) 79LEW/ENE
Norethindrone benzoate
Phase Changes
c/liq 531 K, $\Delta H = 41500$ J·mol^{-1}
$\Delta S = 78.2$ J·mol^{-1}·K^{-1}
Molecular Weight 386.5328
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1 FVR
Evaluation A

$C_{27}H_{36}N_2O_3$ (c) 88FAN/POE
4-*n*-Pentanoyl-4-*n'*-decanoyloxyazobenzene
Phase Changes
c,II/c,I 338.2 K, $\Delta H = 4310$ J·mol^{-1}
$\Delta S = 12.74$ J·mol^{-1}·K^{-1}
c,I/liq 368.6 K, $\Delta H = 28752$ J·mol^{-1}
$\Delta S = 78.01$ J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 405.2 K, $\Delta H = 8000$ J·mol^{-1}
$\Delta S = 19.74$ J·mol^{-1}·K^{-1}
Smectic A-isotropic.
liq/liq 364.7 K, $\Delta H = 5406$ J·mol^{-1}
$\Delta S = 14.82$ J·mol^{-1}·K^{-1}
Smectic A-smectic monotropic 1.
Molecular Weight 436.5930
Wiswesser Line Notation 9VOR DNUNR DV4
Evaluation A

$C_{27}H_{36}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4'-*n*-dodecanoyloxyazobenzene
Phase Changes
c/liq 373.65 K, $\Delta H = 38074$ J·mol^{-1}
$\Delta S = 101.9$ J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 416.15 K, $\Delta H = 7866$ J·mol^{-1}
Smectic A-isotropic liquid transition.
Molecular Weight 436.5930
Wiswesser Line Notation 11VOR DNUNR DV2
Evaluation A

$C_{27}H_{38}O_2$ (c) 72YOU/HAI
4-Methoxy-4'-dodecoxy-*trans*-stilbene
Phase Changes
liq/liq 409 K, $\Delta H = 21880$ J·mol^{-1}
$\Delta S = 53.5$ J·mol^{-1}·K^{-1}
Smectic-liquid transition.
c/liq 415 K, $\Delta H = 58660$ J·mol^{-1}
$\Delta S = 141.3$ J·mol^{-1}·K^{-1}
Crystal-isotropic liquid transition.
Molecular Weight 394.5960
Wiswesser Line Notation 12OR D1U1R DO1 -T
Evaluation B

$C_{27}H_{38}O_2$ (c) 79LEW/EN
Norethindrone heptanoate
Phase Changes
c/liq 340 K, $\Delta H = 21600$ J·mol^{-1}
$\Delta S = 63.5$ J·mol^{-1}·K^{-1}
Molecular Weight 394.5960
Wiswesser Line Notation L E5 B666 OV MUTJ E1 FV6 F1UU1
Evaluation A

$C_{27}H_{46}O$ (c) 88PET/TS
Cholesterol
Phase Changes
c,II/c,I 304.8 K, $\Delta H = 2500$ J·mol^{-1}
$\Delta S = 8.2$ J·mol^{-1}·K^{-1}
Molecular Weight 386.6598
Wiswesser Line Notation L E5 B666 LUTJ A1 E1 FY1&3Y1&1 OQ -A&BI -B&AEFO
Evaluation A

$C_{27}H_{48}$ (liq) 49PAR/MO
11-Phenyleicosane
Heat Capacity 300 K, $C_p = 765.7$ J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.15 K, $S = 867.8$ J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 172.0 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 294.3 K, $\Delta H = 64772$ J·mol^{-1}
$\Delta S = 220.1$ J·mol^{-1}·K^{-1}
Molecular Weight 372.6762
Wiswesser Line Notation 10Y10&R
Evaluation B(C_p),C(S)

$C_{27}H_{50}$ (liq) 63GUD/CA
4-*n*-Nonyltercyclohexyl
Heat Capacity 373 K, $C_p = 820.5$ J·mol^{-1}·K^{-1}
Temperature range 373 to 483 K.
Molecular Weight 374.6920
Wiswesser Line Notation L6TJ AAL6TJ X- AL6TJ X9
Evaluation C

$C_{27}H_{50}O_6$ (liq) 76PHI/MA
Trioctanoin; Glyceryl trioctanoate
Heat Capacity 338 K, $C_p = 920$ J·mol^{-1}·K^{-1}
Temperature range 338 to 413 K.
Molecular Weight 470.6884
Wiswesser Line Notation 7VO1YOV7&1OV7
Evaluation C

$C_{27}H_{54}$ (liq) 49PAR/MOO
11-Cyclohexyleicosane
Heat Capacity 298.15 K, C_p=787.4 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.15 K, S=844.1 J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 174.9 J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 269.9 K, ΔH=48693 J·mol^{-1}
ΔS=180.4 J·mol^{-1}·K^{-1}
Molecular Weight 378.7236
Wiswesser Line Notation L6TJ AY10&10
Evaluation B(C_p),C(S)

$C_{27}H_{54}N_3AsS_6$ (c) 89AIR/DES
Tris(di-*n*-butyldithiocarbamato)arsenic(III)
Heat Capacity 298.15 K, C_p=861 J·mol^{-1}·K^{-1}
Temperature range 385 to 395 K.
Phase Changes
c/liq 397 K, ΔH=30950 J·mol^{-1}
Molecular Weight 688.0253
Wiswesser Line Notation
4N4&YUS&S-AS-SYUS&N4&4&SYUS&N4&4
Evaluation B

$C_{27}H_{54}N_3BiS_6$ (c) 89AIR/DES
Tris(di-*n*-butyldithiocarbamato)bismuth(III)
Heat Capacity 298.15 K, C_p=1056 J·mol^{-1}·K^{-1}
Temperature range 355 to 365 K.
Phase Changes
c/liq 367 K, ΔH=31800 J·mol^{-1}
Molecular Weight 822.0841
Wiswesser Line Notation
4N4&YUS&S-BI-SYUS&N4&4&SYUS&N4&4
Evaluation B

$C_{27}H_{54}N_3PS_6$ (c) 89AIR/DES
Tris(di-*n*-butyldithiocarbamato)phosphorus(III)
Heat Capacity 298.15 K, C_p=962 J·mol^{-1}·K^{-1}
Temperature range 355 to 365 K.
Phase Changes
c/liq 374 K, ΔH=35600 J·mol^{-1}
Molecular Weight 644.0775
Wiswesser Line Notation
4N4&YUS&SPSYUS&N4&4&SYUS&N4&4
Evaluation B

$C_{27}H_{54}N_3SbS_6$ (c) 89AIR/DES
Tris(di-*n*-butyldithiocarbamato)antimony(III)
Heat Capacity 298.15 K, C_p=1049 J·mol^{-1}·K^{-1}
Temperature range 330 to 340 K.
Phase Changes
c/liq 343 K, ΔH=37240 J·mol^{-1}
Molecular Weight 734.8537
Wiswesser Line Notation
4N4&YUS&S-SB-SYUS&N4&4&SYUS&N4&4
Evaluation B

$C_{27}H_{56}$ (c,β) 38VER
n-Heptacosane
Heat Capacity 313 K, C_p=828 J·mol^{-1}·K^{-1}
One temperature. Also data for α form, 1117 J·mol^{-1}·K^{-1} at 328 K, and liquid, 828 J·mol^{-1}·K^{-1} at 338 K.
Molecular Weight 380.7394
Wiswesser Line Notation 27H
Evaluation C

$C_{27}H_{56}$ (c) 55SCH/BUS
n-Heptacosane
Phase Changes
c,II/c,I 320.25 K, ΔH=28953 J·mol^{-1}
ΔS=90.4 J·mol^{-1}·K^{-1}
c,I/liq 331.95 K, ΔH=60417 J·mol^{-1}
ΔS=182.0 J·mol^{-1}·K^{-1}
Molecular Weight 380.7394
Wiswesser Line Notation 27H
Evaluation B

$C_{28}H_{15}N_3O_7$ (c) 79FAR/SHA
o-Phenylenepyrene picric acid
Phase Changes
c/liq 469.6 K, ΔH=39300 J·mol^{-1}
ΔS=83.7 J·mol^{-1}·K^{-1}
Molecular Weight 505.4424
Wiswesser Line Notation L E6 D4 B6666 2AB TJ &WNR BQ CNW ENW WNR BQ CNW ENW
Evaluation B

$C_{28}H_{17}N_3O_7$ (c) 79FAR/SHA
1,2,3,4-Dibenzanthracene-picric acid
Phase Changes
c,II/c,I 446.5 K, ΔH=6700 J·mol^{-1}
ΔS=15.0 J·mol^{-1}·K^{-1}
c/liq 485.2 K, ΔH=44800 J·mol^{-1}
ΔS=92.3 J·mol^{-1}·K^{-1}
Molecular Weight 507.4582
Wiswesser Line Notation L D6 J6 C666J &WNR BQ CNW ENW
Evaluation B

$C_{28}H_{17}N_3O_7$ (c) 79FAR/SHA
Picene-picric acid
Phase Changes
c,II/c,I 391 K, ΔH=3300 J·mol^{-1}
ΔS=8.4 J·mol^{-1}·K^{-1}
c/liq 437.9 K, ΔH=21300 J·mol^{-1}
ΔS=48.6 J·mol^{-1}·K^{-1}
Molecular Weight 507.4582
Wiswesser Line Notation L F6 E6 B666J &WNR BQ CNW ENW
Evaluation B

$C_{28}H_{17}N_3O_7$ (c) 79FAR/SHA
1,2,5,6-Dibenzanthracene-picric acid
Phase Changes
c/liq 493.0 K, ΔH=54000 J·mol^{-1}
ΔS=109.6 J·mol^{-1}·K^{-1}
Molecular Weight 507.4582
Wiswesser Line Notation L G6 D6 B666J &WNR BQ CNW ENW
Evaluation B

$C_{28}H_{18}N_6$ (c) 84RAB/KAR
Phthalonitrile and *m*-phenylene diamine condensation product
Heat Capacity 298.15 K, C_p=446.5 J·mol^{-1}·K^{-1}
Temperature range 60 to 530 K.
Entropy 298.15 K, S=424.3 J·mol^{-1}·K^{-1}
Molecular Weight 438.4904
Wiswesser Line Notation ZR CZ &NCR DCN
Evaluation A

$(C_{28}H_{24}GeSi)_n$ (gls) 78LEB/LEB2
Diphenylsilane-diethynyldi-phenylgermane vitreous copolymer; Polyvinylenediphenylenesilyl,germyl-α, ω-dihydride copolymer
Heat Capacity 298.15 K, $C_p = 566.6$ J·mol^{-1}·K^{-1}
Temperature range for devitrification 280 to 310 K. T(glass)=301 K.
Molecular Weight 461.1931
Wiswesser Line Notation /*-SI-R&R&1U1-GE-R&R&1U1*/
Evaluation A
Average molecular weight, $n = 10{,}000$.

$(C_{28}H_{24}GeSi)_n$ (gls) 78LEB/RAB2
Diphenylsilane-diethynyldi-phenylgermane vitreous copolymer; Polyvinylenediphenylenesilyl, germyl-α, ω-dihydride copolymer
Heat Capacity 298.15 K, $C_p = 566.6$ J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, $S = 583.8$ J·mol^{-1}·K^{-1}
Glass like state.
Molecular Weight 461.1931
Wiswesser Line Notation /*-SI-R&R&1U1-GE-R&R&1U1*/
Evaluation A
T(glass)=301 K.

$C_{28}H_{28}P_2$ (c) 89HUI/VAN
1,4-Bis(diphenylphosphino)butane
Heat Capacity 364 K, $C_p = 354$ J·mol^{-1}·K^{-1}
Temperature range 364 to 444 K.
Phase Changes
c/liq 405.9 K, $\Delta H = 45300$ J·mol^{-1}
Molecular Weight 272.6570
Wiswesser Line Notation RPR&4PR&R
Evaluation B

$(C_{28}H_{30}N_2O_4)_n$ (c) 89CHE/JAN
Poly(azomethine)
Heat Capacity
C_p(liq)=0.9751T+507.78 J/mol·K (305 to 512 K).
Phase Changes
liq/liq 416.0 K, $\Delta H = 21700$ J·mol^{-1}
Disordering transition. 38.5% crystallinity.
liq/liq 512.8 K, $\Delta H = 2100$ J·mol^{-1}
$\Delta S = 4.1$ J·mol^{-1}·K^{-1}
Isotropic transition.
Molecular Weight 458.5560
Wiswesser Line Notation /*NR B1 DO2O2O2OR C1 DNU1R D1*/
Evaluation B
Poly(azomethine) with three ethylene glycol spacers. T(glass)=305 K.

$C_{28}H_{30}O_4$ (c) 84OZC/ASR
4,4′-Dihexanoyloxydiphenyldiacetylene
Phase Changes
c,III/c,II 343 K, $\Delta H = 19000$ J·mol^{-1}
$\Delta S = 55.40$ J·mol^{-1}·K^{-1}
c,II/c,I 396 K, $\Delta H = 1460$ J·mol^{-1}
$\Delta S = 3.682$ J·mol^{-1}·K^{-1}
c,I/liq 407 K, $\Delta H = 26300$ J·mol^{-1}
$\Delta S = 64.64$ J·mol^{-1}·K^{-1}
Solid-nematic.
liq/liq 430 K, $\Delta H = 1710$ J·mol^{-1}
$\Delta S = 3.975$ J·mol^{-1}·K^{-1}
Nematic-isotropic liquid transition.
Molecular Weight 430.5426
Wiswesser Line Notation 5VOR D1UU2UU1R DOV5
Evaluation A

$C_{28}H_{32}Cl_4N_2Zn$ (c) 82FER/SO(
Bis-(tetradecylammonium)zinc tetrachloride
Heat Capacity
Temperature range 360 to 370 K. Data given graphically.
Phase Changes
c,III/c,II 362.5 K, $\Delta H = 9700$ J·mol^{-1}
$\Delta S = 22.5$ J·mol^{-1}·K^{-1}
Low temperature phase—intermediate phase.
c,II/c,I 367 K, $\Delta H = 49690$ J·mol^{-1}
$\Delta S = 7.5$ J·mol^{-1}·K^{-1}
Intermediate phase—high temperature phase.
c,I/liq 438 K, $\Delta H = 7500$ J·mol^{-1}
$\Delta S = 17.1$ J·mol^{-1}·K^{-1}
High temperature phase—isotropic liquid phase.
Molecular Weight 603.7662
Wiswesser Line Notation 14ZH 2 .ZN G4
Evaluation A

$C_{28}H_{32}N_2$ (c) 79KOB/KA
Terephthal-bis-*n*-butylaniline
Heat Capacity
C_p data given graphically only. Temperature range 88 to 330 K.
Phase Changes
c,X/c,IX 99 K, $\Delta H = 280$ J·mol^{-1}
$\Delta S = 2.83$ J·mol^{-1}·K^{-1}
c,IX/c,VIII 240 K, $\Delta H = 1255$ J·mol^{-1}
$\Delta S = 9.0$ J·mol^{-1}·K^{-1}
Molecular Weight 396.5742
Wiswesser Line Notation 4R DNUYR DYVNR D4
Evaluation C

$C_{28}H_{32}O_4Si_4$ (c) 76KUL/DZ
1,1,3,3-Tetramethyl-5,5,7,7,-tetraphenyl-cyclotetrasiloxane
Heat Capacity
C_p not given. Temperature range 12 to 370 K. Data deposited VINIT No. 1191-76, 13 April 1976.
Entropy 298.15 K, $S = 811.3$ J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 186.5 K, $\Delta H = 243$ J·mol^{-1}
$\Delta S = 1.3$ J·mol^{-1}·K^{-1}
c,II/c,I 271.5 K, $\Delta H = 1046$ J·mol^{-1}
$\Delta S = 3.85$ J·mol^{-1}·K^{-1}
c,I/liq 346.21 K, $\Delta H = 27050$ J·mol^{-1}
$\Delta S = 78.13$ J·mol^{-1}·K^{-1}
Molecular Weight 544.9004
Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI-OTJ A1 A1 C1 C1 E ER GR GR
Evaluation B

$C_{28}H_{32}O_4Si_4$ (c) 75MEK/KAI
1,3,5′7′-Tetramethyl-1′,3′,5,7-tetraphenylcyclotetrasiloxane
Heat Capacity 298.15 K, $C_p = 615.5$ J·mol^{-1}·K^{-1}
Temperature range 13 to 390 K.
Entropy 298.15 K, $S = 662.7$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 373.4 K, $\Delta H = 24619$ J·mol^{-1}
$\Delta S = 62.8$ J·mol^{-1}·K^{-1}
Molecular Weight 544.9004
Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI-OTJ A1 AR C1 CR 1 ER G1 GR
Evaluation B

$C_{28}H_{32}O_4Si_4$ (c) 81MEK/KAR

Tetra(methylphenyl)tetrasiloxane

Heat Capacity 298.15 K, $C_p = 615.0$ J·mol^{-1}·K^{-1}

Temperature range 13 to 390 K. Data given graphically.

Entropy 298.15 K, $S = 662.7$ J·mol^{-1}·K^{-1}

Phase Changes

c/liq 373.0 K, $\Delta H = 42731$ J·mol^{-1}

$\Delta S = 121.8$ J·mol^{-1}·K^{-1}

Molecular Weight 544.9004

Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI- O-TJ A1 AR C1 CR E1 ER G1 GR

Evaluation A

$C_{28}H_{34}Cl_3Fe_3N_3O_{13}$ (c) 89KAN/NAK

Hexakis(μ-acetato) (μ_3-oxo)tris(pyridine)iron(II) diiron(III)chloroform

Heat Capacity 300.309 K, $C_p = 932.03$ J·mol^{-1}·K^{-1}

Temperature range 14 to 300 K. Unsmoothed experimental datum.

Phase Changes

c,II/c,I 207.14 K $\Delta H = 5107$ J·mol^{-1}

208.19 K, $\Delta S = 28.10$ J·mol^{-1}·K^{-1}

Two peaks closely centered.

Molecular Weight 894.1889

Wiswesser Line Notation OV1 6 &T6NJ 3 &-FE- 30 &GYGG

Evaluation A

$C_{28}H_{38}FeN_4O_4$ (c) 93KAJ/SOR

Bis[2-[[[3-(1-aziridinyl)propyl]imino]methyl]-6-ethoxyphenolato-N^2,N^2,O^1]-(OC-6-1′2′)-iron (1+) perchlorate complex with benzene

Heat Capacity 297.94 K, $C_p = 910.63$ J·mol^{-1}·K^{-1}

Temperature range 13 to 320 K. Unsmoothed experimental datum.

Phase Changes

c,III/c,II 187 K

First order transition

c,II/c,I 295.3 K

Second or higher order transition

Molecular Weight

Wiswesser Line Notation

Evaluation A

A very broad heat capacity anomaly exists between 100 and 310 K. The phase transitions at 187 and 295.3 K are superimposed over the broad heat capacity anomaly. Enthalpy and entropy changes due to all anomalies were calculated to be: $\Delta H = 34.8 \pm 1.5$ J·mol^{-1}·K^{-1}.

$C_{28}H_{38}N_2O_3$ (c) 88FAN/POE

4-*n*-Pentanoyl-4-*n*′-undecanoyloxyazobenzene

Phase Changes

c,II/c,I 354.4 K, $\Delta H = 4678$ J·mol^{-1}

$\Delta S = 13.20$ J·mol^{-1}·K^{-1}

c,I/liq 368.7 K, $\Delta H = 31355$ J·mol^{-1}

$\Delta S = 85.040$ J·mol^{-1}·K^{-1}

Solid-smectic A.

liq/liq 404.6 K, $\Delta H = 8540$ J·mol^{-1}

$\Delta S = 21.10$ J·mol^{-1}·K^{-1}

Smectic A-isotropic.

liq/liq 363.9 K, $\Delta H = 4807$ J·mol^{-1}

$\Delta S = 13.21$ J·mol^{-1}·K^{-1}

Smectic A-smectic monotropic 1.

liq/c 359.0 K, $\Delta H = 22853$ J·mol^{-1}

$\Delta S = 63.655$ J·mol^{-1}·K^{-1}

Smectic monotropic 1-solid.

Molecular Weight 450.6198

Wiswesser Line Notation 10VOR DNUNR DV4

Evaluation A

$C_{28}H_{38}N_2O_3$ (c) 83FAN/POE

4-Propionyl-4′-*n*-tridecanoyloxyazobenzene

Phase Changes

c/liq 374.65 K, $\Delta H = 44769$ J·mol^{-1}

$\Delta S = 119.5$ J·mol^{-1}·K^{-1}

Solid-smectic A.

liq/liq 416.65 K, $\Delta H = 8075$ J·mol^{-1}

$\Delta S = 19.4$ J·mol^{-1}·K^{-1}

Smectic A-isotropic liquid transition.

Molecular Weight 450.6198

Wiswesser Line Notation 12VOR DNUNR DV2

Evaluation A

$C_{28}H_{40}O_4$ (liq) 81ARU/DAU

4-(2-Methylbutoxy)phenyl ester of 4-*n*-decycloxybenzoic acid (D)

Phase Changes

liq/liq 323.7 K

Smectic C-smectic A liquid transition.

liq/liq 338.15 K, $\Delta H = 17.21$ J·mol^{-1}

Smectic A-isotropic liquid transition.

Molecular Weight 440.6216

Wiswesser Line Notation 10OR DVOR DO1Y2&1

Evaluation C

$C_{28}H_{54}HgO_4$ (liq) 78ADE

Mercuric tetradecanoate; Mercuric myristate

Heat Capacity 415 K, $C_p = 1135.5$ J·mol^{-1}·K^{-1}

Mean value, 413 to 421 K. Data only graphically for solid.

Phase Changes

c,II/c,I 382.4 K, $\Delta H = 57900$ J·mol^{-1}

$\Delta S = 151.4$ J·mol^{-1}·K^{-1}

c,I probably a smectic phase.

c,I/liq 387.0 K, $\Delta H = 40000$ J·mol^{-1}

$\Delta S = 103.4$ J·mol^{-1}·K^{-1}

Molecular Weight 655.3222

Wiswesser Line Notation OV13 2 .HG

Evaluation C

$C_{28}H_{54}O_4Cd$ (c) 78KON/RUF

Cadmium(II) *n*-tetradecanoate

Phase Changes

c/liq 374.7 K, $\Delta H = 43000$ J·mol^{-1}

$\Delta S = 115$ J·mol^{-1}·K^{-1}

Crystal mesophase.

liq/liq 380.4 K, $\Delta H = 1600$ J·mol^{-1}

$\Delta S = 4$ J·mol^{-1}·K^{-1}

Mesophase-liquid.

Molecular Weight 567.1422

Wiswesser Line Notation OV13 2 .CD

Evaluation B

$C_{28}H_{54}O_4Pb$ (c) 76ADE/SIM

Lead(II) *n*-tetradecanoate

Phase Changes

c/liq 372.2 K, $\Delta H = 59100$ J·mol^{-1}

$\Delta S = 159$ J·mol^{-1}·K^{-1}

Crystal-smectic.

liq/liq 382.7 K, $\Delta H = 41600$ J·mol^{-1}

$\Delta S = 109$ J·mol^{-1}·K^{-1}

Smectic-liquid.

Molecular Weight 661.9322

Wiswesser Line Notation OV13 2 .PB

Evaluation B

$C_{28}H_{54}O_4Zn$ (c) 78KON/RUF
Zinc(II) *n*-tetradecanoate
Phase Changes
c/liq 407 K, $\Delta H = 86000$ J·mol^{-1}
$\Delta S = 211$ J·mol^{-1}·K^{-1}
Molecular Weight 520.1122
Wiswesser Line Notation OV13 2 .ZN
Evaluation B

$C_{28}H_{56}Ni_4O_{16}$ (c) 78SOR/YOS
Tetrakis(μ_3-methoxo-2,4-pentanedionato(methanol)nickel(II)
Heat Capacity 284.91 K, $C_p = 1018.5$ J·mol^{-1}·K^{-1}
Temperature range 0.4 to 285 K. Value is unsmoothed experimental datum.
Molecular Weight 883.5408
Wiswesser Line Notation D60-NI-O ADTJ BO1 BO1 D1 F1 4
Evaluation B

$C_{28}H_{56}O_2$ (c) 34KIN/GAR
Ethyl hexacosanate
Phase Changes
c,II/c,I 322.65 K, $\Delta H = 13222$ J·mol^{-1}
β-α transition.
c,I/liq 332.75 K, $\Delta H = 27048$ J·mol^{-1}
α-liq transition.
Molecular Weight 424.7492
Wiswesser Line Notation 25VO2
Evaluation B
Data on the specific heats are given at or near the phase transitions.

$C_{28}H_{58}$ (c) 55SCH/BUS
n-Octacosane
Phase Changes
c,II/c,I 331.15 K, $\Delta H = 35438$ J·mol^{-1}
$\Delta S = 107.0$ J·mol^{-1}·K^{-1}
c,I/liq 334.35 K, $\Delta H = 64643$ J·mol^{-1}
$\Delta S = 193.3$ J·mol^{-1}·K^{-1}
Molecular Weight 394.7662
Wiswesser Line Notation 28H
Evaluation B

$C_{28}H_{58}$ (liq) 69ATK/LAR
n-Octacosane
Heat Capacity 353 K, $C_p = 937$ J·mol^{-1}·K^{-1}
Temperature range 353 to 453 K. Equation only.
Molecular Weight 394.7662
Wiswesser Line Notation 28H
Evaluation C

$C_{28}H_{58}$ (c) 73COM
n-Octacosane
Phase Changes
c,II/c,I 331.25 K, $\Delta H = 35438$ J·mol^{-1}
$\Delta S = 107.0$ J·mol^{-1}·K^{-1}
c,I/liq 334.45 K, $\Delta H = 64642$ J·mol^{-1}
$\Delta S = 193.3$ J·mol^{-1}·K^{-1}
Molecular Weight 394.7662
Wiswesser Line Notation 28H
Evaluation B

$C_{28}H_{58}$ (liq) 91CLA/LE
n-Octacosane
Phase Changes
c,II/c,I 330.7 K, $\Delta H = 33675$ J·mol^{-1}
c,I/liq 334.7 K, $\Delta H = 63385$ J·mol^{-1}
Molecular Weight 394.7662
Wiswesser Line Notation 28H
Evaluation A

$C_{28}H_{58}$ (c) 91DOM/WY
n-Octacosane
Phase Changes
c,II/c,I 330.40 K, $\Delta H = 33660$ J·mol^{-1}
c,I/liq 333.98 K, $\Delta H = 66520$ J·mol^{-1}
Molecular Weight 394.7662
Wiswesser Line Notation 28H
Evaluation A

$C_{29}H_{40}N_2O_3$ (c) 88FAN/PO
4-*n*-Pentanoyl-4-*n*′-dodecanoyloxyazobenzene
Phase Changes
c,III/c,II 315.6 K, $\Delta H = 3033$ J·mol^{-1}
$\Delta S = 9.611$ J·mol^{-1}·K^{-1}
c,II/c,I 347.5 K, $\Delta H = 5230$ J·mol^{-1}
$\Delta S = 15.05$ J·mol^{-1}·K^{-1}
c,I/liq 371.0 K, $\Delta H = 33618$ J·mol^{-1}
$\Delta S = 90.62$ J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 404.4 K, $\Delta H = 8866$ J·mol^{-1}
$\Delta S = 21.92$ J·mol^{-1}·K^{-1}
Smectic A-isotropic.
liq/liq 363.1 K, $\Delta H = 4607$ J·mol^{-1}
$\Delta S = 12.69$ J·mol^{-1}·K^{-1}
Smectic A-smectic monotropic 1.
Molecular Weight 464.6466
Wiswesser Line Notation 11VOR DNUNR DV4
Evaluation A
Smectic monotropic 1-solid transition, 361 K, $\Delta H = 25175$ J/mc
$\Delta S = 70.46$ J/mol·K.

$C_{29}H_{40}N_2O_3$ (c) 83FAN/PO
4-Propionyl-4′-*n*-tetradecanoyloxyazobenzene
Phase Changes
c/liq 375.65 K, $\Delta H = 45898$ J·mol^{-1}
Solid-smectic A.
liq/liq 413.65 K, $\Delta H = 8117$ J·mol^{-1}
Smectic A-isotropic liquid transition.
Molecular Weight 464.6466
Wiswesser Line Notation 13VOR DNUNR DV2
Evaluation A

$C_{29}H_{41}O_2$ (c,I) 69KOS/SU
Galvinoxyl radical; 2,6-Di-*tert*-butyl-4-(3,5-di-tert-butyl-4-oxocyclohex
2,5-dienylidene methyl)phenoxyl
Heat Capacity 298.15 K, $C_p = 654.28$ J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, $S = 670.10$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 81.5 K, $\Delta H = 1504.6$ J·mol^{-1}
$\Delta S = 18.67$ J·mol^{-1}·K^{-1}
Magnetic transition temperature.
Molecular Weight 421.6417
Wiswesser Line Notation L6V DYJ BX1&1&1 DU1R DO CX1&1&
EX1&1&1& FX1&1&1
Evaluation A

$C_{29}H_{42}O_2$ (c) 69KOS/SUG
2,6-Di-tert-butyl-4-(3,5-di-tert-butyl-4-oxocyclohexa-2,5-dienylidene methyl)phenol
Heat Capacity 298.15 K, C_p=654.28 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S=662.24 J·mol^{-1}·K^{-1}
Molecular Weight 422.6496
Wiswesser Line Notation L6V DYJ BX1&1&1 DU1R DQ CX1&1&1 EX1&1&1& FX1&1&1
Evaluation A

$C_{29}H_{42}O_4$ (c) 83ANI/VOR
4-*n*-Hexoxyphenyl-4′-*n*-decyloxybenzoate
Phase Changes
c/liq 334.85 K, ΔH=31700 J·mol^{-1}
Crystal-smectic C.
liq/liq 350.9 K
Smectic C-smectic A.
liq/liq 356.496 K
Smectic A-nematic.
liq/liq 362.18 K, ΔH=1770 J·mol^{-1}
Nematic-isotropic liquid.
Molecular Weight 454.6484
Wiswesser Line Notation 10OR DVOR DO6
Evaluation B

$C_{29}H_{50}O$ (c) 88PET/TSY
β-Sitosterol; 24-β-Ethylcholesterol
Phase Changes
c,II/c,I 342.7 K, ΔH=2900 J·mol^{-1}
ΔS=8.4 J·mol^{-1}·K^{-1}
Molecular Weight 414.7134
Wiswesser Line Notation
Evaluation A

$C_{29}H_{60}$ (c) 55SCH/BUS
n-Nonacosane
Phase Changes
c,II/c,I 331.35 K, ΔH=29706 J·mol^{-1}
ΔS=89.7 J·mol^{-1}·K^{-1}
c,I/liq 336.55 K, ΔH=66107 J·mol^{-1}
ΔS=196.4 J·mol^{-1}·K^{-1}
Molecular Weight 408.7930
Wiswesser Line Notation 29H
Evaluation B

$(C_{30}H_{16}N_4O_4)_n$ (c) 79KAR/SAP
Poly-(*p*,*p*′-diphenylenephthalido)-1,3,4-oxadiazole
Heat Capacity 298.15 K, C_p=515.9 J·mol^{-1}·K^{-1}
Temperature range 60 to 500 K.
Entropy 298.15 K, S=499.6 J·mol^{-1}·K^{-1}
Molecular Weight 496.4810
Wiswesser Line Notation /T56 BHOVT&J BR D-CT5NN DOJ E* BR D- CT5NN DOJ ER D*/
Evaluation A

$(C_{30}H_{16}N_8)_n$ (c) 73KAR/SAP2
Poly(trizaolequinazoline)
Heat Capacity 298 K, C_p=481.2 J·mol^{-1}·K^{-1}
Temperature range 100 to 650 K.
Entropy 298 K, S=441.4 J·mol^{-1}·K^{-1}
Molecular Weight 488.5100
Wiswesser Line Notation /*YUNR& T5N CNNJ B- ET B566 CNN FN HNJ HR D*/
Evaluation B

$(C_{30}H_{20}N_4O_6)_n$ (c) 79KAR/SAP
Poly-(*p*,*p*′-diphenylenephthalido)hydrazide
Heat Capacity 298.15 K, C_p=583.7 J·mol^{-1}·K^{-1}
Temperature range 60 to 500 K.
Entropy 298.15 K, S=545.6 J·mol^{-1}·K^{-1}
Molecular Weight 532.5114
Wiswesser Line Notation /T56 BHOVT&J BR DVMMVR D* BR DVMMV*/
Evaluation A

$(C_{30}H_{20}N_8O_2)_n$ (c) 73KAR/SAP2
Poly(amido-1,2,4-triazole)
Heat Capacity 298 K, C_p=544.3 J·mol^{-1}·K^{-1}
Temperature range 100 to 650 K.
Entropy 298 K, S=514.6 J·mol^{-1}·K^{-1}
Molecular Weight 524.5404
Wiswesser Line Notation /*VMR B- CT5NN DMJ ER C- CT5NN DMJ ER BMVR D*/
Evaluation B

$C_{30}H_{22}$ (c) 79SMI
p-Quinquephenyl
Phase Changes
c/liq 659.6 K, ΔH=42300 J·mol^{-1}
ΔS=64.1 J·mol^{-1}·K^{-1}
Solid-nematic phase change.
liq/liq 688.1 K, ΔH=922 J·mol^{-1}
ΔS=1.34 J·mol^{-1}·K^{-1}
Nematic-isotropic phase change.
Molecular Weight 382.5038
Wiswesser Line Notation RR DR DR DR
Evaluation A

$(C_{30}H_{34}N_2O_5)_n$ (c) 89CHE/JAN
Poly(azomethine)
Heat Capacity
C_p(liq)=1.0417*T*+575.53 (293 to 467 K).
Phase Changes
liq/liq 368.3 K, ΔH=12300 J·mol^{-1}
Disordering transition. 19.1% crystallinity.
liq/liq 467.0 K, ΔH=2300 J·mol^{-1}
ΔS=4.9 J·mol^{-1}·K^{-1}
Isotropic transition.
Molecular Weight 502.6090
Wiswesser Line Notation /*NR B1 DO2O2O2O2OR C1 DNU1R D1*/
Evaluation B
Poly(azomethine) with four ethylene glycol spacers. T(glass)=293 K.

$C_{30}H_{34}O_4$ (c) 84OZC/ASR
4,4′-Diheptanoyloxydiphenyldiacetylene
Phase Changes
c,III/c,II 305 K
c,II/c,I 318 K, ΔH=18900 J·mol^{-1}
ΔS=60.67 J·mol^{-1}·K^{-1}
c,II/c,II, c,II/c,I transitions combined.
c,I/liq 402 K, ΔH=25500 J·mol^{-1}
ΔS=63.47 J·mol^{-1}·K^{-1}
Solid-nematic.
liq/liq 411 K, ΔH=1170 J·mol^{-1}
ΔS=2.845 J·mol^{-1}·K^{-1}
Nematic-isotropic liquid transition.
Molecular Weight 458.5962
Wiswesser Line Notation 6VOR D1UU2UU1R DOV6
Evaluation A

$C_{30}H_{41}NO$ (liq) 81ARU/DAU
4-Octyl-4′-heptyl-α-cyanostilbene
Heat Capacity
Temperature range 320 to 340 K. Data given graphically.
Phase Changes
liq/liq 324.3 K
Smectic C-smectic A liquid transition.
liq/liq 337.3 K, $\Delta S = 1.66\ J \cdot mol^{-1} \cdot K^{-1}$
Smectic A-nematic liquid transition.
liq/liq 338.5 K, $\Delta S = 6.98\ J \cdot mol^{-1} \cdot K^{-1}$
Nematic-isotropic liquid transition.
Molecular Weight 431.6600
Wiswesser Line Notation 8OR D1U1R DYCN&6
Evaluation B
Assume trans isomer.

$C_{30}H_{42}N_2O_3$ (c) 88FAN/POE
4-*n*-Pentanoyl-4-*n*′-tridecanoyloxyazobenzene
Phase Changes
c,II/c,I 361.5 K, $\Delta H = 6088\ J \cdot mol^{-1}$
$\Delta S = 16.84\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 371.6 K, $\Delta H = 37070\ J \cdot mol^{-1}$
$\Delta S = 99.76\ J \cdot mol^{-1} \cdot K^{-1}$
Solid-smectic A.
liq/liq 402.9 K, $\Delta H = 9234\ J \cdot mol^{-1}$
$\Delta S = 22.92\ J \cdot mol^{-1} \cdot K^{-1}$
Smectic A-isotropic.
liq/liq 361.9 K, $\Delta H = 4477\ J \cdot mol^{-1}$
$\Delta S = 12.37\ J \cdot mol^{-1} \cdot K^{-1}$
Smectic A-smectic monotropic 1.
Molecular Weight 478.6734
Wiswesser Line Notation 12VOR DNUNR DV4
Evaluation A

$C_{30}H_{42}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-pentadecanoyloxyazobenzene
Phase Changes
c/liq 376.65 K, $\Delta H = 51505\ J \cdot mol^{-1}$
$\Delta S = 136.7\ J \cdot mol^{-1} \cdot K^{-1}$
Solid-smectic A.
liq/liq 412.15 K, $\Delta H = 8452\ J \cdot mol^{-1}$
$\Delta S = 20.5\ J \cdot mol^{-1} \cdot K^{-1}$
Smectic A-isotropic liquid transition.
Molecular Weight 478.6734
Wiswesser Line Notation 14VOR DNUNR DV2
Evaluation A

$C_{30}H_{46}$ (c) 83KRA/BEC
3,4-Dimethyl-3,4-bis(4-*tert*-butylphenyl)hexane
Heat Capacity 298 K, $C_p = 631.3\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature. C_p given as $0.371\ cal \cdot K^{-1} \cdot g^{-1}$.
Molecular Weight 406.6934
Wiswesser Line Notation 1XR DX2&2&X2&2&R DX
Evaluation B

$C_{30}H_{58}O_4$ (liq) 76PHI/MAT
Di-*n*-decyl sebacate
Heat Capacity 368 K, $C_p = 1004\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 368 to 240 K.
Molecular Weight 482.7858
Wiswesser Line Notation 10OV8VO10
Evaluation C

$C_{30}H_{58}O_4Pb$ (c,II) 78ADE/SIN
Lead(II) pentadecanoate
Heat Capacity 380 K, $C_p = 1430\ J \cdot mol^{-1} \cdot K^{-1}$
Mean value, 376 to 380 K. Data only graphically for c,III.
Phase Changes
c,III/c,II 374.7 K, $\Delta H = 64100\ J \cdot mol^{-1}$
$\Delta S = 171\ J \cdot mol^{-1} \cdot K^{-1}$
c,II and c,I are mesophases.
c,II/c,I 384.6 K, $\Delta H = 48100\ J \cdot mol^{-1}$
$\Delta S = 125\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 689.9858
Wiswesser Line Notation OV14 2 .PB
Evaluation C

$C_{30}H_{62}$ (liq) 91TRE/CC
2,6,10,15,19,23-Hexamethyltetracosane
Heat Capacity 298.15 K, $C_p = 886.36\ J \cdot mol^{-1} \cdot K^{-1}$
One temperature.
Molecular Weight 422.8198
Wiswesser Line Notation 1Y1&3Y1&3Y1&3Y1&3Y1&3Y1&1
Evaluation B

$C_{30}H_{62}$ (c,II) 31GAR/VA
n-Triacontane
Heat Capacity 301 K, $C_p = 808.8\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 289 to 373 K. Mean value 16 to 38 °C, β-form.
Phase Changes
c,II/c,I 332.2 K, $\Delta H = 36484\ J \cdot mol^{-1}$
$\Delta S = 109.8\ J \cdot mol^{-1} \cdot K^{-1}$
β-α transition.
c,I/liq 338.7 K, $\Delta H = 68827\ J \cdot mol^{-1}$
$\Delta S = 203.2\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 422.8198
Wiswesser Line Notation 30H
Evaluation B (C_p), D (Phase changes)

$C_{30}H_{62}$ (c) 55SCH/BU
n-Triacontane
Phase Changes
c,II/c,I 335.15 K
c,I/liq 338.55 K
Molecular Weight 422.8198
Wiswesser Line Notation 30H
Evaluation B

$C_{30}H_{62}$ (c) 73CO
n-Triacontane
Phase Changes
c,II/c,I 335.25 K, $\Delta H = 37489\ J \cdot mol^{-1}$
$\Delta S = 111.8\ J \cdot mol^{-1} \cdot K^{-1}$
c,I/liq 338.65 K, $\Delta H = 68827\ J \cdot mol^{-1}$
$\Delta S = 203.2\ J \cdot mol^{-1} \cdot K^{-1}$
Molecular Weight 422.8198
Wiswesser Line Notation 30H
Evaluation B

$C_{30}H_{62}$ (c) 81HC
n-Triacontane
Heat Capacity 300 K, $C_p = 558\ J \cdot mol^{-1} \cdot K^{-1}$
Temperature range 300 to 500 K. $C_v = 1.30\ J \cdot g^{-1} \cdot K^{-1}$.
Molecular Weight 422.8198
Wiswesser Line Notation 30H
Evaluation D

$C_{31}H_{44}N_2O_3$ (c) 88FAN/POE
4-*n*-Pentanoyl-4-*n*′-Tetradecanoyloxyazobenzene
Phase Changes
c,III/c,II 325.1 K, $\Delta H = 3234$ J·mol^{-1}
$\Delta S = 9.950$ J·mol^{-1}·K^{-1}
c,II/c,I 354.4 K, $\Delta H = 6000$ J·mol^{-1}
$\Delta S = 16.93$ J·mol^{-1}·K^{-1}
c,I/liq 373.5 K, $\Delta H = 38116$ J·mol^{-1}
$\Delta S = 102.05$ J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 402.6 K, $\Delta H = 9544$ J·mol^{-1}
$\Delta S = 23.71$ J·mol^{-1}·K^{-1}
Smectic A-isotropic.
Molecular Weight 492.7702
Wiswesser Line Notation 13VOR DNUNR DV4
Evaluation A

$C_{31}H_{44}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-hexadecanoyloxyazobenzene
Phase Changes
c/liq 378.65 K, $\Delta H = 53011$ J·mol^{-1}
$\Delta S = 140.0$ J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 410.65 K, $\Delta H = 8619$ J·mol^{-1}
$\Delta S = 21.0$ J·mol^{-1}·K^{-1}
Smectic A-isotropic liquid transition
Molecular Weight 492.7002
Wiswesser Line Notation 15VOR DNUNR DV2
Evaluation A

$C_{31}H_{52}O_3$ (c) 88BAG/GUR
α-Tocopherol acetate
Heat Capacity 293.75 K, $C_p = 898$ J·mol^{-1}·K^{-1}
Temperature range 273 to 334 K. Unsmoothed experimental datum.
Molecular Weight 472.7500
Wiswesser Line Notation T66 BOT&J C3Y1&3Y1&3Y1&1 C1 G1 HOV1 I1 J1
Evaluation B

$C_{31}H_{64}$ (liq) 45FIS/NAY
11-*n*-Decylheneicosane
Heat Capacity 300 K, $C_p = 949.8$ J·mol^{-1}·K^{-1}
Temperature range 12 to 296 K (Penn State), 80 to 297 K (Stanford); at 300 K, $C_p = 949.8$ J·mol^{-1}·K^{-1} (Penn State), 963.2 J·mol^{-1}·K^{-1} (Stanford).
Entropy 298.15 K, $S = 1086.2$ J·mol^{-1}·K^{-1}
Penn State entropy above. From Stanford data, with extrapolation of 218.0 J·mol^{-1}·K^{-1}, $S = 1098.3$ J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 282.34 K, $\Delta H = 71207$ J·mol^{-1}
$\Delta S = 252.20$ J·mol^{-1}·K^{-1}
Stanford data give $\Delta H = 71044$ J·mol^{-1}; Tm 282.2 K.
Molecular Weight 436.8466
Wiswesser Line Notation 10Y10&10
Evaluation B
Impurity from melting data, 3.4 to 3.5 mol%.

$C_{31}H_{64}$ (c,β) 38VER
n-Hentriacontane
Heat Capacity 323 K, $C_p = 912$ J·mol^{-1}·K^{-1}
One temperature. Also data for α form, 1774 J·mol^{-1}·K^{-1} at 338 K, and liquid 1096 J·mol^{-1}·K^{-1} at 348 K.
Molecular Weight 436.8466
Wiswesser Line Notation 31H
Evaluation C

$(C_{32}H_{20}N_4)_n$ (c) 74KAR/RAB
Poly-[2,2′-(*p*-phenylene-1,1-diphenyl-5,5′-dibenzimidazole]
Heat Capacity 298.15 K, $C_p = 537.2$ J·mol^{-1}·K^{-1}
Temperature range 50 to 500 K.
Entropy 298.15 K, $S = 469.0$ J·mol^{-1}·K^{-1}
Molecular Weight 460.5370
Wiswesser Line Notation /T56 BN DNJ CR D* H- HT56 BN DNJ CR D*& DR/
Evaluation A

$C_{32}H_{22}Ge$ (c) 75LEB/MIL3
1,1-Diethynyl-2,3,4,5-tetraphenyl-1-germacyclo-pentadiene
Heat Capacity 298.15 K, $C_p = 556.5$ J·mol^{-1}·K^{-1}
Temperature range 62 to 309 K.
Entropy 298.15 K, $S = 625.1$ J·mol^{-1}·K^{-1}
Molecular Weight 479.1367
Wiswesser Line Notation T5-GE- AHJ A1UU1 A1UU1 BR CR DR ER
Evaluation B

$(C_{32}H_{22}Ge)_n$ (gls) 75LEB/MIL3
Poly-1,1-diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene
Heat Capacity 298.15 K, $C_p = 489.5$ J·mol^{-1}·K^{-1}
Temperature range 62 to 307 K.
Entropy 298.15 K, $S = 524.7$ J·mol^{-1}·K^{-1}
Molecular Weight 479.1367
Wiswesser Line Notation /T5-GE- BUTJ A1UU1 A1UU1 BR* CR* DR ER/
Evaluation B

$(C_{32}H_{24}N_4O_2)_n$ (c) 74KAR/RAB
Poly-[N-terphthalyl-bis-(N′-phenyl-*o*-diphenylamine)]
Heat Capacity 298.15 K, $C_p = 612.1$ J·mol^{-1}·K^{-1}
Temperature range 50 to 500 K.
Entropy 298.15 K, $S = 601.2$ J·mol^{-1}·K^{-1}
Molecular Weight 496.5674
Wiswesser Line Notation /*VMR BMR ER CMVR* DMR/
Evaluation A

$C_{32}H_{26}$ (c) 31SMI/AND
Pentaphenylethane
Heat Capacity 298.5 K, $C_p = 473.6$ J·mol^{-1}·K^{-1}
Temperature range 102 to 346 K. Value is unsmoothed experimental datum.
Molecular Weight 410.5574
Wiswesser Line Notation RYR&XR&R&R
Evaluation C

$C_{32}H_{38}Fe_3N_4O_{13}$ (c) 85OH/KAM
μ_3-Oxo-tris(pyridine)hexakis(acetato) iron(II) diiron pyridine
Heat Capacity 300 K, $C_p = 930$ J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K. Data given graphically. Value estimated from graph.
Phase Changes
c,V/c,IV 111.4 K
c,IV/c,III 112.0 K
c,III/c,II 185.8 K
c,II/c,I 191.5 K
Molecular Weight 854.2122
Wiswesser Line Notation OV1 6 &T6NJ 3 &-FE- O &T6NJ
Evaluation C

$C_{32}H_{38}Fe_3N_4O_{13}$ (c) 86SOR/KAJ
μ_3-Oxo-tris(pyridine)hexakis(acetato) iron(II)-diiron pyridine
Heat Capacity 300 K, $C_p = 928.91$ J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Phase Changes
c,V/c,IV 111.4 K
c,IV/c,III 112.0 K, $\Delta H = 503$ J·mol^{-1}, $\Delta S = 4.61$ J·mol^{-1}·K^{-1}
c,V/c,IV and c,IV/c,III combined.
c,III/c,II 185.8 K
c,II/c,I 191.5 K, $\Delta H = 4440$ J·mol^{-1}, $\Delta S = 26.04$ J·mol^{-1}·K^{-1}
c,III/c,II and c,II/c,I combined.
Molecular Weight 854.2122
Wiswesser Line Notation OV1 6 &T6NJ 3 &-FE- 3 O &T6NJ
Evaluation A

$C_{32}H_{38}Mn_3N_4O_{13}$ (c) 89JAN/VIN
Hexakis-(μ-acetato) (μ_3-oxo)tris(pyridine) trimanganese·pyridine
Phase Changes
c,II/c,I 184.65 K, $\Delta H = 6460$ J·mol^{-1}, $\Delta S = 35.77$ J·mol^{-1}·K^{-1}
Molecular Weight 851.4852
Wiswesser Line Notation OV1 6 &T6NJ 3 &-MN- O &T6NJ
Evaluation A

$C_{32}H_{38}Mn_3N_4O_{13}$ (c) 89NAK/SOR
Hexakis-(μ-acetato)(μ_3-oxo)tris(pyridine)trimanganese·pyridine
Heat Capacity 299.804 K, $C_p = 926.56$ J·mol^{-1}·K^{-1}
Temperature range 14 to 302 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 184.65 K, $\Delta H = 6460$ J·mol^{-1}, $\Delta S = 35.77$ J·mol^{-1}·K^{-1}
Molecular Weight 851.4852
Wiswesser Line Notation OV1 6 &T6NJ 3 &-MN- O &T6NJ
Evaluation A

$C_{32}H_{38}O_4$ (c) 84OZC/ASR
4,4′-Dioctanoyloxydiphenyldiacetylene
Phase Changes
c,II/c,I 359 K, $\Delta H = 35400$ J·mol^{-1}, $\Delta S = 98.70$ J·mol^{-1}·K^{-1}
c,I/liq 406 K, $\Delta H = 34000$ J·mol^{-1}, $\Delta S = 83.76$ J·mol^{-1}·K^{-1}
Solid-nematic.
liq/liq 412 K, $\Delta H = 21800$ J·mol^{-1}, $\Delta S = 5.272$ J·mol^{-1}·K^{-1}
Nematic-isotropic liquid transition.
Molecular Weight 486.6498
Wiswesser Line Notation 7VOR D1UU2UU1R DOV7
Evaluation A

$C_{32}H_{39}ClO_2$ (c) 79LEW/ENE
Norethindrone-6-(4-chlorophenyl)-hexanoate
Phase Changes
c/liq 413 K, $\Delta H = 28800$ J·mol^{-1}, $\Delta S = 69.7$ J·mol^{-1}·K^{-1}
Molecular Weight 491.1119
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1 FV5R DG
Evaluation A

$C_{32}H_{46}N_2O_3$ (c) 88FAN/POE
4-*n*-Pentanoyl-4-*n*′-pentadecanoyloxyazobenzene
Phase Changes
c,II/c,I 368.9 K, $\Delta H = 9117$ J·mol^{-1}, $\Delta S = 24.71$ J·mol^{-1}·K^{-1}
c,I/liq 374.8 K, $\Delta H = 42702$ J·mol^{-1}, $\Delta S = 113.93$ J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 401.2 K, $\Delta H = 9836$ J·mol^{-1}, $\Delta S = 24.52$ J·mol^{-1}·K^{-1}
Smectic A-isotropic.
Molecular Weight 506.7270
Wiswesser Line Notation 14VOR DNUNR DV4
Evaluation A

$C_{32}H_{46}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-heptadecanoyloxyazobenzene
Phase Changes
c/liq 379.65 K, $\Delta H = 58743$ J·mol^{-1}, $\Delta S = 154.7$ J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 409.65 K, $\Delta H = 8703$ J·mol^{-1}, $\Delta S = 21.2$ J·mol^{-1}·K^{-1}
Smectic A-isotropic liquid transition.
Molecular Weight 506.7270
Wiswesser Line Notation 16VOR DNUNR DV2
Evaluation A

$C_{32}H_{50}$ (c) 83KRA/BEC
2,4,5,7-Tetramethyl-4,5-bis(4-*tert*-butylphenyl)octane
Heat Capacity 298 K, $C_p = 683.9$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.376 cal.K^{-1}.g^{-1}.
Molecular Weight 434.7470
Wiswesser Line Notation 1XR DX1Y&X1Y&R DX
Evaluation B

$C_{32}H_{50}$ (c) 83KRA/BEC
4,5-Diethyl-4,5-bis-(4-*tert*-butylphenyl)octane
Heat Capacity 298 K, $C_p = 618.5$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.340 cal.K^{-1}.g^{-1}.
Molecular Weight 434.7470
Wiswesser Line Notation 1XR DX2&3&X2&3&R DX
Evaluation B

$C_{32}H_{54}O_4$ (gls) 84OVC/MOS
Diisododecyl phthalate
Heat Capacity 297.50 K, $C_p = 909$ J·mol^{-1}·K^{-1}
Temperature range 6 to 300 K. Unsmoothed experimental datum.
Entropy 298.15 K, $S = 959$ J·mol^{-1}·K^{-1}
Molecular Weight 502.7762
Wiswesser Line Notation 4Y2&1Y2&1OVR BVO1Y2&1Y2&4
Evaluation A
T(glass) = 188 K.

$C_{32}H_{62}O_4Cd$ (c) 78KON/RUF
Cadmium(II) *n*-hexadecanoate
Phase Changes
c/liq 380.4 K, $\Delta H = 23000$ J·mol^{-1}
$\Delta S = 60$ J·mol^{-1}·K^{-1}
Crystal-mesophase(1).
liq/liq 387.1 K, $\Delta H = 15300$ J·mol^{-1}
$\Delta S = 40$ J·mol^{-1}·K^{-1}
Mesophase(1)-mesophase(2).
liq/liq 399 K, $\Delta H = 4800$ J·mol^{-1}
$\Delta S = 12$ J·mol^{-1}·K^{-1}
Mesophase(2)-liquid.
Molecular Weight 623.2494
Wiswesser Line Notation OV15 2 .CD
Evaluation B

$C_{32}H_{62}O_4Pb$ (c) 76ADE/SIM
Lead(II) *n*-hexadecanoate
Phase Changes
c/liq 373.4 K, $\Delta H = 55000$ J·mol^{-1}
$\Delta S = 147$ J·mol^{-1}·K^{-1}
Crystal-smectic(1).
liq/liq 380.6 K, $\Delta H = 40000$ J·mol^{-1}
$\Delta S = 100$ J·mol^{-1}·K^{-1}
Smectic(1)-smectic(2).
liq/liq 384.2 K, $\Delta H = 46400$ J·mol^{-1}
$\Delta S = 121$ J·mol^{-1}·K^{-1}
Smectic(2)-liquid.
Molecular Weight 718.0394
Wiswesser Line Notation OV15 2 .PB
Evaluation B

$C_{32}H_{62}O_4Zn$ (c) 78KON/RUF
Zinc(II) *n*-hexadecanoate
Phase Changes
c/liq 407 K, $\Delta H = 93000$ J·mol^{-1}
$\Delta S = 229$ J·mol^{-1}·K^{-1}
Molecular Weight 576.2194
Wiswesser Line Notation OV15 2 .ZN
Evaluation B

$C_{32}H_{64}HgO_4$ (liq) 78ADE
Mercuric hexadecanoate; Mercuric palmitate
Heat Capacity 410 K, $C_p = 1217.3$ J·mol^{-1}·K^{-1}
Mean value, 396 to 421 K. Data only graphically for solid.
Phase Changes
c,II/c,I 383.4 K, $\Delta H = 49500$ J·mol^{-1}
$\Delta S = 129.1$ J·mol^{-1}·K^{-1}
c,I probably a smectic phase.
c,I/liq 390.3 K, $\Delta H = 59500$ J·mol^{-1}
$\Delta S = 152.4$ J·mol^{-1}·K^{-1}
Molecular Weight 713.4452
Wiswesser Line Notation OV15 2 .HG
Evaluation C
Data on the specific heats are given at or near the phase transitions.

$C_{32}H_{64}O_2$ (c) 34KIN/GAR
Ethyl triacontanate
Phase Changes
c,II/c,I 334.65 K, $\Delta H = 16196$ J·mol^{-1}
β-α transition.
c,I/liq 341.45 K, $\Delta H = 36073$ J·mol^{-1}
α-liq transition.
Molecular Weight 480.8564
Wiswesser Line Notation 29VO2
Evaluation B

$C_{32}H_{66}$ (c,α) 38VER
n-Dotriacontane
Heat Capacity 338 K, $C_p = 1059$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 450.8734
Wiswesser Line Notation 32H
Evaluation C

$C_{32}H_{66}$ (c,β) 38VER
n-Dotriacontane
Heat Capacity 333 K, $C_p = 1038$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 450.8734
Wiswesser Line Notation 32H
Evaluation C

$C_{32}H_{66}$ (liq) 38VER
n-Dotriacontane
Heat Capacity 348 K, $C_p = 1356$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 450.8734
Wiswesser Line Notation 32H
Evaluation C

$C_{32}H_{66}$ (c) 49PAR/MOO
n-Dotriacontane
Heat Capacity 298.15 K, $C_p = 877.4$ J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Entropy 298.15 K, $S = 851.4$ J·mol^{-1}·K^{-1}
Extrapolation below 80 K, 214.8 J·mol^{-1}·K^{-1}.
Molecular Weight 450.8734
Wiswesser Line Notation 32H
Evaluation B(C_p),C(S)

$C_{32}H_{66}$ (c) 73COM
n-Dotriacontane
Phase Changes
c,II/c,I 338.65 K, $\Delta H = 41376$ J·mol^{-1}
$\Delta S = 122.2$ J·mol^{-1}·K^{-1}
c,I/liq 343.45 K, $\Delta H = 76567$ J·mol^{-1}
$\Delta S = 222.9$ J·mol^{-1}·K^{-1}
Molecular Weight 450.8734
Wiswesser Line Notation 32H
Evaluation B

$C_{32}H_{66}$ (c) 81HOE
n-Dotriacontane
Heat Capacity 300 K, $C_p = 806$ J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K. $C_p = 1.77$ J·g^{-1}·K^{-1}.
Molecular Weight 450.8734
Wiswesser Line Notation 32H
Evaluation B

$C_{32}H_{72}CdCl_4N_2$ (c) 85RIC/CAV
Bis-hexadecylammonium tetrachlorocadmium
Phase Changes
c,IV/c,III 346 K, $\Delta H = 32000$ J·mol^{-1}
$\Delta S = 93$ J·mol^{-1}·K^{-1}
c,III/c,II 352 K, $\Delta H = 8000$ J·mol^{-1}
$\Delta S = 23$ J·mol^{-1}·K^{-1}
c,II/c,I 356 K, $\Delta H = 26500$ J·mol^{-1}
$\Delta S = 74$ J·mol^{-1}·K^{-1}
Molecular Weight 739.1562
Wiswesser Line Notation -16-ZH 2 .CD G4
Evaluation B

$C_{32}H_{72}CdCl_4N_2$ (c) 89CHA/HOU
Bis(*n*-hexadecylammonium)tetrachlorocadmate
Phase Changes
c,IV/c,III 345 K, $\Delta H = 40400$ J·mol^{-1}
$\Delta S = 117.2$ J·mol^{-1}·K^{-1}
Monoclinic to ortho II.
c,III/c,II 352 K, $\Delta H = 7700$ J·mol^{-1}
$\Delta S = 21.6$ J·mol^{-1}·K^{-1}
Ortho II to ortho I.
c,II/c,I 356 K, $\Delta H = 31500$ J·mol^{-1}
$\Delta S = 88.1$ J·mol^{-1}·K^{-1}
Ortho I to tetragonal.
Molecular Weight 739.1562
Wiswesser Line Notation 16ZH 2 .CD G4
Evaluation A

$C_{33}H_{34}O_2$ (c) 79LEW/ENE
Norethindrone *trans*-4-hexylcyclohexylcarboxylate
Phase Changes
c/liq 398 K, $\Delta H = 22600$ J·mol^{-1}
$\Delta S = 56.8$ J·mol^{-1}·K^{-1}
Molecular Weight 462.6304
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1 FV- -AL6TJ
Evaluation A

$C_{33}H_{34}O_2$ (c) 79LEW/ENE
Norethindrone biphenyl-4-carboxylate
Phase Changes
c/liq 462 K, $\Delta H = 31600$ J·mol^{-1}
Molecular Weight 462.6304
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1 FVR DR
Evaluation A

$C_{33}H_{40}O_2$ (c) 79LEW/ENE
Norethindrone 4-cyclohexylbenzoate
Phase Changes
c/liq 482 K, $\Delta H = 36800$ J·mol^{-1}
$\Delta S = 65.6$ J·mol^{-1}·K^{-1}
Molecular Weight 468.6778
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1 FVR D- -AL6TJ
Evaluation A

$C_{33}H_{48}N_2O_3$ (c) 88FAN/POE
4-*n*-Pentanoyl-4-*n*′-hexadecanoyloxyazobenzene
Phase Changes
c,III/c,II 333.9 K, $\Delta H = 4686$ J·mol^{-1}
$\Delta S = 14.03$ J·mol^{-1}·K^{-1}
c,II/c,I 361.8 K, $\Delta H = 7146$ J·mol^{-1}
$\Delta S = 19.75$ J·mol^{-1}·K^{-1}
c,I/liq 377.4 K, $\Delta H = 45627$ J·mol^{-1}
$\Delta S = 120.90$ J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 399.6 K, $\Delta H = 10067$ J·mol^{-1}
$\Delta S = 25.19$ J·mol^{-1}·K^{-1}
Smectic A-isotropic.
Molecular Weight 520.7538
Wiswesser Line Notation 15VOR DNUNR DV4
Evaluation A

$C_{33}H_{48}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-octadecanoyloxyazobenzene
Phase Changes
c/liq 380.65 K, $\Delta H = 59622$ J·mol^{-1}
$\Delta S = 156.6$ J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 408.65 K, $\Delta H = 8954$ J·mol^{-1}
$\Delta S = 21.9$ J·mol^{-1}·K^{-1}
Smectic A-isotropic liquid transition.
Molecular Weight 520.7538
Wiswesser Line Notation 17VOR DNUNR DV2
Evaluation A

$C_{33}H_{48}O_2$ (c) 79LEW/ENE
Norethindrone *trans*-3-(4-butylcyclohexyl)propionate
Phase Changes
c/liq 374 K, $\Delta H = 22500$ J·mol^{-1}
$\Delta S = 60.2$ J·mol^{-1}·K^{-1}
Molecular Weight 476.7410
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1 FV2- -AL6TJ D4
Evaluation A

$C_{33}H_{62}O_6$ (liq) 76PHI/MAT
Tridecanoin; Glyceryl tridecanoate
Heat Capacity 313 K, $C_p = 1109$ J·mol^{-1}·K^{-1}
Temperature range 313 to 388 K.
Molecular Weight 554.8492
Wiswesser Line Notation 9VO1YOV9&1OV9
Evaluation C

$C_{33}H_{68}$ (c) 30PAR/HUF
n-Tritriacontane
Heat Capacity 294.4 K, $C_p = 900.8$ J·mol^{-1}·K^{-1}
Temperature range 94 to 294 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S = 877.8$ J·mol^{-1}·K^{-1}
Extrapolation below 90 K, 267 J·mol^{-1}·K^{-1}.
Molecular Weight 464.9002
Wiswesser Line Notation 33H
Evaluation B(C_p),C(S)

$C_{33}H_{68}$ (liq) 32SPA/TIC
n-Tritriacontane
Heat Capacity 353 K, $C_p = 1112.5$ J·mol^{-1}·K^{-1}
Temperature range 80 to 110 °C.
Phase Changes
c/liq 344.2 K, $\Delta H = 105039$ J·mol^{-1}
$\Delta S = 305.2$ J·mol^{-1}·K^{-1}
Molecular Weight 464.9002
Wiswesser Line Notation 33H
Evaluation B

$(C_{34}H_{18}N_6O)_n$ (c) 84KAR/SHV
Polybenzimidazoloquinazole
Heat Capacity 298.15 K, $C_p = 523.2$ J·mol^{-1}·K^{-1}
Temperature range 60 to 600 K.
Entropy 298.15 K, $S = 453.2$ J·mol^{-1}·K^{-1}
Molecular Weight 526.5560
Wiswesser Line Notation /T D6 C656 BN LNJ K* OO- OT D6 C656 BN LNJ KR D*/
Evaluation B

$(C_{34}H_{20}N_4O)_n$ (c) 77KAR/RAB
Poly[2,2′-(1,4-phenylene)-7,7′-oxy-bis(3-phenylquinoxaline)]
Heat Capacity 300 K, $C_p = 600$ J·mol^{-1}·K^{-1}
Temperature range 100 to 700 K. Data given graphically. Value estimated from graph.
Entropy 300 K, $S = 449.8$ J·mol^{-1}·K^{-1}
Molecular Weight 576.6558
Wiswesser Line Notation /T66 BN ENJ CR D* HO- HT66 BN ENJ CR DR D*/
Evaluation C(C_p,S); A(Phase changes)
T(glass) = 556.0 K.

$(C_{34}H_{22}N_6O_3)_n$ (c) 84KAR/SHV
Bis-(*o*-aminophenyl)-2,2′-dibenzimidazole oxide, intermediate polymer
Heat Capacity 298.15 K, $C_p = 699.2$ J·mol^{-1}·K^{-1}
Temperature range 60 to 600 K.
Entropy 298.15 K, $S = 594.8$ J·mol^{-1}·K^{-1}
Molecular Weight 562.5864
Wiswesser Line Notation /*VR DVMR B- CT56 BM DNJ HO-HT56 BM DNJ CR BM*/
Evaluation B

$C_{34}H_{42}O_4$ (c) 84OZC/ASR
4,4′-Dinonanoyloxydiphenyldiacetylene
Phase Changes

c,II/c,I	326 K,	$\Delta H = 19500$ J·mol^{-1}
		$\Delta S = 59.79$ J·mol^{-1}·K^{-1}
c,I/liq	400 K,	$\Delta H = 33500$ J·mol^{-1}
		$\Delta S = 83.76$ J·mol^{-1}·K^{-1}

Solid-nematic.

liq/liq	401 K,	$\Delta H = 14600$ J·mol^{-1}
		$\Delta S = 3.640$ J·mol^{-1}·K^{-1}

Nematic-isotropic liquid transition.
Molecular Weight 514.7034
Wiswesser Line Notation 8VOR D1UU2UU1R DOV8
Evaluation A

$C_{34}H_{50}N_2O_3$ (c) 88FAN/POE
4-*n*-Pentanoyl-4-*n*′-heptadecanoyloxyazobenzene
Phase Changes

c,II/c,I	371.5 K,	$\Delta H = 9217$ J·mol^{-1}
		$\Delta S = 24.81$ J·mol^{-1}·K^{-1}
c,I/liq	377.4 K,	$\Delta H = 46497$ J·mol^{-1}
		$\Delta S = 123.20$ J·mol^{-1}·K^{-1}

Solid-smectic A.

liq/liq	397.0 K,	$\Delta H = 9979$ J·mol^{-1}
		$\Delta S = 25.14$ J·mol^{-1}·K^{-1}

Smectic A-isotropic.
Molecular Weight 534.7806
Wiswesser Line Notation 16VOR DNUNR DV4
Evaluation A

$C_{34}H_{54}$ (c) 83KRA/BEC
4,5-Dipropyl-4,5-bis(4-*tert*-butylphenyl)octane
Heat Capacity 298 K, $C_p = 724.2$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.374 cal.K^{-1}.g^{-1}.
Molecular Weight 462.8006
Wiswesser Line Notation 1XR DX3&3&X3&3&R DX
Evaluation B

$C_{34}H_{64}O_4$ (liq) 76PHI/MAT
Di-*n*-dodecyl sebacate
Heat Capacity 368 K, $C_p = 1117$ J·mol^{-1}·K^{-1}
Temperature range 368 to 408 K.
Molecular Weight 536.8772
Wiswesser Line Notation 12OV8VO12
Evaluation C

$C_{34}H_{66}O_4Pb$ (c,III) 78ADE/SIM
Lead(II) heptadecanoate
Heat Capacity
Data only graphically for c,III.
Phase Changes

c,III/c,II	378.7 K,	$\Delta H = 68000$ J·mol^{-1}
		$\Delta S = 180$ J·mol^{-1}·K^{-1}

c,II, and c,I, are mesophases.

c,II/c,I	387.4 K,	$\Delta H = 55100$ J·mol^{-1}
		$\Delta S = 142$ J·mol^{-1}·K^{-1}

Molecular Weight 746.0930
Wiswesser Line Notation OV16 2 .PB
Evaluation C

$C_{34}H_{70}$ (c) 31GAR/VAN
n-Tetratriacontane
Heat Capacity 303 K, $C_p = 887.4$ J·mol^{-1}·K^{-1}
Temperature range 293 to 373 K. Mean value 20 to 40 °C. β-form.
Phase Changes

c,II/c,I	341.1 K,	$\Delta H = 48032$ J·mol^{-1}
		$\Delta S = 140.8$ J·mol^{-1}·K^{-1}

β-α transition.

c,I/liq	345.6 K,	$\Delta H = 79956$ J·mol^{-1}
		$\Delta S = 231.4$ J·mol^{-1}·K^{-1}

Molecular Weight 478.9270
Wiswesser Line Notation 34H
Evaluation B

$C_{34}H_{70}$ (liq) 69ATK/LAR
n-Tetratriacontane
Heat Capacity 353 K, $C_p = 1149$ J·mol^{-1}·K^{-1}
Temperature range 353 to 453 K. Equation only.
Molecular Weight 478.9270
Wiswesser Line Notation 34H
Evaluation C

$C_{34}H_{70}$ (c) 73COM
n-Tetratriacontane
Phase Changes

c,III/c,II	342.25 K	
c,II/c,I	342.65 K,	$\Delta H = 48032$ J·mol^{-1}
		$\Delta S = 140.2$ J·mol^{-1}·K^{-1}
c,I/liq	345.95 K,	$\Delta H = 79956$ J·mol^{-1}
		$\Delta S = 231.1$ J·mol^{-1}·K^{-1}

Molecular Weight 478.9270
Wiswesser Line Notation 34H
Evaluation B

$C_{35}H_{52}N_2O_3$ (c) 88FAN/POE
4-*n*-Pentanoyl-4-*n*′-octadecanoyloxyazobenzene
Phase Changes

c,III/c,II	339.6 K,	$\Delta H = 5305$ J·mol^{-1}
		$\Delta S = 15.62$ J·mol^{-1}·K^{-1}
c,II/c,I	367.5 K,	$\Delta H = 8268$ J·mol^{-1}
		$\Delta S = 22.50$ J·mol^{-1}·K^{-1}
c,I/liq	379.3 K,	$\Delta H = 51827$ J·mol^{-1}
		$\Delta S = 136.64$ J·mol^{-1}·K^{-1}

Solid-smectic A.

liq/liq	397.3 K,	$\Delta H = 10447$ J·mol^{-1}
		$\Delta S = 26.30$ J·mol^{-1}·K^{-1}

Smectic A-isotropic.
Molecular Weight 548.8074
Wiswesser Line Notation 17VOR DNUNR DV4
Evaluation A

$C_{35}H_{72}$ (c,II) 31GAR/VAN

n-Pentatriacotane

Heat Capacity 302 K, $C_p = 915.9\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 290 to 373 K. Mean value, 17 to 41 °C.

Phase Changes

c,II/c,I 344.7 K, $\Delta H = 41087\ J \cdot mol^{-1}$, $\Delta S = 119.2\ J \cdot mol^{-1} \cdot K^{-1}$

β-α transition.

c,I/liq 347.2 K, $\Delta H = 86400\ J \cdot mol^{-1}$, $\Delta S = 248.8\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 492.9538

Wiswesser Line Notation 35H

Evaluation B

$C_{36}H_{18}$ (c) 79FAR/SHA

Decacyclene; Diacenaphtho[1,2-j:1′,2′-1]-fluoranthene

Phase Changes

c,II/c,I 533 K

c/liq 562.0 K, $\Delta H = 45200\ J \cdot mol^{-1}$, $\Delta S = 80.4\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 450.5382

Wiswesser Line Notation L E6 E-6 D5 P6 P-6 O5 C6566 3AC-P- K&J

Evaluation B

$C_{36}H_{24}$ (c) 67MAG

1,3,5-Tri-2-naphthylbenzene

Heat Capacity 300 K, $C_p = 481\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 200 to 560 K. Estimated, data graphically only. Also data for glass.

Phase Changes

c/liq 472 K, $\Delta H = 42425\ J \cdot mol^{-1}$, $\Delta S = 89.9\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 456.5856

Wiswesser Line Notation L66J C- R CCL66J& E- CL66J

Evaluation C

$C_{36}H_{30}OSi_2$ (c) 86DZH/KUL

Hexaphenyldisiloxane

Heat Capacity 298.15 K, $C_p = 681\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 4 to 300 K. $C_p(c) = 124 + 1.726T + 5.6 \times 10^{-1} T^2$ (150 to 300 K).

Entropy 298.15 K, $S = 754.4\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 534.8034

Wiswesser Line Notation R-SI-R&R&O-SI-R&R&R

Evaluation A

$C_{36}H_{30}O_3Si_3$ (c) 82KUL/DZH

Hexaphenylcyclotrisiloxane

Heat Capacity 298.15 K, $C_p = 683.7\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 4.7 to 300 K. Data given graphically except for data at 298.15 K.

Entropy 298.15 K, $S = 735.5\ J \cdot mol^{-1} \cdot K^{-1}$

Molecular Weight 594.8877

Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ AR AR CR CR ER ER

Evaluation B

$C_{36}H_{46}Fe_3N_4O_{13}$ (c) 87SOR/SHI

Mixed valence iron oxo-centered complex with acetate and 3-methyl pyridine

Heat Capacity 299.635 K, $C_p = 1094.7\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 12 to 350 K. Unsmoothed experimental datum.

Phase Changes

c,V/c,IV 181 K

c,IV/c,III 263.5 K

c,III/c,II 271.5 K

c,II/c,I 282.2 K

Molecular Weight 910.3194

Wiswesser Line Notation -FE-3 O & T6NJ C1 3 & OV1 6 & T6NJ C1

Evaluation A

Cumulative enthalpy and entropy changes due to the four phase transitions were: $\Delta H = 3410\ J \cdot mol^{-1}$, $\Delta S = 13.71\ J \cdot mol^{-1} \cdot K^{-1}$.

$C_{36}H_{46}O_4$ (c) 84OZC/ASR

4,4′-Didecanoyloxydiphenyldiacetylene

Phase Changes

c,II/c,I 308 K, $\Delta H = 44900\ J \cdot mol^{-1}$, $\Delta S = 122.1\ J \cdot mol^{-1} \cdot K^{-1}$

c,I/liq 403 K, $\Delta H = 42200\ J \cdot mol^{-1}$, $\Delta S = 104.6\ J \cdot mol^{-1} \cdot K^{-1}$

Solid-isotropic.

Molecular Weight 542.7570

Wiswesser Line Notation 9VOR D1UU2UU1R DOV9

Evaluation A

$C_{36}H_{48}N_2O_2$ (c) 92CHE/JIN

N,N′-Bis(4-*n*-octyloxybenzal)-1,4-phenylenediamine

Heat Capacity 298.15 K, $C_p = 805.69\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 130 to 550 K. $C_p(liq) = 1433.2 - 0.3084T$ J/K·mo (530 to 550 K).

Phase Changes

c,III/liq $\Delta H = 44360\ J \cdot mol^{-1}$, $\Delta S = 106.04\ J \cdot mol^{-1} \cdot K^{-1}$

Total for the series of transitions over temperature range 385.50 t 504.76 K.

Molecular Weight 540.7874

Wiswesser Line Notation 8OR DYUNR DNUYR DO8

Evaluation B

$C_{36}H_{48}Ni_4O_{16}$ (c) 83SOR/MUR

Tetra-μ_3-methoxy-tetrakis-[salicylaldehydato (methanol)nickel(II)]

Heat Capacity 284.664 K, $C_p = 1038.4\ J \cdot mol^{-1} \cdot K^{-1}$

Temperature range 0.4 to 288 K. Unsmoothed experimental datum.

Molecular Weight 971.5656

Wiswesser Line Notation VHR BO .NI O1 &O1 &4

Evaluation A

$C_{36}H_{60}O_{30}$ (c) 90RRI/WAI

α-Cyclodextrin; Cyclohexaamylose

Heat Capacity 298.15 K, $C_p = 1153\ J \cdot mol^{-1} \cdot K^{-1}$

Estimated value.

Molecular Weight 972.8520

Wiswesser Line Notation /T5OTJ B* CQ DQ EQ* F1Q/ 6

Evaluation B

$C_{36}H_{70}O_4Cd$ (c) 78KON/RUF
Cadmium(II) *n*-octadecanoate
Phase Changes
c/liq 380 K, $\Delta H = 19600$ J·mol^{-1}
$\Delta S = 51$ J·mol^{-1}·K^{-1}
Crystal-mesophase(1).
liq/liq 386.2 K, $\Delta H = 22800$ J·mol^{-1}
$\Delta S = 59$ J·mol^{-1}·K^{-1}
Mesophase(1)-mesophase(2).
liq/liq 391.2 K, $\Delta H = 26200$ J·mol^{-1}
$\Delta S = 67$ J·mol^{-1}·K^{-1}
Mesophase(2)-liquid.
Molecular Weight 679.3566
Wiswesser Line Notation OV17 2 .CD
Evaluation B

$C_{36}H_{70}HgO_4$ (liq) 78ADE
Mercuric octadecanoate; Mercuric stearate
Heat Capacity 410 K, $C_p = 1377.2$ J·mol^{-1}·K^{-1}
Mean value, 391 to 433 K. Data only graphically for solid.
Phase Changes
c,II/c,I 355.2 K, $\Delta H = 4400$ J·mol^{-1}
$\Delta S = 12.4$ J·mol^{-1}·K^{-1}
c,I/liq 383.2 K, $\Delta H = 116500$ J·mol^{-1}
$\Delta S = 296.3$ J·mol^{-1}·K^{-1}
Molecular Weight 767.5366
Wiswesser Line Notation OV17 2 .HG
Evaluation C

$C_{36}H_{70}O_4Pb$ (c) 76ADE/SIM
Lead(II) *n*-octadecanoate
Phase Changes
c/liq 381.2 K, $\Delta H = 62600$ J·mol^{-1}
$\Delta S = 164$ J·mol^{-1}·K^{-1}
Crystal-smectic.
liq/liq 387.2 K, $\Delta H = 56900$ J·mol^{-1}
$\Delta S = 147$ J·mol^{-1}·K^{-1}
Smectic-liquid.
Molecular Weight 774.1466
Wiswesser Line Notation OV17 2 .PB
Evaluation B

$C_{36}H_{70}O_4Zn$ (c) 78KON/RUF
Zinc(II) *n*-octadecanoate
Phase Changes
c/liq 403 K, $\Delta H = 103000$ J·mol^{-1}
$\Delta S = 256$ J·mol^{-1}·K^{-1}
Molecular Weight 632.3266
Wiswesser Line Notation OV17 2 .ZN
Evaluation B

$C_{36}H_{74}$ (c) 55SCH/BUS
n-Hexatriacontane
Phase Changes
c,III/c,II 345.25 K, $\Delta H = 9916$ J·mol^{-1}
$\Delta S = 28.7$ J·mol^{-1}·K^{-1}
c,II/c,I 346.95 K, $\Delta H = 30543$ J·mol^{-1}
$\Delta S = 88.0$ J·mol^{-1}·K^{-1}
c,I/liq 349.05 K, $\Delta H = 88826$ J·mol^{-1}
$\Delta S = 254.5$ J·mol^{-1}·K^{-1}
Molecular Weight 506.9806
Wiswesser Line Notation 36H
Evaluation B

$C_{36}H_{74}$ (liq) 69ATK/LAR
n-Hexatriacontane
Heat Capacity 353 K, $C_p = 1206$ J·mol^{-1}·K^{-1}
Temperature range 353 to 453 K. Equation only.
Molecular Weight 506.9806
Wiswesser Line Notation 36H
Evaluation C

$C_{36}H_{74}$ (c) 73COM
n-Hexatriacontane
Phase Changes
c,III/c,II 345.35 K, $\Delta H = 9916$ J·mol^{-1}
$\Delta S = 28.7$ J·mol^{-1}·K^{-1}
c,II/c,I 347.05 K, $\Delta H = 30543$ J·mol^{-1}
$\Delta S = 88.0$ J·mol^{-1}·K^{-1}
c,I/liq 349.15 K, $\Delta H = 130666$ J·mol^{-1}
$\Delta S = 374.2$ J·mol^{-1}·K^{-1}
Molecular Weight 506.9806
Wiswesser Line Notation 36H
Evaluation B

$C_{36}H_{74}$ (c) 81HOE
n-Hexatriacontane
Heat Capacity 300 K, $C_p = 840$ J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K. $C_v = 1.64$ J·g^{-1}·K^{-1}.
Molecular Weight 506.9806
Wiswesser Line Notation 36H
Evaluation B

$C_{36}H_{80}CdCl_4N_2$ (c) 84WHI
Bis(octadecylammonium) cadmium tetrachloride
Heat Capacity 300 K, $C_p = 1010$ J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K. Data given graphically. Value estimated from graph.
Phase Changes
c,V/c,IV 349.6 K, $\Delta H = 49500$ J·mol^{-1}
$\Delta S = 132$ J·mol^{-1}·K^{-1}
c,IV/c,III 356.0 K, $\Delta H = 2300$ J·mol^{-1}
$\Delta S = 6.5$ J·mol^{-1}·K^{-1}
c,III/c,II 359.5 K, $\Delta H = 3500$ J·mol^{-1}
$\Delta S = 9.6$ J·mol^{-1}·K^{-1}
c,II/c,I 365.6 K, $\Delta H = 34300$ J·mol^{-1}
$\Delta S = 95$ J·mol^{-1}·K^{-1}
Molecular Weight 795.2634
Wiswesser Line Notation 18ZH 2 .CD G4
Evaluation C(C_p); A(Phase changes)

$C_{37}H_{54}Si$ (liq) 60BAR/BOL
Tribenzyl-*n*-hexadecylsilane
Heat Capacity 313 K, $C_p = 904$ J·mol^{-1}·K^{-1}
Temperature range 40 to 240 °C.
Molecular Weight 526.9191
Wiswesser Line Notation 16 SI 1R&1R&1R
Evaluation B

$C_{38}H_{28}B_2F_8FeN_8$ (c) 87KUL/IYE
Bis(1,10-phenanthroline-2-carbaldehyde phenylhydrazone) iron(II) ditetrafluoroborate
Phase Changes
c,II/c,I 280.3 K, $\Delta H = 15600$ J·mol^{-1}
$\Delta S = 55.5$ J·mol^{-1}·K^{-1}
Spin-state transition.
Molecular Weight 826.1470
Wiswesser Line Notation T B666 CN NNϕJ D1UNMR ϕ-FE-ϕT B666 CN NNϕJ D1UNMR &B-F4 2
Evaluation A

$C_{38}H_{28}Cl_2FeN_8O_8$ (c) 87KUL/IYE
Bis(1,10-phenanthroline-2-carbaldehyde phenylhydrazone) iron(II) diperchlorate
Phase Changes
c,II/c,I 244.8 K, $\Delta H = 15800$ J·mol^{-1}
$\Delta S = 64.6$ J·mol^{-1}·K^{-1}
Spin-state transition.
Molecular Weight 851.4410
Wiswesser Line Notation T B666 CN NNϕJ D1UNMR ϕ-FE-ϕT B666 CN NNϕJ D1UNMR &G-O4 2
Evaluation A

$C_{38}H_{36}O_4Si_4$ (c) 82KUL/DZH2
1,1,3,3,5,5-Hexaphenyl-7,7-dimethylcyclotetrasiloxane
Heat Capacity 298.15 K, $C_p = 815.5$ J·mol^{-1}·K^{-1}
Temperature range 12 to 340 K.
Entropy 298.15 K, $S = 865.7$ J·mol^{-1}·K^{-1}
Molecular Weight 669.0420
Wiswesser Line Notation T8-SI-O-SI-O-SI-OJ AR AR C1 C1 ER ER GR GR
Evaluation A

$C_{38}H_{50}O_4$ (c) 84OZC/ASR
4,4′-Diundecanoyloxydiphenyldiacetylene
Phase Changes
c,III/c,II 339 K, $\Delta H = 18100$ J·mol^{-1}
$\Delta S = 53.54$ J·mol^{-1}·K^{-1}
c,II/c,I 359 K, $\Delta H = 7590$ J·mol^{-1}
$\Delta S = 21.14$ J·mol^{-1}·K^{-1}
c,I/liq 399 K, $\Delta H = 36200$ J·mol^{-1}
$\Delta S = 90.85$ J·mol^{-1}·K^{-1}
Solid-isotropic.
Molecular Weight 570.8106
Wiswesser Line Notation 1OOVR D1UU2UU1R DOV10
Evaluation A

$C_{38}H_{62}$ (c) 83KRA/BEC
5,6-Dibutyl-5,6-bis(4-*tert*-butylphenyl)decane
Heat Capacity 298 K, $C_p = 805.5$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.371 cal.K^{-1}.g^{-1}.
Molecular Weight 518.9078
Wiswesser Line Notation 1XR DX4&4&X4&4&R DX
Evaluation B

$(C_{38}H_{70}O_8)_n$ (liq) 75PHI/WAL
Poly(hexamethylene sebacate)
Heat Capacity 328.15 K, $C_p = 1290$ J·mol^{-1}·K^{-1}
Temperature range 328.15 to 408.15 K.
Phase Changes
c/liq 306 K
Molecular Weight 654.9662
Wiswesser Line Notation 60V8VO6VO8VO6
Evaluation B

$C_{38}H_{70}O_8$ (liq) 76PHI/MAT
Dihexyl hexamethylene-1,6-disebacate
Heat Capacity 328 K, $C_p = 1293$ J·mol^{-1}·K^{-1}
Temperature range 328 to 408 K.
Molecular Weight 654.9662
Wiswesser Line Notation 6OV8VO6OV8VO6
Evaluation C

$C_{38}H_{74}O_4$ (liq) 76PHI/MAT
Di-*n*-tetradecylsebacate
Heat Capacity 343 K, $C_p = 1247$ J·mol^{-1}·K^{-1}
Temperature range 343 to 433 K.
Molecular Weight 595.0002
Wiswesser Line Notation 14OV8VO14
Evaluation C

$C_{38}H_{74}O_4Pb$ (c,II) 78ADE/SIM
Lead(II) nonadecanoate
Heat Capacity
Data only graphically for c,III.
Phase Changes
c,III/c,II 383.8 K, $\Delta H = 75900$ J·mol^{-1}
$\Delta S = 198$ J·mol^{-1}·K^{-1}
c,II and c,I are mesophases.
c,II/c,I 389.1 K, $\Delta H = 64300$ J·mol^{-1}
$\Delta S = 165$ J·mol^{-1}·K^{-1}
Molecular Weight 802.2002
Wiswesser Line Notation OV18 2 .PB
Evaluation C

$C_{39}H_{30}N_6$ (c) 84LEB/BYK
Hexaphenylisomelamine
Heat Capacity 298.15 K, $C_p = 672.4$ J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, $S = 706.5$ J·mol^{-1}·K^{-1}
Molecular Weight 582.7062
Wiswesser Line Notation T6NYNYNYJ AR BUNR CR DUNR ER FUNR
Evaluation A

$C_{39}H_{30}N_6$ (c) 84LEB/BYK
Hexaphenylmelamine
Heat Capacity 298.15 K, $C_p = 665.8$ J·mol^{-1}·K^{-1}
Temperature range 10 to 330 K.
Entropy 298.15 K, $S = 673.7$ J·mol^{-1}·K^{-1}
Molecular Weight 582.7062
Wiswesser Line Notation T6N CN ENJ BNR&R DNR&R FNR&R
Evaluation A

$C_{39}H_{74}O_6$ (liq) 47CHA/SIN
Trilaurin; Glyceryl trilaurate
Heat Capacity 330.7 K, $C_p = 1355.6$ J·mol^{-1}·K^{-1}
Temperature range 90 to 370 K. Value is unsmoothed experimental datum.
Entropy 298.15 K, $S = 1071.5$ J·mol^{-1}·K^{-1}
For c,β: Extrapolation below 90 K, 339 J·mol^{-1}·K^{-1}.
Phase Changes
c,β/liq 319.5 K, $\Delta H = 123510$ J·mol^{-1}
$\Delta S = 386.6$ J·mol^{-1}·K^{-1}
Molecular Weight 639.0100
Wiswesser Line Notation 11VO1YOV11&1OV11
Evaluation C

$C_{39}H_{74}O_6$ (liq) 76PHI/MAT
Trilaurin; Glyceryl trilaurate
Heat Capacity 323 K, $C_p = 1305$ J·mol^{-1}·K^{-1}
Temperature range 323 to 398 K.
Molecular Weight 639.0100
Wiswesser Line Notation 11VO1YOV11&1OV11
Evaluation C

$C_{40}H_{54}O_4$ (c) 84OZC/ASR
4,4′-Didodecanoyloxydiphenyldiacetylene
Phase Changes
c,II/c,I 374 K, $\Delta H = 50200$ J·mol^{-1}
$\Delta S = 134.1$ J·mol^{-1}·K^{-1}
c,I/liq 401 K, $\Delta H = 44000$ J·mol^{-1}
$\Delta S = 109.7$ J·mol^{-1}·K^{-1}
Solid-isotropic.
Molecular Weight 598.8642
Wiswesser Line Notation 11OVR D1UU2UU1R DOV11
Evaluation A

$C_{40}H_{76}N_2O_4 \cdot 61H_2O$ (liq) 89STR/STU
Bis-(tetra-*n*-butylammonium) *m*-phthalate clathrate hydrate
Phase Changes
c/liq 288.65 K, $\Delta H = 334000$ J·mol^{-1}
Molecular Weight 1747.9786
Wiswesser Line Notation QVR CVQ &K4&4&4&4 2 &QH 61
Evaluation A

$C_{40}H_{76}N_2O_4 \cdot 62H_2O$ (liq) 89STR/STU
Bis-(tetra-*n*-butylammonium) *o*-phthalate clathrate hydrate
Phase Changes
c/liq 293.45 K, $\Delta H = 382000$ J·mol^{-1}
Molecular Weight 1765.9938
Wiswesser Line Notation QVR BVQ &K4&4&4&4 2 &QH 62
Evaluation A

$C_{40}H_{76}N_2O_4 \cdot 63H_2O$ (liq) 89STR/STU
Bis-(tetra-*n*-butylammonium) *p*-phthalate clathrate hydrate
Phase Changes
c/liq 283.75 K, $\Delta H = 323000$ J·mol^{-1}
Molecular Weight 1784.009
Wiswesser Line Notation QVR DVQ &K4&4&4&4 2 &QH 63
Evaluation A

$C_{41}H_{72}O_2$ (c) 67BAR/POR
Cholesteryl myristate
Heat Capacity
C_p data given graphically only. Temperature range 270 to 370 K.
Phase Changes
c/liq 346.8 K, $\Delta H = 46690$ J·mol^{-1}
$\Delta S = 134.6$ J·mol^{-1}·K^{-1}
Solid-smectic transition.
liq/liq 352.9 K, $\Delta H = 1300$ J·mol^{-1}
$\Delta S = 3.7$ J·mol^{-1}·K^{-1}
Solid-cholesteric transition.
liq/liq 358.7 K, $\Delta H = 1025$ J·mol^{-1}
$\Delta S = 2.9$ J·mol^{-1}·K^{-1}
Cholesteric-isotropic transition.
Molecular Weight 597.0186
Wiswesser Line Notation L E5 B666 LUTJ A1 E1 FY1&3Y1&1 OOV13
Evaluation B

$C_{41}H_{72}O_2$ (c) 86KIS/IWA
Cholesteryl myristate
Phase Changes
c,I/liq 344.6 K, $\Delta H = 47100$ J·mol^{-1}
Solid-smectic transition.
liq/liq 353.0 K, $\Delta H = 1600$ J·mol^{-1}
Smectic-cholesteric.
liq/liq 358.3 K, $\Delta H = 1100$ J·mol^{-1}
Cholesteric-isotropic.
Molecular Weight 597.0186
Wiswesser Line Notation L E5 B666 LUTJ A1 E1 FY1&3Y1&1 OOV13
Evaluation A

$C_{42}H_{66}O_{12}$ (c) 79SOR/TSU
Benzene-hexa-*n*-hexanoate
Heat Capacity 300 K, $C_p = 1300$ J·mol^{-1}·K^{-1}
Temperature range 13 to 393 K. Data given graphically. C_p value is a graphical estimate.
Phase Changes
c,IV/c,III 251.58 K, $\Delta H = 25660$ J·mol^{-1}
$\Delta S = 102.67$ J·mol^{-1}·K^{-1}
c,III/c,II 291.46 K, $\Delta H = 12270$ J·mol^{-1}
$\Delta S = 46.11$ J·mol^{-1}·K^{-1}
c,II/c,I 348.27 K, $\Delta H = 16260$ J·mol^{-1}
$\Delta S = 46.68$ J·mol^{-1}·K^{-1}
c,I/liq 368.74 K, $\Delta H = 33500$ J·mol^{-1}
$\Delta S = 90.86$ J·mol^{-1}·K^{-1}
Molecular Weight 762.9762
Wiswesser Line Notation 5OVR BVO5 CVO5 DVO5 EVO5 FVO5
Evaluation B(C_p); A(Phase changes)

$C_{42}H_{66}O_{12}$ (c) 80SOR/TSU
Benzene-hexa-*n*-hexanoate
Heat Capacity 298.15 K, $C_p = 1294.9$ J·mol^{-1}·K^{-1}
Temperature range 13 to 393 K.
Entropy 298.15 K, $S = 1380.0$ J·mol^{-1}·K^{-1}
Phase Changes
c,IV/c,III 251.58 K, $\Delta H = 25665$ J·mol^{-1}
$\Delta S = 102.7$ J·mol^{-1}·K^{-1}
Transition has a large amount of first-order character.
c,III/c,II 291.46 K, $\Delta H = 12272$ J·mol^{-1}
$\Delta S = 46.69$ J·mol^{-1}·K^{-1}
Anomalous transition.
c,II/c,I 348.27 K, $\Delta H = 16259$ J·mol^{-1}
$\Delta S = 46.69$ J·mol^{-1}·K^{-1}
c,I/liq 368.74 K, $\Delta H = 33501$ J·mol^{-1}
$\Delta S = 90.88$ J·mol^{-1}·K^{-1}
Molecular Weight 762.9762
Wiswesser Line Notation 5OVR BVO5 CVO5 DVO5 EVO5 FVO5
Evaluation A

$C_{42}H_{70}O_{35}$ (c) 90BRI/WAD
β-Cyclodextrin; Cycloheptaamylose
Heat Capacity 298.15 K, $C_p = 1342$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 1134.9940
Wiswesser Line Notation /T5OTJ B* CQ DQ EQ* F1Q/ 7
Evaluation B

$C_{42}H_{70}O_{35} \cdot 11H_2O$ (c) 87HAN/MAT
β-Cyclodextrin undecahydrate; Cycloheptaamylose undecahydrate
Heat Capacity 299.53 K, $C_p = 2093$ J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 226 K, $\Delta S = 45.0$ J·mol^{-1}·K^{-1}
Molecular Weight 1333.1612
Wiswesser Line Notation /T5OTJ B* CQ DQ EO* F1Q/ 7
Evaluation A
T(glass) = 150 K.

$C_{42}H_{72}O_{12}$ (c) 84KOH/PRA
Hexa-*o*-hexanoyl-scyllo-inositol
Phase Changes
c/liq 341.6 K, $\Delta H = 21150$ J·mol^{-1}
Solid-discotic.
liq/liq 472.6 K, $\Delta H = 8840$ J·mol^{-1}
Discotic-isotropic.
Molecular Weight 769.0236
Wiswesser Line Notation L6TJ AOV5 BOV5 COV5 DOV5 EOV5 FOV5
Evaluation A

$C_{42}H_{82}O_4$ (liq) 76PHI/MAT
Di-*n*-hexadecyl sebacate
Heat Capacity 353 K, $C_p = 1460$ J·mol^{-1}·K^{-1}
Temperature range 353 to 384 K.
Molecular Weight 651.1074
Wiswesser Line Notation 16OV8VO16
Evaluation C

$C_{42}H_{86}$ (liq) 69ATK/LAR
n-Dotetracontane
Heat Capacity 353 K, $C_p = 1425$ J·mol^{-1}·K^{-1}
Temperature range 353 to 453 K. Equation only.
Molecular Weight 591.1414
Wiswesser Line Notation 42H
Evaluation C

$C_{43}H_{26}AsN_8$ (c) 77KOS/SOR2
Methyltriphenylarsonium bis[7,7,8,8-tetracyanoquinodimethanide]
Heat Capacity 300 K, $C_p = 879.74$ J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Entropy 300 K, $S = 982.05$ J·mol^{-1}·K^{-1}
Molecular Weight 729.6536
Wiswesser Line Notation L6Y DYJ AYCN&CN DYCN&CN 2 &1-AS-R&R&
Evaluation A

$C_{43}H_{26}N_8P$ (c) 70KOS/IID
Methyltriphenylphosphonium bis(7,7,8,8-tetracyanoquinodimethanide)
Heat Capacity 300 K, $C_p = 858$ J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K. Data given graphically only. Value estimated from graph.
Molecular Weight 685.7058
Wiswesser Line Notation L6Y DYJ AYCN&CN DYCN&CN 2 &1PR&R&R
Evaluation C

$C_{43}H_{26}N_8P$ (c,II) 77KOS/SOR2
Methyltriphenylphosphonium bis(7,7,8,8-tetracyanoquinodimethanide)
Heat Capacity 300 K, $C_p = 859.26$ J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Entropy 300 K, $S = 922.69$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 315.65 K, $\Delta H = 2030$ J·mol^{-1}
$\Delta S = 6.43$ J·mol^{-1}·K^{-1}
Molecular Weight 685.7058
Wiswesser Line Notation L6Y DYJ AYCN&CN DYCN&CN 2 &1PR&R&R
Evaluation A

$C_{43}H_{76}O_2$ (c) 86KIS/IWA
Cholesteryl palmitate
Phase Changes
c,I/liq 350.4 K, $\Delta H = 56200$ J·mol^{-1}
$\Delta S = 160.4$ J·mol^{-1}·K^{-1}
Solid-smectic transition.
liq/liq 349.9 K, $\Delta H = 1700$ J·mol^{-1}
$\Delta S = 4.86$ J·mol^{-1}·K^{-1}
Smectic-cholesteric.
liq/liq 355.0 K, $\Delta H = 1300$ J·mol^{-1}
$\Delta S = 3.66$ J·mol^{-1}·K^{-1}
Cholesteric-isotropic.
Molecular Weight 625.0722
Wiswesser Line Notation L E5 B666 LUTJ A1 E1 FY1&3Y1&1 OOV15
Evaluation A

$C_{45}H_{78}O_2$ (c) 86KIS/IWA
Cholesteryl oleate
Phase Changes
c,I/liq 321.1 K, $\Delta H = 2900$ J·mol^{-1}
Solid$_1$-isotropic. Solid$_2$-isotropic also given:
317.4 K, $\Delta H = 2700$ J·mol^{-1}
$\Delta S = 8.51$ J·mol^{-1}·K^{-1}
liq/liq 315.9 K, $\Delta H = 1300$ J·mol^{-1}
$\Delta S = 4.12$ J·mol^{-1}·K^{-1}
Smectic-cholesteric liquid transition.
liq/liq 321.0 K, $\Delta H = 840$ J·mol^{-1}
$\Delta S = 2.62$ J·mol^{-1}·K^{-1}
Cholesteric-isotropic liquid transition.
Molecular Weight 651.1100
Wiswesser Line Notation L E5 B666 LUTJ A1 E1 FY1&3Y1&1 OOV8U9
Evaluation A

$C_{45}H_{78}O_2$ (c) 88VOE/MAR
Cholesteryl oleate
Phase Changes
c,I/liq 314.52 K, $\Delta H = 19500$ J·mol^{-1}
Crystalline/Smectic A.
liq/liq 322.24 K, $\Delta H = 980$ J·mol^{-1}
Smectic A/Cholesteric.
liq/liq 326.73 K, $\Delta H = 18$ J·mol^{-1}
Cholesteric/BPI.
liq/liq 327.54 K, $\Delta H = 12$ J·mol^{-1}
BPI/BPII.
liq/liq 328.02 K, $\Delta H = 485$ J·mol^{-1}
BPII/Isotropic.
Molecular Weight 651.1100
Wiswesser Line Notation L E5 B666 LUTJ A1 E1 FY1&3Y1&1 OOV8U9
Evaluation A

$C_{45}H_{80}O_2$ (c) 86KIS/IWA
Cholesteryl stearate
Phase Changes
c,I/liq 355.4 K, $\Delta H = 67500$ J·mol^{-1}
$\Delta S = 189.9$ J·mol^{-1}·K^{-1}
Solid-isotropic liquid transition.
liq/liq 349.0 K, $\Delta H = 1800$ J·mol^{-1}
$\Delta S = 5.16$ J·mol^{-1}·K^{-1}
Smectic-cholesteric liquid transition.
liq/liq 353.0 K, $\Delta H = 1700$ J·mol^{-1}
$\Delta S = 4.82$ J·mol^{-1}·K^{-1}
Cholesteric-isotropic liquid transition.
Molecular Weight 653.1258
Wiswesser Line Notation L E5 B666 LUTJ A1 E1 FY1&3Y1&1 OOV17
Evaluation A

$C_{45}H_{86}O_6$ (liq) 47CHA/SIN
Trimyristin; Glyceryl trimyristate
Heat Capacity 331.5 K, $C_p = 1555.2$ J·mol^{-1}·K^{-1}
Temperature range 89 to 365 K. Value is unsmoothed experimental datum. Data for c,α, 192 to 247 K.
Entropy 298.15 K, $S = 1246.0$ J·mol^{-1}·K^{-1}
For c,β. Extrapolation below 90 K, 381.2 J·mol^{-1}·K^{-1}.
Phase Changes
c,α/liq 305.5 K, $\Delta H = 104685$ J·mol^{-1}
$\Delta S = 342.7$ J·mol^{-1}·K^{-1}
c,β/liq 330.2 K, $\Delta H = 152195$ J·mol^{-1}
$\Delta S = 460.9$ J·mol^{-1}·K^{-1}
Molecular Weight 723.1708
Wiswesser Line Notation 13VO1YOV13&1OV13
Evaluation C

$C_{45}H_{86}O_6$ (liq) 76PHI/MAT

Trimyristin; Glyceryl trimyristate

Heat Capacity 333 K, $C_p = 1481$ J·mol^{-1}·K^{-1}

Temperature range 333 to 433 K.

Molecular Weight 723.1708

Wiswesser Line Notation 13VO1YOV13&1OV13

Evaluation C

$C_{46}H_{47}N_7O_2$ (c) 40CAM/CAM

p-Nitrosodimethylaniline-*β*-naphthylamine complex; *β*-Naphthylamine-*p*-nitrosodimethylaniline complex

Heat Capacity 293 K, $C_p = 857.7$ J·mol^{-1}·K^{-1}

One temperature.

Molecular Weight 729.9230

Wiswesser Line Notation ONR DN1&1 2 &L66J CZ3

Evaluation C

$C_{46}H_{90}O_4$ (liq) 76PHI/MAT

Di-*n*-octadecyl sebacate

Heat Capacity 353 K, $C_p = 1481$ J·mol^{-1}·K^{-1}

Temperature range 353 to 354 K.

Molecular Weight 707.2146

Wiswesser Line Notation 18OV8VO18

Evaluation C

$C_{48}H_{40}O_4Si_4$ (c) 82KUL

Octaphenylcyclotetrasiloxane

Heat Capacity 298.15 K, $C_p = 932.5$ J·mol^{-1}·K^{-1}

Temperature range 12 to 300 K.

Entropy 298.15 K, $S = 1044$ J·mol^{-1}·K^{-1}

Molecular Weight 793.1836

Wiswesser Line Notation T8SIOSIOSIOSIOJ AR AR CR CR ER ER GR GR

Evaluation A

$C_{48}H_{78}O_{12}$ (c) 79SOR/TSU

Benzene-hexa-*n*-heptanoate

Heat Capacity 300 K, $C_p = 1500$ J·mol^{-1}·K^{-1}

Temperature range 13 to 393 K. Data given graphically. C_p value is a graphical estimate.

Phase Changes

c,IV/c,III 129 K, $\Delta H = 1120$ J·mol^{-1}; $\Delta S = 8.46$ J·mol^{-1}·K^{-1}

c,III/c,II 222.80 K

c,II/c,I 230.81 K, $\Delta H = 11500$ J·mol^{-1}; $\Delta S = 50.44$ J·mol^{-1}·K^{-1}

Combination of transition c,III/c,II and c,II/c,I.

c,I/liq 353.79 K, $\Delta H = 32210$ J·mol^{-1}; $\Delta S = 91.08$ J·mol^{-1}·K^{-1}

Solid-mesophase.

liq/liq 359.28 K, $\Delta H = 21540$ J·mol^{-1}; $\Delta S = 59.93$ J·mol^{-1}·K^{-1}

Mesophase-liquid transition.

Molecular Weight 847.1370

Wiswesser Line Notation 6OVR BVO6 CVO6 DVO6 EVO6 FVO6

Evaluation A(Phase changes), B(C_p)

$C_{48}H_{78}O_{12}$ (c) 81SOR/SUG

Benzene-hexa-*n*-heptanoate

Heat Capacity 298.15 K, $C_p = 1505.0$ J·mol^{-1}·K^{-1}

Temperature range 13 to 393 K.

Entropy 298.15 K, $S = 1530.1$ J·mol^{-1}·K^{-1}

Phase Changes

c,IV/c,III 129 K, $\Delta H = 1120$ J·mol^{-1}; $\Delta S = 8.46$ J·mol^{-1}·K^{-1}

Anomalous or diffuse first-order transition.

c,III/c,II 222.80 K

Anomalous transition. c,II/c,I 230.81 K

First order transition.

c,I/meso 353.79 K, $\Delta H = 32210$ J·mol^{-1}; $\Delta S = 91.08$ J·mol^{-1}·K^{-1}

meso/iso 359.28 K, $\Delta H = 21540$ J·mol^{-1}; $\Delta S = 59.93$ J·mol^{-1}·K^{-1}

Triple point is 353.81 K.

Molecular Weight 847.1370

Wiswesser Line Notation 6OVR BVO6 CVO6 DVO6 EVO6 FVO6

Evaluation A

$C_{48}H_{80}O_{40}$ (c) 90BRI/WAD

γ-Cyclodextrin; Cyclooctaamylose

Heat Capacity 298.15 K, $C_p = 1568$ J·mol^{-1}·K^{-1}

One temperature.

Molecular Weight 1297.1360

Wiswesser Line Notation /T5OTJ B* CQ DQ EQ* F1Q/ 8

Evaluation B

$C_{48}H_{98}$ (liq) 69ATK/LAR

n-Octatetracontane

Heat Capacity 353 K, $C_p = 1595$ J·mol^{-1}·K^{-1}

Temperature range 353 to 453 K. Equation only.

Molecular Weight 675.3022

Wiswesser Line Notation 48H

Evaluation C

$C_{51}H_{98}O_6$ (liq) 47CHA/SIN

Tripalmitin; Glyceryl tripalmitate

Heat Capacity 338.8 K, $C_p = 1753.1$ J·mol^{-1}·K^{-1}

Temperature range 87 to 369 K. Value is unsmoothed experimental datum. Data for c,*α*, 195 to 252 K.

Entropy 298.15 K, $S = 1387.4$ J·mol^{-1}·K^{-1}

For c,*β*: extrapolation below 90 K, 415.1 J·mol^{-1}·K^{-1}.

Phase Changes

c,*α*/liq 317.9 K, $\Delta H = 126335$ J·mol^{-1}; $\Delta S = 397.4$ J·mol^{-1}·K^{-1}

c,*β*/liq 338.9 K, $\Delta H = 179370$ J·mol^{-1}; $\Delta S = 529.3$ J·mol^{-1}·K^{-1}

Molecular Weight 807.3316

Wiswesser Line Notation 15VO1YOV15&1OV15

Evaluation C

$C_{51}H_{98}O_6$ (liq) 76PHI/MAT

Tripalmitin; Glyceryl tripalmitate

Heat Capacity 343 K, $C_p = 1665$ J·mol^{-1}·K^{-1}

Temperature range 343 to 418 K.

Molecular Weight 807.3316

Wiswesser Line Notation 15VO1YOV15&1OV15

Evaluation C

$C_{54}H_{72}O_{12}$ (c,III) 90SOR/ASA
2,3,6,7,10,11-Hexa-*n*-hexyloxytriphenylene
Heat Capacity 298.15 K, $C_p = 1498.3$ J·mol^{-1}·K^{-1}
Temperature range 17 to 397 K.
Entropy 298.15 K, $S = 1396.546$ J·mol^{-1}·K^{-1}
Phase Changes

c,VI/c,V	105.90 K,	$\Delta H = 1160$ J·mol^{-1}
		$\Delta S = 13.43$ J·mol^{-1}·K^{-1}
c,V/c,IV	220.86 K,	$\Delta H = 1950$ J·mol^{-1}
		$\Delta S = 5.56$ J·mol^{-1}·K^{-1}
c,IV/c,III	233.91 K,	$\Delta H = 1300$ J·mol^{-1}
		$\Delta S = 8.83$ J·mol^{-1}·K^{-1}
c,III/c,II	330.81 K,	$\Delta H = 3060$ J·mol^{-1}
		$\Delta S = 9.59$ J·mol^{-1}·K^{-1}
c,II/c,I	337.10 K,	$\Delta H = 2510$ J·mol^{-1}
		$\Delta S = 7.46$ J·mol^{-1}·K^{-1}

Molecular Weight 913.1556
Wiswesser Line Notation L B6 H666J DOR EOR JOR KOR POR OOR
Evaluation A
c,I/liq, 340.27K, $\Delta H = 39050$ J·mol^{-1}, $\Delta S = 114.91$ J·mol^{-1}·K^{-1}; discotic liq/isotropic liq, 371.17K, $\Delta H = 5240$ J·mol^{-1}, $\Delta S = 14.13$ J·mol^{-1}·K^{-1}.

$C_{54}H_{90}O_{12}$ (c) 82SOR/YOS
Benzene-hexa-*n*-octanoate
Heat Capacity 298.15 K, $C_p = 2131.3$ J·mol^{-1}·K^{-1}
Temperature range 13 to 393 K.
Entropy 298.15 K, $S = 1514.2$ J·mol^{-1}·K^{-1}
Phase Changes

c,II/c,I	301.89 K,	$\Delta H = 48960$ J·mol^{-1}
		$\Delta S = 164.01$ J·mol^{-1}·K^{-1}
c,I/liq	355.10 K,	$\Delta H = 46070$ J·mol^{-1}
		$\Delta S = 129.81$ J·mol^{-1}·K^{-1}

Solid-columnar mesophase transition.

liq/liq	357.09 K,	$\Delta H = 19220$ J·mol^{-1}
		$\Delta S = 53.77$ J·mol^{-1}·K^{-1}

Columnar mesophase-isotropic liquid transition.
Molecular Weight 931.2978
Wiswesser Line Notation 7OVR BOV7 COV7 DOV7 EOV7 FOV7
Evaluation A

$C_{54}H_{96}O_{12}$ (c) 84KOH/PRA
Hexa-*o*-octanoyl-scyllo-inositol
Phase Changes

c/liq	348.6 K,	$\Delta H = 43330$ J·mol^{-1}
		$\Delta S = 124.3$ J·mol^{-1}·K^{-1}

Solid-discotic.

liq/liq	471.6 K,	$\Delta H = 9470$ J·mol^{-1}
		$\Delta S = 20.08$ J·mol^{-1}·K^{-1}

Discotic-isotropic.
Molecular Weight 937.3452
Wiswesser Line Notation L6TJ AOV7 BOV7 COV7 DOV7 EOV7 FOV7
Evaluation A

$C_{54}H_{98}O_{12}$ (liq) 75PHI/WAL
Dihexyl bis(hexamethylene-1,6-)trisebacate
Heat Capacity 333.15 K, $C_p = 1850$ J·mol^{-1}·K^{-1}
Temperature range 333.15 to 433.15 K.
Phase Changes

c/liq	322 K

Molecular Weight 939.3610
Wiswesser Line Notation 6OV8VO6VO8VO6VO8VO6
Evaluation B

$C_{54}H_{98}O_{12}$ (liq) 76PHI/MAT
Dihexyl bis(hexamethylene-1,6-)trisebacate
Heat Capacity 333 K, $C_p = 1828$ J·mol^{-1}·K^{-1}
Temperature range 333 to 433 K.
Molecular Weight 939.3610
Wiswesser Line Notation 6OV8VO6VO8VO6VO8VO6
Evaluation C

$C_{54}H_{104}O_6$ (c) 84SIM/HOC
Trimargarin; Glyceryl trimargarate
Heat Capacity 300 K
Temperature range 190 to 350 K. Heat capacity given for the following solid state phases: (J·mol^{-1}·K^{-1}); β (mp, 338 K)=1393; $\beta 1'$ (mp, 335 K) 1518; $\beta 2'$ (mp, 333 K)=1621; α (mp, 323 K)=1759.
Molecular Weight 849.4120
Wiswesser Line Notation 16VO1YOV16&1OV16
Evaluation B

$C_{57}H_{110}O_6$ (liq) 47CHA/SIN
Tristearin; Glyceryl tristearate
Heat Capacity 346.5 K, $C_p = 1969.0$ J·mol^{-1}·K^{-1}
Temperature range 96 to 372 K. Value is unsmoothed experimental datum. Data for c,α, 192 to 226 K.
Entropy 298.15 K, $S = 1534.7$ J·mol^{-1}·K^{-1}
For c,β: extrapolation below 90 K, 462.8 J·mol^{-1}·K^{-1}.
Phase Changes

c,α/liq	327.2 K,	$\Delta H = 145080$ J·mol^{-1}
		$\Delta S = 443.4$ J·mol^{-1}·K^{-1}
c,β/liq	345.7 K,	$\Delta H = 203260$ J·mol^{-1}
		$\Delta S = 588.0$ J·mol^{-1}·K^{-1}

Molecular Weight 891.4924
Wiswesser Line Notation 17VO1YOV17&10V17
Evaluation C

$C_{57}H_{110}O_6$ (liq) 76PHI/MAT
Tristearin; Glyceryl tristearate
Heat Capacity 353 K, $C_p = 1975$ J·mol^{-1}·K^{-1}
Temperature range 353 to 453 K.
Molecular Weight 891.4924
Wiswesser Line Notation 17VO1YOV17&10V17
Evaluation C

$C_{57}H_{110}O_6$ (c) 84SIM/HOC
Tristearin; Glyceryl tristearate
Heat Capacity 300 K
Temperature range 190 to 350 K. Heat capacity given for the following solid state phases: (J·mol^{-1}·K^{-1}); β (mp, 345 K)=1436; $\beta 1'$ (mp, 337 K)=1544; $\beta 2'$ (mp, 334 K)=1615; α (mp, 328 K)=1846.
Molecular Weight 891.4924
Wiswesser Line Notation 17VO1YOV17&10V17
Evaluation B

C_{60} (c) 91ATA/TAN
Fullerene
Heat Capacity
Temperature range 80 to 300 K. Data given graphically only.
Phase Changes

c,II/c,I	230 K

Anomaly from 160 to 260 K.
Molecular Weight 720.6600
Wiswesser Line Notation C60
Evaluation B
Anomaly extends from 180 to 260 K, peaking at 230 K.

C_{60} (c) 91DWO/FAB
Fullerene
Phase Changes
c/c 257 K, $\Delta H = 6945$ J·mol^{-1}
Molecular Weight 720.6600
Wiswesser Line Notation C60
Evaluation B
Transition enthalpy changes with sample history, in particular, the degree of crystallinity.

C_{60} (c) 91DWO/SZW2
Fullerene
Phase Changes
c,II/c,I 257.2 K, $\Delta H = 2710$ J·mol^{-1}
Molecular Weight 720.6600
Wiswesser Line Notation
Evaluation B

C_{60} (amorp) 92BYS/DID
Fullerene
Heat Capacity
Temperature range 210 to 290 K, graphical data only.
Phase Changes
c/c 260 K, $\Delta H = 2100$ J·mol^{-1}
He atmosphere
c/c 260 K, $\Delta H = 600$ J·mol^{-1}
Ar atmosphere
Molecular Weight 720.6600
Wiswesser Line Notation C60
Evaluation B
Amorphous powder.

C_{60} (c) 92BYS/DID
Fullerene
Heat Capacity
Temperature range 210 to 290 K, graphical data only.
Phase Changes
c/c 240 K, $\Delta H = 4900$ J·mol^{-1}
He atmosphere
c/c 240 K, $\Delta H = 5300$ J·mol^{-1}
Ar atmosphere
c/c 265 K, $\Delta H = 1000$ J·mol^{-1}
He atmosphere
c/c 265 K, $\Delta H = 500$ J·mol^{-1}
Ar atmosphere
Molecular Weight 720.6600
Wiswesser Line Notation C60
Evaluation B
Crushed single crystals.

C_{60} (c) 92JIN/CHE
Fullerene
Heat Capacity 298.15 K, $C_p = 536.9$ J·mol^{-1}·K^{-1}
Temperature range 120 to 560 K.
Phase Changes
c,II/c,I 256 K, $\Delta H = 6990$ J·mol^{-1}
$\Delta S = 27.3$ J·mol^{-1}·K^{-1}
Molecular Weight 720.6600
Wiswesser Line Notation C60
Evaluation A

C_{60} (c) 92MAT/SUG
Fullerene
Heat Capacity 300 K, $C_p = 550$ J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Data given graphically, only. Value estimated from graph.
Phase Changes
c,II/c,I 257.6 K, $\Delta H = 7540$ J·mol^{-1}
$\Delta S = 30.0$ J·mol^{-1}·K^{-1}
Excess entropy at 240 and 254 K.
Molecular Weight 720.6600
Wiswesser Line Notation C60
Evaluation A
T(glass)=86 K.

C_{60} (c) 92STE/CHI2
Fullerene
Heat Capacity 300 K, $C_p = 556.46$ J·mol^{-1}·K^{-1}
Temperature range 300 to 800 K. $C_{sat}(c) = -136.9 + 2.442(T/K) - 2.56\times10^{-4}(T/K)^2 - 6.5\times10^{-7}(T/K)^3$J/K·mol (300 to 800 K). Value calculated from equation.
Molecular Weight 720.6600
Wiswesser Line Notation C60
Evaluation A

$C_{60}O$ (c) 92VAU/IIEI
Fullerene epoxide
Phase Changes
c,II/c,I 278 K, $\Delta H = 4420$ J·mol^{-1}
Molecular Weight 736.6594
Wiswesser Line Notation C-60-O
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86HEC/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid I)
Heat Capacity 298.651 K, $C_p = 2016.6$ J·mol^{-1}·K^{-1}
Temperature range 12 to 425 K. Unsmoothed experimental datum.
Phase Changes
c,I/liq 362.6 K, $\Delta H = 24210$ J·mol^{-1}
$\Delta S = 66.76$ J·mol^{-1}·K^{-1}
Crystal/discotic.
liq/liq 402.16 K, $\Delta H = 3626$ J·mol^{-1}
$\Delta S = 9.02$ J·mol^{-1}·K^{-1}
Discotic/Isotropic liquid.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J COV8 DOV8 IOV8 JOV8 OOV8 POV8
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86HEC/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid II)
Heat Capacity 299.036 K, $C_p = 2082.0$ J·mol^{-1}·K^{-1}
Temperature range 12 to 425 K. Unsmoothed experimental datum.
Phase Changes
c,II/liq 359.7 K, $\Delta H = 25440$ J·mol^{-1}
$\Delta S = 71.12$ J·mol^{-1}·K^{-1}
Crystal/discotic.
liq/liq 402.16 K, $\Delta H = 3626$ J·mol^{-1}
$\Delta S = 9.02$ J·mol^{-1}·K^{-1}
Discotic/isotropic liquid.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J COV8 DOV8 IOV8 JOV8 OOV8 POV8
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86HEC/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid III)
Heat Capacity 298.428 K, $C_p = 1956.1$ J·mol^{-1}·K^{-1}
Temperature range 12 to 425 K. Unsmoothed experimental datum.
Phase Changes
c,III/c,I 290 K, $\Delta H = 15320$ J·mol^{-1}
$\Delta S = 52.8$ J·mol^{-1}·K^{-1}
Expected phase transition, but not observed.
c,III/liq 348 K, $\Delta H = 34770$ J·mol^{-1}
$\Delta S = 99.91$ J·mol^{-1}·K^{-1}
Crystal/discotic.
liq/liq 402.16 K, $\Delta H = 3626$ J·mol^{-1}
$\Delta S = 9.02$ J·mol^{-1}·K^{-1}
Discotic/isotropic liquid.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J COV8 DOV8 IOV8 JOV8 OOV8 POV8
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86VAN/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
Heat Capacity 298.651 K, $C_p = 2016.6$ J·mol^{-1}·K^{-1}
Temperature range 12 to 365 K. Unsmoothed experimental datum for "Solid-I".
Phase Changes
c/liq 362.6 K, $\Delta H = 24210$ J·mol^{-1}
$\Delta S = 66.76$ J·mol^{-1}·K^{-1}
Solid I-discotic.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J EOV7 FOV7 KOV7 LOV7 QOV7 ROV7
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86VAN/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
Heat Capacity 299.036 K, $C_p = 2082.0$ J·mol^{-1}·K^{-1}
Temperature range 12 to 425 K. Unsmoothed experimental datum for "solid-II".
Phase Changes
c/liq 359.7 K, $\Delta H = 25440$ J·mol^{-1}
$\Delta S = 71.12$ J·mol^{-1}·K^{-1}
Solid II-discotic.
liq/liq 402.16 K, $\Delta H = 3626$ J·mol^{-1}
$\Delta S = 9.02$ J·mol^{-1}·K^{-1}
Discotic-isotropic liquid transition.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J EOV7 FOV7 KOV7 LOV7 QOV7 ROV7
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86VAN/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
Heat Capacity 298.428 K, $C_p = 1956.1$ J·mol^{-1}·K^{-1}
Temperature range 12 to 348 K. Unsmoothed experimental datum for "Solid-III".
Phase Changes
c/liq 348 K, $\Delta H = 34770$ J·mol^{-1}
$\Delta S = 9.02$ J·mol^{-1}·K^{-1}
Solid III -discotic.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J EOV7 FOV7 KOV7 LOV7 QOV7 ROV7
Evaluation A

$C_{66}H_{120}O_{12}$ (c) 84KOH/PRA
Hexa-*o*-decanoyl-scyllo-inositol
Phase Changes
c/liq 357.1 K, $\Delta H = 53070$ J·mol^{-1}
$\Delta S = 148.6$ J·mol^{-1}·K^{-1}
Solid-discotic liquid transition.
liq/liq 461.8 K, $\Delta H = 10280$ J·mol^{-1}
$\Delta S = 22.26$ J·mol^{-1}·K^{-1}
Discotic-isotropic liquid transition.
Molecular Weight 1105.6668
Wiswesser Line Notation L6TJ AOV9 BOV9 COV9 DOV9 EOV9 FOV9
Evaluation A

$C_{78}H_{108}$ (c) 90PRA/KOH
2,3,6,7,10,11-Hexakis(1-decynyl)triphenylene
Phase Changes
c/liq 314.15 K, $\Delta H = 63000$ J·mol^{-1}
Crystal/isotropic.
Molecular Weight 1045.7112
Wiswesser Line Notation L B6 H666J D1UU9 E1UU9 J1UU9 K1UU9 Q1UU9
Evaluation C

$C_{84}H_{90}$ (c) 90PRA/KOH
Hexakis[(4-pentylphenyl)ethynyl]benzene
Phase Changes
c/liq 443.55 K, $\Delta H = 44100$ J·mol^{-1}
Crystal/nematic-discotic.
liq/liq 458.05 K, $\Delta H = 200$ J·mol^{-1}
Nematic-discotic/isotropic.
Molecular Weight 1099.6350
Wiswesser Line Notation 5R1UU1R B1UU1R5 &C1UU1R5 &D1UU1R5 &E1UU1R5 &F1UU1R5
Evaluation C

$C_{90}H_{102}$ (c) 90PRA/KOH
Hexakis[(4-hexylphenyl)ethynyl]benzene
Phase Changes
c/liq 397.55 K, $\Delta H = 38900$ J·mol^{-1}
Crystal/nematic-discotic.
liq/liq 416.05 K, $\Delta H = 200$ J·mol^{-1}
Nematic-discotic/isotropic.
Molecular Weight 1183.7958
Wiswesser Line Notation 6R1UU1R B1UU1R6 &C1UU1R6 &D1UU1R6 &E1UU1R6 &F1UU1R6
Evaluation C

$C_{96}H_{96}$ (c) 90PRA/KOH
2,3,6,7,10,11-Hexakis[(4-pentylphenyl)ethynyl] triphenylene
Phase Changes
c/liq 429.95 K, $\Delta H = 36700$ J·mol^{-1}
Crystal/nematic-discotic.
liq/liq 510.25 K, $\Delta H = 100$ J·mol^{-1}
Nematic-discotic/isotropic.
Molecular Weight 1249.8144
Wiswesser Line Notation L B6 H666J D1UU1R5 E1UU1R5 J1UU1R5 K1UU1R5 P1UU1R5 Q1UU1R5
Evaluation C

$C_{108}H_{120}$ (c) 90PRA/KOH
2,3,6,7,10,11-Hexakis[(4-heptylphenyl)ethynyl] triphenylene
Phase Changes
c/liq 395.15 K, $\Delta H = 41100$ J·mol^{-1}
Crystal/nematic-discotic.
liq/liq 449.75 K, $\Delta H = 100$ J·mol^{-1}
Nematic-discotic/isotropic.
Molecular Weight 1418.1360
Wiswesser Line Notation L B6 H666J D1UU1R7 E1UU1R7 J1UU1R7 K1UU1R7 P1UU1R7 Q1UU1R7
Evaluation C

$C_{203}H_{288}O_{14}$ (c) 87AWA/SUG
Galvinoxyl hydrogalvinoxyl (6:1) radical
Heat Capacity 299.62 K, $C_p = 634.81$ J·mol^{-1}·K^{-1}
Temperature range 12 to 303 K. Unsmoothed experimental datum.
Molecular Weight 2952.4998
Evaluation A

$C_{290}H_{411}O_{20}$ (c) 87AWA/SUG
Galvinoxyl hydrogalvinoxyl (9:1) radical
Heat Capacity 298.45 K, $C_p = 631.92$ J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K. Unsmoothed experimental datum.
Phase Changes
c,II/c,I 71 K, $\Delta H = 718$ J·mol^{-1}
$\Delta S = 10.11$ J·mol^{-1}·K^{-1}
Diamagnetic low temperature- paramagnetic high temperature phase transition in 9:1 crystal.
Molecular Weight 4217.4249
Evaluation A

$C_{508}H_{752}N_{130}O_{150}S_{12}Zn$ (c) 69HUT/COL
Bovine zinc insulin, anhydrous
Heat Capacity 298.15 K
$C_p = 125.4$ J·100g^{-1}·K^{-1}. Temperature range 10 to 310 K.
Entropy 298.15 K
$S = 131.5$ J·100g^{-1}·K^{-1}. Anhydrous protein from beef pancreas and consists of a sequence of 96 amino acids.
Molecular Weight 11530.4098
Evaluation A

$C_{508}H_{752}N_{130}O_{150}S_{12}Zn$ (c) 69HUT/COL
Bovine zinc insulin, hydrated
Heat Capacity 298.15 K
$C_p = 132.0$ J·100g^{-1}·K^{-1}. Temperature range 10 to 310 K.
Entropy 298.15 K
$S = 136.1$ J·100g^{-1}·K^{-1}. Anhydrous protein from beef pancreas and consists of a sequence of 96 amino acids. Hydrated bovine zinc insulin contains 4.0% water and would require the addition of 26.7 moles of H_2O to the empirical formula.
Molecular Weight 11530.4098
Evaluation A

$C_{1077}H_{1736}N_{304}O_{343}S_{12}$ (c) 69HUT/COL
Bovine chymotrypsinogen A, anhydrous
Heat Capacity 298.15 K
$C_p = 129.3$ J·100g^{-1}·K^{-1}. Temperature range is 10 to 310 K.
Entropy 298.15 K
$S = 135.0$ J·100g^{-1}·K^{-1}. Empirical formula and molecular weight calculated from compositional data on chymotrypsinogen in 69HUT/COL which shows a sequence of 245 amino acids.
Molecular Weight 24816.1124
Evaluation A

$C_{1077}H_{1736}N_{304}O_{343}S_{12}$ (c) 69HUT/COL
Bovine chymotrypsinogen A, hydrated
Heat Capacity 298.15 K
$C_p = 160.4$ J·100g^{-1}·K^{-1}. Temperature range 10 to 310 K.
Entropy 298.15 K
$S = 152.1$ J·100g^{-1}·K^{-1}. Empirical formula and molecular weight calculated from compositional data on chymotrypsinogen in 69HUT/COL which shows a sequence of 245 amino acids. Hydrated bovine chymotrypsinogen A contains 10.7% water and would require the addition of 165 moles of H_2O to the empirical formula.
Molecular Weight 24816.1124
Evaluation A

8. Compound Name—Formula—CASRN Index

A

Acenaphthene	$C_{12}H_{10}$	83-32-9
Acenaphthene picric acid	$C_{18}H_{11}N_3O_7$	4599-99-9
Acenaphthylene	$C_{12}H_8$	208-96-8
Acetal	$C_6H_{14}O_2$	105-57-7
Acetaldehyde	C_2H_4O	75-07-0
Acetaldehyde dibutyl acetal	$C_{10}H_{22}O_2$	871-22-7
Acetaldoxime	C_2H_5NO	107-29-9
Acetamide	C_2H_5NO	60-35-5
Acetamide nitrate	$C_2H_6N_2O_4$	75238-15-2
Acetamide-salicylic acid complex	$C_9H_{11}NO_4$	unavailable
Acetanilide	C_8H_9NO	103-84-4
Acetic acid	$C_2H_4O_2$	64-19-7
Acetic anhydride	$C_4H_6O_3$	108-24-7
Acetoacetic ester	$C_6H_{10}O_3$	141-97-9
Acetone	C_3H_6O	67-64-1
Acetone clathrate hydrate	$C_3H_6O \cdot 17H_2O$	18879-06-6
Acetonitrile	C_2H_3N	75-05-8
Acetophenone	C_8H_8O	98-86-2
Acetophenone diethyl ketal	$C_{12}H_{18}O_2$	4316-37-4
1-Aceto-3-stearin	$C_{23}H_{44}O_5$	27177-85-1
Acetylacetone, enol form	$C_5H_8O_2$	1522-20-9
N-Acetyl-L-alanine amide	$C_5H_{10}N_2O_2$	15962-47-7
N-Acetylalanine-N′-methylamide	$C_6H_{12}N_2O_2$	19701-83-8
Acetyl chloride	C_2H_3ClO	75-36-5
Acetylferrocene	$C_{12}H_{12}FeO$	1271-55-2
N-Acetylglycine amide	$C_4H_8N_2O_2$	2620-63-5
N-Acetylglycine-N′-methylamide	$C_5H_{10}N_2O_2$	7606-79-3
N-Acetylisoleucine-N′-methylamide	$C_9H_{18}N_2O_2$	32483-16-2
N-Acetyl-D-leucine amide	$C_8H_{16}N_2O_2$	16624-68-3
N-Acetylleucine-N′-methylamide	$C_9H_{18}N_2O_2$	32483-15-1
17-(Acetyloxy)-(17α)-19-norpregn-4-en-20-yn-3-one	$C_{22}H_{28}O_3$	51-98-9
N-Acetylphenylalanine-N′-methylamide	$C_{12}H_{16}N_2O_2$	17186-60-6
N-Acetylproline-N′-methylamide	$C_8H_{14}N_2O_2$	120328-71-4
N-Acetylvaline-N′-methylamide	$C_8H_{16}N_2O_2$	33067-46-8
Acridine	$C_{13}H_9N$	260-94-6
Acrylamide	C_3H_5NO	79-06-1
Acrylic acid	$C_3H_4O_2$	79-10-7
Acrylonitrile	C_3H_3N	107-13-1
Adamantane	$C_{10}H_{16}$	281-23-2
Adamantane-1-carboxylic acid methyl ester	$C_{12}H_{18}O_2$	711-01-3
1-Adamantyl carboxamide	$C_{11}H_{17}NO$	5511-18-2
1-Adamantyl cyanide	$C_{11}H_{15}N$	23074-42-2
1-Adamantyl isonitrile	$C_{11}H_{15}N$	22110-53-8
1-Adamantyl methyl ketone	$C_{12}H_{18}O$	1660-04-4
Adenine	$C_5H_5N_5$	73-24-5
Adipic acid	$C_6H_{10}O_4$	124-04-9
Adonitol	$C_5H_{12}O_5$	488-81-3
Alanine(D)	$C_3H_7NO_2$	338-69-2
Alanine(DL)	$C_3H_7NO_2$	302-72-7
Alanine(L)	$C_3H_7NO_2$	56-41-7
β-Alanine	$C_3H_7NO_2$	107-95-9
α,α-Alanylalanine(DL)	$C_6H_{12}N_2O_3$	2867-20-1
α,α-Alanylalanine(L)	$C_6H_{12}N_2O_3$	1948-31-8
β-Alanyl-β-alanine	$C_6H_{12}N_2O_3$	34322-87-7
α-Alanylasparagine(DL)	$C_7H_{13}N_3O_4$	1999-41-3
Alanylasparagine hydrate(DL)	$C_7H_{13}N_3O_4 \cdot H_2O$	unavailable
Alanylglycine	$C_5H_{10}N_2O_3$	687-69-4
Alanylglycine(DL)	$C_5H_{10}N_2O_3$	1188-01-8
β-Alanylglycine	$C_5H_{10}N_2O_3$	2672-88-0
Alanylglycylglycine(DL)	$C_7H_{13}N_3O_4$	927-21-9
α-Alanylglycylglycine	$C_7H_{13}N_3O_4$	927-21-9
Alanylnorleucine(DL)	$C_9H_{18}N_2O_3$	19079-66-4
N-DL-Alanyl-DL-norleucine	$C_9H_{18}N_2O_3$	19079-66-4
α-Alanylnorleucine(DL)	$C_9H_{18}N_2O_3$	19079-66-4
Alanylvaline(DL)	$C_8H_{15}N_2O_3$	1999-46-8
α-Alanylvaline(DL)	$C_8H_{16}N_2O_3$	1999-46-8
Allantoin	$C_4H_6N_4O_3$	97-59-6
Alloxan	$C_4H_2N_2O_4$	50-71-5
Allyl acetate	$C_5H_8O_2$	591-87-7
Allylcyclohexane	C_9H_{16}	2114-42-3
Allylcyclopentane	C_8H_{14}	3524-75-2
4-Allylguaiacol	$C_{10}H_{12}O_2$	97-53-0
Allyl isothiocyanate	C_4H_5NS	57-06-7
N-Allyl-N′-phenylthiourea	$C_{10}H_{12}N_2S$	7341-63-1
N-Allylpyrazole tricarbonyliron	$C_9H_8FeN_2O_3$	40672-10-4
Aluminum acetylacetonate	$C_{15}H_{21}AlO_6$	13963-57-0
Aminoantipyrene	$C_{11}H_{13}N_3O$	83-07-8
p-Aminoazobenzene	$C_{12}H_{11}N_3$	60-09-3
p-Aminobenzenesulfonamide	$C_6H_8N_2O_2S$	63-74-1
2-Aminobenzoic acid	$C_7H_7NO_2$	118-92-3
3-Aminobenzoic acid	$C_7H_7NO_2$	99-05-8
4-Aminobenzoic acid	$C_7H_7NO_2$	150-13-0
2-Aminobiphenyl	$C_{12}H_{11}N$	90-41-5
1-Aminobutane	$C_4H_{11}N$	109-73-9
2-Aminobutanoic acid	$C_4H_9NO_2$	1492-24-6
2-Aminobutanoic acid(L)	$C_4H_9NO_2$	1492-24-6
2-Aminobutanoic acid(DL)	$C_4H_9NO_2$	2835-81-6
4-Aminobutanoic acid	$C_4H_9NO_2$	56-12-2
α-Aminobutyric acid	$C_4H_9NO_2$	80-60-4
α-Aminobutyric acid(DL)	$C_4H_9NO_2$	56-12-2
α-Aminobutyric acid(L)	$C_4H_9NO_2$	1492-24-6
γ-Aminobutyric acid	$C_4H_9NO_2$	56-12-2
α-Aminocaproic acid(DL)	$C_6H_{13}NO_2$	616-06-8
α-Aminocaproic acid(L)	$C_6H_{13}NO_2$	327-57-1
m-Aminocinnamic acid	$C_9H_9NO_2$	1664-56-8
2-Aminoethanesulfonic acid	$C_2H_7NO_3S$	107-35-7
Aminoethanoic acid	$C_2H_5NO_2$	56-40-6
N-(2-Aminoethyl-N′-[(2-aminoethyl)2-aminoethyl]piperazine	$C_{10}H_{25}N_5$	110-85-0
N-[(2-Aminoethyl)2-aminoethyl]piperazine	$C_8H_{20}N_4$	31295-54-2
N-(2-Aminoethyl)piperazine	$C_6H_{15}N_3$	140-31-8
1-Aminohexane	$C_6H_{15}N$	111-26-2
6-Aminohexanoic acid	$C_6H_{13}NO_2$	60-32-2
2-Amino-2-hydroxymethyl-1,3-propanediol	$C_4H_{11}NO_3$	77-86-1
2-Amino-3-hydroxypropanoic acid(DL)	$C_3H_7NO_3$	302-84-1
2-Amino-3-hydroxypropanoic acid(L)	$C_3H_7NO_3$	56-45-1
α-Aminoisovaleric acid	$C_5H_{11}NO_2$	640-68-6
α-Aminoisovaleric acid(D)	$C_5H_{11}NO_2$	640-68-6
α-Aminoisovaleric acid(DL)	$C_5H_{11}NO_2$	516-06-3
Aminomethane	CH_5N	74-89-5
2-Amino-3-methylbutanoic acid(D)	$C_5H_{11}NO_2$	640-68-6
2-Amino-3-methylbutanoic acid(DL)	$C_5H_{11}NO_2$	516-06-3
2-Amino-3-methylbutanoic acid(L)	$C_5H_{11}NO_2$	72-18-4
3-Amino-5-methylisoxazole	$C_4H_6N_2O$	1072-67-9
2-Amino-3-methylpentanoic acid(L)	$C_6H_{13}NO_2$	73-32-5
2-Amino-4-methylpentanoic acid(DL)	$C_6H_{13}NO_2$	328-39-2
2-Amino-4-methylpentanoic acid(L)	$C_6H_{13}NO_2$	61-90-5
2-Amino-2-methyl-1,3-propanediol	$C_4H_{11}NO_2$	115-69-5
2-Amino-2-methylpropanol	$C_4H_{11}NO$	124-68-5
2-Aminonaphthalene	$C_{10}H_9N$	91-59-8
8-Aminooctanoic acid	$C_8H_{17}NO_2$	1002-57-9
1-Aminopentane	$C_5H_{13}N$	110-58-7
5-Aminopentanoic acid	$C_5H_{11}NO_2$	660-88-8
2-Aminophenol	C_6H_7NO	95-55-6
3-Aminophenol	C_6H_7NO	591-27-5
4-Aminophenol	C_6H_7NO	123-30-8
1-Aminopropane	C_3H_9N	107-10-8
2-Aminopropane	C_3H_9N	75-31-0
2-Aminopropanoic acid(D)	$C_3H_7NO_2$	338-69-2
2-Aminopropanoic acid(DL)	$C_3H_7NO_2$	302-72-7
2-Aminopropanoic acid(L)	$C_3H_7NO_2$	56-41-7
3-Aminopropanoic acid	$C_3H_7NO_2$	107-95-9
Aminosuccinic acid(L)	$C_4H_7NO_4$	56-84-8
α-Aminovaleric acid(L)	$C_5H_{11}NO_2$	6600-40-4
Ammonium acid butanedioate	$C_4H_9NO_4$	38457-08-8

Ammonium acid isophthalate	$C_8H_9NO_4$	50961-33-6
Ammonium acid 2-methylsuccinate	$C_5H_{11}NO_4$	61478-85-1
Ammonium acid oxalate	$C_2H_5NO_4$	5972-72-5
Ammonium acid *m*-phthalate	$C_8H_9NO_4$	50961-33-6
Ammonium acid *o*-phthalate	$C_8H_9NO_4$	17735-77-2
Ammonium acid pyrotartrate	$C_5H_{11}NO_4$	61478-85-1
Ammonium acid succinate	$C_4H_9NO_4$	38457-08-8
Ammonium acid tartrate	$C_4H_9NO_6$	3095-65-6
Ammonium benzoate	$C_7H_9NO_2$	1863-63-4
Ammonium carbamate	$CH_6N_2O_2$	111-78-0
Ammonium cinnamate	$C_9H_{11}NO_2$	25459-05-6
Ammonium hydrogen oxalate hemihydrate	$C_2H_5NO_4 \cdot 0.5H_2O$	37541-72-3
Ammonium hydrogen oxalate hemihydrate-d_6	$C_2D_5NO_4 \cdot 0.5D_2O$	76585-14-3
Ammonium isophthalate	$C_8H_{12}N_2O_4$	18996-38-8
Ammonium oxalate	$C_2H_8N_2O_4$	1113-38-8
Ammonium phthalate	$C_8H_{12}N_2O_4$	523-24-0
Ammonium *m*-phthalate	$C_8H_{12}N_2O_4$	18996-38-8
Ammonium *o*-phthalate	$C_8H_{12}N_2O_4$	523-24-0
Ammonium purpurate	$C_8H_8N_6O_6$	3051-09-0
Ammonium succinate	$C_4H_{12}N_2O_4$	2226-88-2
Ammonium tartrate	$C_4H_{12}N_2O_6$	3164-29-2
Ammonium tetraphenyl borate	$C_{24}H_{24}BN$	14637-34-4
Ammonium tetraphenyl boron	$C_{24}H_{24}BN$	14637-34-4
Ammonium thiocyanate	CH_4N_2S	1762-95-4
n-Amyl acetate	$C_7H_{14}O_2$	628-63-7
n-Amyl alcohol	$C_5H_{12}O$	71-41-0
tert-Amyl alcohol	$C_5H_{12}O$	75-85-4
n-Amylamine	$C_5H_{13}N$	110-58-7
n-Amylammonium chloride	$C_5H_{14}ClN$	142-65-4
n-Amyl bromide	$C_5H_{11}Br$	110-53-2
Amyl butanoate	$C_9H_{18}O_2$	540-18-1
n-Amyl chloride	$C_5H_{11}Cl$	543-59-9
tert-Amyl ethyl ether	$C_7H_{16}O$	17952-11-3
n-Amyl iodide	$C_5H_{11}I$	628-17-1
n-Amyl mercaptan	$C_5H_{12}S$	110-66-7
tert-Amyl mercaptan	$C_5H_{12}S$	1679-09-0
tert-Amyl methyl ether	$C_6H_{14}O$	994-05-8
Amyl propionate	$C_8H_{16}O_2$	624-54-4
5α-Androstane-3-one-17β-ol	$C_{19}H_{30}O_2$	521-18-6
Androstanolone	$C_{19}H_{30}O_2$	521-18-6
Aniline	C_6H_7N	62-53-3
Aniline formaldehyde	$C_6H_7N \cdot CH_2O$	unavailable
Aniline hydrobromide	$C_6H_7N \cdot HBr$	542-11-0
Anisaldazine	$C_{16}H_{16}N_2O_2$	2299-73-2
p-Anisic acid	$C_8H_8O_3$	100-09-4
p-Anisidine	C_7H_9NO	104-94-9
Anisole	C_7H_8O	100-66-3
Anthracene	$C_{14}H_{10}$	120-12-7
Anthracene picric acid	$C_{20}H_{13}N_3O_7$	5937-78-0
Anthracene TCNB	$C_{24}H_{12}N_4$	747-42-2
Anthracene-1,2,4,5-tetracyanobenzene	$C_{24}H_{12}N_4$	747-42-2
Anthracene-1,3,5-trinitrobenzene adduct	$C_{20}H_{13}N_3O_6$	2499-09-4
Anthraquinone	$C_{14}H_8O_2$	84-65-1
Anthrone	$C_{14}H_{10}O$	90-44-8
Antimony triphenyl	$C_{18}H_{15}Sb$	603-36-1
Antipyrene	$C_{11}H_{12}N_2O$	60-80-0
Arabinitol(D)	$C_5H_{12}O_5$	488-82-4
Arabinose(D)	$C_5H_{10}O_5$	28697-53-2
Arabinose(L)	$C_5H_{10}O_5$	87-72-9
Arabitol(D)	$C_5H_{12}O_5$	488-82-4
Arginine(D)	$C_6H_{14}N_4O_2$	157-06-2
Arginine hydrochloride(L)	$C_6H_{15}ClN_4O_2$	627-75-8
Arginine phosphate monohydrate(L)	$C_6H_{14}N_4O_2 \cdot H_3PO_4 \cdot H_2O$	80887-43-0
Asparagine(L)	$C_4H_8N_2O_3$	70-47-3
Asparagine hydrate(L)	$C_4H_8N_2O_3 \cdot H_2O$	5794-13-8
Aspartic acid(L)	$C_4H_7NO_4$	56-84-8
1-Azabicyclo[2.2.2]octane	$C_7H_{13}N$	100-76-5
3-Azabicyclo[3.2.2]nonane	$C_8H_{15}N$	283-24-9
Azacymantrene	$C_7H_4MnNO_3$	32761-36-7
Azaferrocene	C_9H_9FeN	11077-12-6
Azelaic acid	$C_9H_{16}O_4$	123-99-9
Azobenzene	$C_{12}H_{10}N_2$	103-33-3
cis-Azobenzene	$C_{12}H_{10}N_2$	17082-12-1
tert-Azobenzene	$C_{12}H_{10}N_2$	1080-16-6
2,2′-Azodiisobutyrodinitrile	$C_8H_{12}N_4$	78-67-1
p-Azoxyanisole	$C_{14}H_{14}N_2O_3$	1562-94-3
p-Azoxyanisoylphenetole	$C_{15}H_{16}N_2O_3$	56095-14-8
p-Azoxyphenetole	$C_{16}H_{18}N_2O_3$	4792-83-0

B

Baked carbon	C	7440-44-0
Barbituric acid	$C_4H_4N_2O_3$	67-52-7
Barium dicalcium propionate	$C_{18}H_{30}BaCa_2O_{12}$	17115-98-9
1,2-Benzacenaphthene	$C_{16}H_{10}$	206-44-0
Benzaldehyde	C_7H_6O	100-52-7
Benzamide	C_7H_7NO	55-21-0
Benzanilide	$C_{13}H_{11}NO$	93-98-1
1,2-Benzanthracene picric acid	$C_{24}H_{15}N_3O_7$	72454-41-2
Benzanthrene	$C_{17}H_{12}$	56-55-3
Benzene	C_6H_6	71-43-2
Benzene-d_6	C_6D_6	1076-43-3
Benzene chromium dicarbonyl thiocarbonyl	$C_9H_6CrO_2S$	63356-86-5
Benzene chromium tricarbonyl	$C_9H_6CrO_3$	12082-08-5
Benzene-hexa-*n*-heptanoate	$C_{48}H_{78}O_{12}$	65201-70-9
Benzene-hexa-*n*-hexanoate	$C_{42}H_{66}O_{12}$	65201-69-6
Benzene-hexa-*n*-octanoate	$C_{54}H_{90}O_{12}$	65201-71-0
Benzene:hexafluorobenzene complex	$C_{12}H_6F_6$	783-33-5
Benzenesulfonamide	$C_6H_7NO_2S$	98-10-2
9,10-*o*-Benzeno-9,10-dihydroanthracene	$C_{20}H_{14}$	477-75-8
1,2-Benzfluorene picric acid	$C_{23}H_{15}N_3O_7$	72454-42-3
2,3-Benzfluorene picric acid	$C_{23}H_{15}N_3O_7$	72454-43-4
Benzhydrol	$C_{13}H_{12}O$	91-01-0
Benzil	$C_{14}H_{10}O_2$	134-81-6
Benzimidazole	$C_7H_6N_2$	51-17-2
Benzo[c]cinnoline	$C_{12}H_8N_2$	230-17-1
1,2-Benzofluorene	$C_{17}H_{12}$	238-84-6
2,3-Benzofluorene	$C_{17}H_{12}$	243-17-4
2,3-Benzofuran	C_8H_6O	271-89-6
Benzoic acid	$C_7H_6O_2$	65-85-0
Benzonitrile	C_7H_5N	100-47-0
9,10-Benzophenanthrene	$C_{18}H_{12}$	217-59-4
Benzo(d,e,f)phenanthrene	$C_{16}H_{10}$	129-00-0
Benzophenone	$C_{13}H_{10}O$	119-61-9
3,3′4,4′-Benzophenonetetracarboxylic-dianhydride-2,2-dimethyl-1,3-(4-aminophenoxy)-propane condensation polymer	$(C_{34}H_{24}N_2O_7)_n$	136922-70-8
7,8-Benzoquinoline	$C_{13}H_9N$	230-27-3
p-Benzoquinone	$C_6H_4O_2$	106-51-4
Benzothiazole	C_7H_5NS	95-16-9
Benzothiophene	C_8H_6S	95-15-8
Benzotriazole	$C_6H_5N_3$	95-14-7
Benzotrichloride	$C_7H_5Cl_3$	98-07-7
Benzotrifluoride	$C_7H_5F_3$	98-08-8
Benzoxazole	C_7H_5NO	273-53-0
N-Benzoyl-*o*-aminodiphenylamine	$C_{19}H_{16}N_2O$	34237-88-2
Benzoyl chloride	C_7H_5ClO	98-88-4
Benzoylferrocene	$C_{17}H_{14}FeO$	1272-44-2
Benzoyl formic acid	$C_8H_6O_3$	611-73-4
Benzoylglycine	$C_9H_9NO_3$	495-69-2
Benzo[a]pyrene picric acid	$C_{26}H_{15}N_3O_7$	72454-44-5
1-Benzo[b]pyrrole	C_8H_7N	120-72-9
17-(Benzoyloxy)-(17α)-19-norpregn-4-en-20-yn-3-one	$C_{27}H_{30}O_3$	71203-39-9
Benzyl acetate	$C_9H_{10}O_2$	140-11-4
Benzyl alcohol	C_7H_8O	100-51-6

Benzylamine	C_7H_9N	100-46-9
Benzyl chloride	C_7H_7Cl	100-44-7
Benzyl ethanoate	$C_9H_{10}O_2$	140-11-4
Benzyl methacrylate	$C_{11}H_{12}O_2$	2495-37-6
Beryllium oxyacetate	$C_{12}H_{18}Be_4O_{13}$	19049-40-2
Betaine calcium chloride dihydrate	$C_5H_{11}CaCl_2NO_2 \cdot 2H_2O$	90268-02-3
Betaine phosphate	$C_5H_{14}NO_6P$	58823-88-4
1-Bicyclo[1.1.0]butyl cyanide	C_5H_5N	16955-35-4
cis-Bicyclo[5.3.0]decane	$C_{10}H_{18}$	16189-46-1
Bicyclo[2.2.1]heptane	C_7H_{12}	279-23-2
Bicyclo[4.1.0]heptane	C_7H_{12}	286-08-8
Bicyclo[2.2.1]heptene	C_7H_{10}	498-66-8
Bicyclo[2.2.1]hept-2,5-diene	C_7H_8	121-46-0
endo-Bicyclo[2.2.1]-5-heptene-2,3-dicarboxylic acid anhydride	$C_9H_8O_3$	129-64-6
Bicyclohexyl	$C_{12}H_{22}$	92-51-3
1-Bicyclo[3.1.0]hexyl cyanide	C_7H_9N	31357-72-9
cis-Bicyclo[6.1.0]nonane	C_9H_{16}	13757-43-2
Bicyclo[3.3.1]nonan-9-one	$C_9H_{14}O$	17931-55-4
Bicyclo[2.2.2]octane	C_8H_{14}	280-33-1
cis-Bicyclo[3.3.0]octane	C_8H_{14}	1755-05-1
trans-Bicyclo[3.3.0]octane	C_8H_{14}	5597-89-7
cis-Bicyclo[4.2.0]octane	C_8H_{14}	28282-35-1
Bicyclo[2.2.2]octene-2	C_8H_{12}	931-64-6
Bicyclopentyl	$C_{10}H_{18}$	1636-39-1
1-Bicyclo[2.1.0]pentyl cyanide	C_6H_7N	31357-71-8
Bicyclo[3.3.3]undecane	$C_{11}H_{20}$	29415-95-0
Biferrocenium triiodide	$C_{20}H_{16}Fe_2I_3$	39470-17-2
2,2′-Biindanyl	$C_{18}H_{18}$	39060-95-2
2,2′-Binaphthyl	$C_{20}H_{14}$	612-78-2
β,β'-Binaphthyl	$C_{20}H_{14}$	612-78-2
β,β'-Binaphthyl picric acid	$C_{26}H_{17}N_3O_7$	72454-45-6
p,p′-Biphenol	$C_{12}H_{10}O_2$	92-88-6
Biphenyl	$C_{12}H_{10}$	92-52-4
Biphenyl-d_{10}	$C_{12}D_{10}$	1486-01-7
[1,1′-Biphenyl]-2-amine	$C_{12}H_{11}N$	90-41-5
17-[([1,1′-Biphenyl]-4-ylcarbonyl)oxy]-(17α)-19-norpregn-4-en-20-yn-3-one	$C_{33}H_{34}O_3$	71203-40-2
Bis-[N-(1-acetyl-2-propylidene) (2-pyridylmethyl)amine]iron(III)phosphorus hexafluoride	$C_{22}H_{26}F_6FeN_3O_2P$	90790-59-3
Bis-(*o*-aminophenyl)-2,2′-dibenzimidazole oxide	$C_{26}H_{20}N_6O$	25829-64-5
Bis-(*o*-aminophenyl)-2,2′-dibenzimidazole oxide, intermediate polymer	$(C_{34}H_{22}N_6O_3)_n$	56592-63-3
Bis-(4-aminophenyl)ether	$C_{12}H_{12}N_2O$	101-80-4
Bis(4-aminophenyl)methane	$C_{13}H_{14}N_2$	101-77-9
1,3-Bis[5-(*o*-aminophenyl)-1,2,4-triazole-3-yl]benzene	$C_{16}H_{18}N_8$	31688-47-8
Bis(benzene)chromium	$C_{12}H_{10}Cr$	1271-54-1
Bis(benzene)chromium bromide	$C_{12}H_{12}CrBr$	11078-20-9
Bis(benzene)chromium chloride	$C_{12}H_{12}CrCl$	11078-19-6
Bis(benzene)chromium iodide	$C_{12}H_{12}CrI$	12089-29-1
Bis-(2,2′-bi-5-methyl-2-thiazoline)diisothiocyanato iron(II)	$C_{18}H_{24}FeN_6S_6$	67903-91-7
Bis(biphenyl)chromium iodide	$C_{24}H_{20}CrI$	12099-17-1
trans-Bis[1,2-bis(diethylphosphino)ethane] diiodochromium(II)	$C_{20}H_{48}CrI_2P_4$	124858-26-0
Bis-(2,2′-bi-2-thiazoline)diisoselenocyanato iron(II) selenoisocyanato iron (II)	$C_{14}H_{16}FeN_6S_4Se_2$	67903-90-6
Bis-(2,2′-bi-2-thiazoline)diisothiocyanato iron(II)	$C_{14}H_{16}FeN_6S_6$	60105-57-9
2,2-Bis(bromomethyl)-1,3-dibromopropane	$C_5H_8Br_4$	3229-00-3
3,3-Bis(4-carboxyphenyl)phthalide dihydrazide	$C_{16}H_{18}N_4O_4$	19261-73-5
2,2-Bis(chloromethyl)-1,3-dichloropropane	$C_5H_8Cl_4$	3228-99-7
3,3-Bis-(chloromethyl)oxacyclobutane	$C_5H_8Cl_2O$	78-71-7
3,3-Bis-(chloromethyl)polyoxacyclobutane	$(C_5H_8Cl_2O)_n$	25323-58-4
2,2-Bis-(4-cyanatophenyl)propane	$C_{17}H_{14}N_2O_2$	1156-51-0
Bis(cyclohexylmethyl)cyclohexane	$C_{20}H_{36}$	unavailable
Bis(cyclopentane)-2,2-dimethylbutane adduct	$C_{22}H_{48}$	unavailable
Bis-decylammonium tetrachlorocadmium	$C_{20}H_{48}CdCl_4N_2$	53188-91-3
1,2-Bis(difluoramino)propane	$C_3H_6F_4N_2$	15403-25-3
1,1-Bis(dimethylcyclohexyl)ethane	$C_{18}H_{34}$	unavailable
Bis(N,N-dimethyldithiocarbamato) iron(III) bromide	$C_6H_{12}BrFeN_2S_4$	23672-37-0
Bis[dimethyl(ethylenedithio)diselenadithiafulvalene} dicyanoaurate(I)	$C_{22}H_{22}AuN_2S_8Se_4$	110321-46-3
Bis-(dimethylthiocarbamoyl)disulfide	$C_6H_{12}N_2S_4$	137-26-8
Bis-(dimethylthiocarbamoyl)sulfide	$C_6H_{12}N_2S_3$	97-74-7
1,4-Bis(diphenylphosphino)butane	$C_{28}H_{28}P_2$	7688-25-7
Bis(dodecylammonium) tetrachlorocadmate (II)	$C_{24}H_{56}CdCl_4N_2$	79001-08-6
Bis(dodecylammonium) tetrachloromanganate (II)	$C_{24}H_{56}Cl_4MnN_2$	75899-75-2
Bis(dodecylammonium) tetrachlorozincate (II)	$C_{24}H_{56}Cl_4N_2Zn$	57947-14-3
Bis(2-ethoxyethyl) ether	$C_8H_{18}O_3$	112-36-7
Bis(ethylbenzene)chromium	$C_{16}H_{20}Cr$	12212-68-0
1,1-Bis(ethylcyclohexyl)ethane	$C_{18}H_{34}$	98803-07-7
Bis(ethylcyclohexyl)methane	$C_{17}H_{32}$	98028-64-0
Bis(2-ethylhexyl)azelate	$C_{25}H_{48}O_4$	103-24-1
Bis(2-ethylhexyl)nonadioate	$C_{25}H_{48}O_4$	103-24-1
Bis(2-ethylhexyl)phthalate	$C_{24}H_{38}O_4$	117-81-7
2,2-Bis(fluoromethyl)-1,3-difluoropropane	$C_5H_8F_4$	338-23-8
Bis(*n*-heptylammonium) tetrachlorocadmate	$C_{14}H_{36}CdCl_4N_2$	88353-51-0
Bis(*n*-heptylammonium) tetrachloromanganate	$C_{14}H_{36}Cl_4MnN_2$	63441-99-0
4,4′-Bis(*n*-heptyloxy)axoxybenzene	$C_{26}H_{38}N_2O_3$	2635-26-0
Bis-hexadecylammonium tetrachlorocadmium	$C_{32}H_{72}CdCl_4N_2$	98394-09-1
Bis-hexadecylammonium tetrachlorocadmate	$C_{32}H_{72}CdCl_4N_2$	98394-09-1
Bis-hydroxyethylpiperazine	$C_8H_{18}N_2O_2$	122-96-3
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane	$C_5H_{12}O_4$	115-77-5
2,2-Bis(hydroxymethyl)propionic acid	$C_5H_{10}O_4$	4767-03-7
2,2-Bis(iodomethyl)-1,3-diiodopropane	$C_5H_8I_4$	1522-88-9
1,3-Bis-(1-isocyanato-1-methylethyl)benzene	$C_{14}H_{16}N_2O_2$	2778-42-9
1,4-Bis-(1-isocyanato-1-methylethyl)benzene	$C_{14}H_{16}N_2O_2$	2778-41-8
Bis(isopropylbenzene)chromium	$C_{18}H_{24}Cr$	38744-20-0
Bis-(4-(N-maleicimido)phenyl)methane	$C_{21}H_{14}N_2O_4$	unavailable
Bis(mesitylene)chromium iodide	$C_{18}H_{24}CrI$	12148-59-1
N,N′-Bis(*m*-methoxyphenyl) terephthalamide	$C_{22}H_{20}N_2O_4$	6957-81-0
N,N′-Bis(*p*-methoxyphenyl) terephthalamide	$C_{22}H_{20}N_2O_4$	7144-15-7
Bis[N-(3-methoxysalicylidene)isopropylamine] nickel (II)	$C_{22}H_{28}N_2NiO_4$	39277-14-0
Bis(methylammonium) hexabromotellurate (IV)	$C_2H_{12}Br_6N_2Te$	67143-09-1
Bis(methylammonium) hexachloroplatinate	$C_2H_{12}Cl_6N_2Pt$	58204-00-5
Bis(methylammonium) hexachlorotellurate	$C_2H_{12}Cl_6N_2Te$	40937-40--
Bis(methylammonium) hexaiodotellurate	$C_2H_{12}I_6N_2Te$	67194-30-1
Bis(methylammonium-d_6) hexachlorostannate (IV)	$C_2D_{12}Cl_6N_2Sn$	114481-22-0
1,2-Bis(methyldiallylammonium)ethane dibromide	$C_{16}H_{34}N_2$	51523-43--
Bis(3-methylpentane-2,4-dionato)copper(II)	$C_{12}H_{18}CuO_4$	14781-49-8
Bismuth triphenyl	$C_{18}H_{15}Bi$	603-33-8
Bis(nitrato)(1,4,8,11-tetraazacyclotetradecane) copper (II)	$C_{10}H_{24}N_4 \cdot Cu(NO_3)_2$	73746-94-8
Bis-(4-nitrophenyl) ether	$C_{12}H_8N_2O_5$	101-63-3
Bis(octadecylammonium) cadmium tetrachloride	$C_{36}H_{80}CdCl_4N_2$	90836-90-1
Bis-octylammonium tetrachlorocadmium	$C_{16}H_{40}CdCl_4N_2$	98394-08-2
N,N′-Bis(4-*n*-octyloxybenzal)-1,4-phenylenediamine	$C_{36}H_{48}N_2O_2$	29273-90-3

Bis-pentylammonium tetrachlorozincate	$C_{10}H_{22}Cl_4N_2Zn$	73180-46-8
Bis(1,10-phenanthroline-2-carbaldehyde-phenylhydrazone) iron (II) diperchlorate	$C_{38}H_{28}Cl_2O_4Ni$	108224-19-7
Bis(1,10-phenanthroline-2-carbaldehydephenylhydrazone) iron (II) ditetrafluoroborate	$C_{38}H_{28}B_2F_8FeN_8$	53261-61-3
2,2-Bis(phenyl-4-glycidoxy)propane	$C_{21}H_{24}O_4$	500008-19-5
1,4-Bis(phenylglyoxaloyl)benzene	$C_{22}H_{14}O_4$	3363-97-1
Bis-(3-phthalyl anhydride) ether	$C_{16}H_6O_7$	1823-59-2
Bis-(3-phthalyl anhydride) sulfone	$C_{16}H_6O_8S$	2421-28-5
Bis-(3-phthalyl anhydride) ketone	$C_{17}H_6O_7$	2540-99-0
Bis(propylammonium) tetrachloroplumbate(II)	$C_6H_{20}Cl_4N_2Pb$	120015-72-7
Bis(pyridine)copper bromide	$C_{10}H_{10}Br_2CuN_2$	6845-03-0
Bis(pyridine)copper chloride	$C_{10}H_{10}Cl_2CuN_2$	13408-58-7
Bis-(pyridine)silicon tetrachloride	$C_{10}H_{10}Cl_4N_2Si$	17731-26-9
Bis-(tetra-*n*-butylammonium) *m*-phthalate clathrate hydrate	$C_{40}H_{76}N_2O_4 \cdot 61H_2O$	123227-97-4
Bis-(tetra-*n*-butylammonium) *o*-phthalate clathrate hydrate	$C_{40}H_{76}N_2O_4 \cdot 62H_2O$	123227-96-3
Bis-(tetra-*n*-butylammonium) *p*-phthalate clathrate hydrate	$C_{40}H_{76}N_2O_4 \cdot 63H_2O$	123227-98-5
Bis-(tetradecylammonium) zinc tetrachloride	$C_{28}H_{32}Cl_4N_2Zn$	73170-02-2
Bis-(tetraethylammonium) tetrachloronickelate	$C_{16}H_{40}Cl_4N_2Ni$	5964-71-6
Bis-(tetraethylammonium) tetrachlorozincate	$C_{16}H_{40}Cl_4N_2Zn$	5964-74-9
Bis-(tetrafluoropropyl)carbonate	$C_7H_6F_8O_3$	1422-70-4
Bis-(tetramethylammonium iodide) tridecasilver iodide	$C_8H_{24}Ag_{13}I_{15}N_2$	56685-61-1
Bis-(tetramethylammonium) tetrabromocuprate	$C_8H_{24}Br_4CuN_2$	15692-22-5
Bis-(tetramethylammonium) tetrachloroferrate	$C_8H_{24}Cl_4FeN_2$	15649-95-3
Bis-(tetramethylammonium) tetrachloromanganate	$C_8H_{24}Cl_4MnN_2$	16594-83-5
Bis-(tetramethylammonium) tetrachlorozincate	$C_8H_{24}Cl_4N_2Zn$	14240-97-2
Bis-(tetramethylammonium) tetraiodocadmate	$C_8H_{24}CdI_4N_2$	37753-91-6
1,4-Bis-(2,2,6,6-tetramethyl-4-oxy-1-oxylpiperidyl)butadiyne	$C_{22}H_{36}N_2O_4$	14306-88-8
Bis(toluene)chromium iodide	$C_{14}H_{16}CrI$	12087-59-1
1,4-Bis(triallylammonium)butene-2-dibromide	$C_{22}H_{38}Br_2N_2$	51523-45-6
1,2-Bis(triallylammonium)ethane dibromide	$C_{20}H_{36}Br_2N_2$	51523-42-3
1,3-Bis(triallylammonium)propane dibromide	$C_{21}H_{38}Br_2N_2$	51523-44-5
1,4-Bis(triethylammonium)butane dibromide	$C_{16}H_{38}Br_2N_2$	1067-62-5
1,10-Bis(triethylammonium)decane dibromide	$C_{22}H_{50}Br_2N_2$	51523-41-2
1,2-Bis(triethylammonium)ethane dibromide	$C_{14}H_{34}Br_2N_2$	10238-71-8
1,6-Bis(triethylammonium)hexane dibromide	$C_{18}H_{42}Br_2N_2$	7072-43-7
1,8-Bis(triethylammonium)octane dibromide	$C_{20}H_{46}Br_2N_2$	51523-40-1
1,5-Bis(triethylammonium)pentane dibromide	$C_{17}H_{40}Br_2N_2$	7128-82-7
1,3-Bis(triethylammonium)propane dibromide	$C_{15}H_{36}Br_2N_2$	7072-41-5
Bis(2,4,6-trimethylcyclohexyl)methane	$C_{19}H_{36}$	unavailable
1,3-Bis(trimethylsilyl)propane	$C_9H_{24}Si_2$	2295-05-8
Bis(*m*-xylene)chromium iodide	$C_{16}H_{20}CrI$	35165-78-7
2,2′-Bitetralin	$C_{20}H_{22}$	27426-98-8
Biuret	$C_2H_5N_3O_2$	108-19-0
Bovine chymotrypsinogen A, anhydrous	$C_{1077}H_{1736}N_{304}O_{343}S_{12}$	9035-75-0
Bovine chymotrypsinogen A, hydrated	$C_{1077}H_{1736}N_{304}O_{343}S_{12}$	9035-75-0
Bovine zinc insulin, anhydrous	$C_{508}H_{752}N_{130}O_{150}S_{12}Zn$	11070-73-8
Bovine zinc insulin, hydrated	$C_{508}H_{752}N_{130}O_{150}S_{12}Zn$	11070-73-8
Bromobenzene	C_6H_5Br	108-86-1
2-Bromobenzoic acid	$C_7H_5BrO_2$	88-65-3
3-Bromobenzoic acid	$C_7H_5BrO_2$	585-76-2
4-Bromobenzoic acid	$C_7H_5BrO_2$	586-76-5
Bromo bis(N,N-diethyldithiocarbamate) iron (III)	$C_{10}H_{20}BrFeN_2S_4$	54163-77-8
1-Bromobutane	C_4H_9Br	109-65-9
1-Bromo-2-chloroethane	C_2H_4BrCl	107-04-0
1-Bromo-2-chloro-1,1,2-trifluoroethane	$C_2HBrClF_3$	354-06-3
2-Bromo-2-chloro-1,1,1-trifluoroethane	$C_2HBrClF_3$	151-67-7
Bromocyclohexane	$C_6H_{11}Br$	108-85-0
Bromoethane	C_2H_5Br	74-96-4
Bromoethene	C_2H_3Br	593-60-2
Bromoform	$CHBr_3$	75-25-2
1-Bromoheptane	$C_7H_{15}Br$	629-04-9
1-Bromohexane	$C_6H_{13}Br$	111-25-1
2-Bromoiodobenzene	C_6H_4BrI	583-55-1
3-Bromoiodobenzene	C_6H_4BrI	591-18-4
4-Bromoiodobenzene	C_6H_4BrI	589-87-7
Bromomethane	CH_3Br	74-83-9
1-Bromo-3-methylbutane	$C_5H_{11}Br$	107-82-4
1-Bromo-2-methylpropane	C_4H_9Br	78-77-3
2-Bromo-2-methylpropane	C_4H_9Br	507-19-7
2-Bromonaphthalene	$C_{10}H_7Br$	580-13-2
Bromopentafluorobenzene	C_6BrF_5	344-04-7
1-Bromopentane	$C_5H_{11}Br$	110-53-2
4-Bromophenol	C_6H_5BrO	106-41-2
1-Bromopropane	C_3H_7Br	106-94-5
2-Bromopropane	C_3H_7Br	75-26-3
2-Bromothiophene	C_4H_3BrS	1003-09-4
Bromotrichloromethane	$CBrCl_3$	75-62-7
Bromotrifluoromethane	$CBrF_3$	75-63-8
Bullvalene	$C_{10}H_{10}$	1005-51-2
1,2-Butadiene	C_4H_6	590-19-2
1,3-Butadiene	C_4H_6	106-99-0
Butadiene-propylene copolymer	$(C_7H_{12})_n$	24991-43-3
Butanal	C_4H_8O	123-72-8
n-Butane	C_4H_{10}	106-97-8
1,4-Butanediamide	$C_4H_8N_2O_2$	110-14-5
1,4-Butanedinitrile	$C_4H_4N_2$	110-61-2
1,4-Butanedioic acid	$C_4H_6O_4$	110-15-6
1,3-Butanediol	$C_4H_{10}O_2$	107-88-0
1,4-Butanediol	$C_4H_{10}O_2$	110-63-4
2,3-Butanediol	$C_4H_{10}O_2$	513-85-9
Butanenitrile	C_4H_7N	109-74-0
1,2,3,4-Butanetetrol	$C_4H_{10}O_4$	149-32-6
1-Butanethiol	$C_4H_{10}S$	109-79-5
2-Butanethiol	$C_4H_{10}S$	513-53-1
Butanoic acid	$C_4H_8O_2$	107-92-6
1-Butanol	$C_4H_{10}O$	71-36-3
2-Butanol	$C_4H_{10}O$	78-92-2
Butanone	C_4H_8O	78-93-3
Butanoyl chloride	C_4H_7ClO	141-75-3
2-Butenal	C_4H_6O	123-73-9
1-Butene	C_4H_8	106-98-9
cis-2-Butene	C_4H_8	590-18-1
trans-2-Butene	C_4H_8	624-64-6
cis-2-Butenedioic acid	$C_4H_4O_4$	110-16-7
trans-2-Butenedioic acid	$C_4H_4O_4$	110-17-8
1-Butene polysulfone	$(C_4H_8O_2S)_n$	25104-10-3
2-*n*-Butoxy-1-ethanol	$C_6H_{14}O_2$	111-76-2
1-*n*-Butoxy-2-methoxyethane	$C_7H_{16}O_2$	500005-29-8
2-*n*-Butoxyethanol	$C_6H_{14}O_2$	111-76-2
2-(2-Butoxyethoxy)ethanol	$C_8H_{18}O_3$	112-34-5
N-*n*-Butylacetamide	$C_6H_{13}NO$	1119-49-9
N-*tert*-Butylacetamide	$C_6H_{13}NO$	762-84-5
n-Butyl acetate	$C_6H_{12}O_2$	123-86-4
tert-Butyl acetate	$C_6H_{12}O_2$	540-88-5

Butyl acrylate	$C_7H_{12}O_2$	141-32-2
n-Butyl alcohol	$C_4H_{10}O$	71-36-3
sec-Butyl alcohol	$C_4H_{10}O$	78-92-2
tert-Butyl alcohol	$C_4H_{10}O$	75-65-0
tert-Butylaldehyde	$C_5H_{10}O$	630-19-3
n-Butylamine	$C_4H_{11}N$	109-73-9
tert-Butylamine	$C_4H_{11}N$	75-64-9
tert-Butylammonium perchlorate	$C_4H_{12}ClNO_4$	18720-49-5
n-Butylbenzene	$C_{10}H_{14}$	104-51-8
sec-Butylbenzene	$C_{10}H_{14}$	135-98-8
tert-Butylbenzene	$C_{10}H_{14}$	98-06-6
n-Butyl bromide	C_4H_9Br	109-65-9
tert-Butyl bromide	C_4H_9Br	507-19-7
Butyl butanoate	$C_8H_{16}O_2$	109-21-7
Butylchloral	$C_4H_5Cl_3O$	76-36-8
n-Butyl chloride	C_4H_9Cl	109-69-3
sec-Butyl chloride	C_4H_9Cl	78-86-4
tert-Butyl chloride	C_4H_9Cl	507-20-0
tert-Butyl cyanide	C_5H_9N	630-18-2
n-Butylcyclohexane	$C_{10}H_{20}$	1678-93-9
tert-Butylcyclohexane	$C_{10}H_{20}$	3178-22-1
17-[3-(4-Butylcyclohexyl)-1-oxopropoxy]-17α, 17(trans)-19-norpregn-4-en-20-yn-3-one	$C_{33}H_{48}O_3$	71203-38-8
n-Butylcyclopentane	C_9H_{18}	2040-95-1
α-*n*-Butyldecalin	$C_{14}H_{26}$	92369-80-7
α-*sec*-Butyldecalin	$C_{14}H_{26}$	92369-82-9
tert-Butyldecalin	$C_{14}H_{26}$	27193-30-2
1,4-Butylene glycol-ethylene glycol-adipic acid oligomer	$C_{12}H_{22}O_6$	26570-73-0
N-*n*-Butylethanamide	$C_6H_{13}NO$	1119-49-9
n-Butyl ethanoate	$C_6H_{12}O_2$	123-86-4
Butyl *p*-(*p*-ethoxyphenoxycarbonyl) phenylcarbonate	$C_{20}H_{22}O_6$	16494-24-9
tert-Butylethylene	C_6H_{12}	558-37-2
tert-Butyl ethyl ether	$C_6H_{14}O$	637-92-3
Butylglycol	$C_6H_{14}O_2$	111-76-2
n-Butyl iodide	C_4H_9I	542-69-8
sec-Butyl iodide	C_4H_9I	513-48-4
n-Butyl mercaptan	$C_4H_{10}S$	109-79-5
sec-Butyl mercaptan	$C_4H_{10}S$	513-53-1
tert-Butyl mercaptan	$C_4H_{10}S$	75-66-1
Butyl methacrylate	$C_8H_{14}O_2$	97-88-1
n-Butyl methanoate	$C_5H_{10}O_2$	592-84-7
Butyl 2-methyl-2-propenoate	$C_8H_{14}O_2$	97-88-1
n-Butyl methyl sulfide	$C_5H_{12}S$	628-29-5
5-Butyl-5-nonanol	$C_{13}H_{28}O$	597-93-3
Butyl octadecanoate	$C_{12}H_{24}O_2$	123-95-5
Butyl ester of pentanoic acid	$C_9H_{18}O_2$	591-68-4
tert-Butyl peroxybenzoate	$C_{11}H_{14}O_3$	614-45-9
Butyl silicate	$C_{16}H_{36}O_4Si$	4766-57-8
Butylurea	$C_5H_{12}N_2O$	592-31-4
tert-Butylurea	$C_5H_{12}N_2O$	1118-12-3
1-Butyne	C_4H_6	107-00-6
2-Butyne	C_4H_6	503-17-3
n-Butyraldehyde	C_4H_8O	123-72-8
n-Butyric acid	$C_4H_8O_2$	107-92-6
γ-Butyrolactone	$C_4H_6O_2$	96-48-0
Butyryl chloride	C_4H_7ClO	141-75-3

C

Cadmium dimethyl	C_2H_6Cd	506-82-1
Cadmium(II) *n*-dodecanoate	$C_{24}H_{46}O_4Cd$	2605-44-9
Cadmium(II) *n*-hexadecanoate	$C_{32}H_{62}O_4Cd$	6427-86-7
Cadmium(II) *n*-octadecanoate	$C_{36}H_{70}O_4Cd$	2223-93-0
Cadmium(II) *n*-tetradecanoate	$C_{28}H_{54}O_4Cd$	10196-67-5
Caffeine	$C_8H_{10}N_4O_2$	58-08-2
Caffeine, anhydrous	$C_8H_{10}N_4O_2$	58-08-2
Calcium oxalate monohydrate	$C_2CaO_4 \cdot H_2O$	5794-28-5
Camphor	$C_{10}H_{16}O$	76-22-2
Camphor(D)	$C_{10}H_{16}O$	464-49-3
Camphor(DL)	$C_{10}H_{16}O$	21368-68-3
Cane sugar	$C_{12}H_{22}O_{11}$	57-50-1
Capraldehyde	$C_{10}H_{20}O$	112-31-2
Capric acid	$C_{10}H_{20}O_2$	334-48-5
Capric aldehyde	$C_{10}H_{20}O$	112-31-2
n-Caproic acid	$C_6H_{12}O_2$	142-62-1
6-Caprolactam	$C_6H_{11}NO$	105-60-2
ϵ-Caprolactam	$C_6H_{11}NO$	105-60-2
6-Caprolactone	$C_6H_{10}O_2$	502-44-3
ϵ-Caprolactone	$C_6H_{10}O_2$	502-44-3
Capryl alcohol	$C_8H_{18}O$	111-87-5
Caprylaldehyde	$C_8H_{16}O$	124-13-0
Caprylene	C_8H_{16}	111-66-0
Caprylic acid	$C_8H_{16}O_2$	124-07-2
Carbamylurea	$C_2H_5N_3O_2$	108-19-0
Carbazole	$C_{12}H_9N$	86-74-8
Carbazole-1,3,5-trinitrobenzene adduct	$C_{18}H_{12}N_4O_6$	6268-68--
4-Carbomethoxyhomocubane	$C_{11}H_{12}O_2$	40317-63-1
Carbon	C	7440-44-0
Carbon, baked	C	7440-44-0
Carbon, diamond	C	7782-40-3
Carbon diselenide	CSe_2	506-80-0
Carbon disulfide	CS_2	75-15-0
Carbon, glassy	C	7440-44-0
Carbon, GPCO graphite	C	7782-42-5
Carbon, graphite	C	7782-42-5
Carbon, graphite, single-crystal	C	7782-42-5
Carbon, irradiated graphite	C	7782-42-5
Carbon, natural graphite	C	7782-42-5
Carbon, pyrolytic graphite	C	7782-42-5
Carbon tetrabromide	CBr_4	558-13--
Carbon tetrachloride	CCl_4	56-23-5
Carbon tetrafluoride	CF_4	75-73-0
Carbonyl chloride	CCl_2O	75-44-5
Carbonyl sulfide	COS	463-58-
Carbisopropoxy methyl methacrylate	$C_9H_{14}O_4$	23684-11-9
m-Carborane	$C_2H_{12}B_{10}$	16986-24-0
1,7-Carborane-12	$C_2H_{12}B_{10}$	16986-24-0
4-Carboxypentacyclo [4.3.0.0^{2,5}.0^{3,8}.0^{4,7}] nonane	$C_{10}H_{10}O_2$	15844-05-0
Carvoxime(DL)	$C_{10}H_{15}NO$	22327-39-5
Carvoxime(L)	$C_{10}H_{15}NO$	2244-16--
Castor oil	$C_{18}H_{34}O_3$	8001-79--
Catechol	$C_6H_6O_2$	120-80-9
Cellulose nitrate	$(C_6H_8N_2O_9)_n$	9004-70-0
Cerium isothiocyanate heptahydrate	$C_3CeN_3S_3 \cdot 7H_2O$	16648-21-8
Cerium(III) oxalate	$C_6O_{12}Ce_2$	13266-83-0
Cesium butyrate	$C_4H_7CsO_2$	38869-25-9
Cesium propionate	$C_3H_5CsO_2$	38869-24-8
Cetane	$C_{16}H_{34}$	50-81-7
n-Cetyl alcohol	$C_{16}H_{34}O$	36653-82--
Chloral	C_2HCl_3O	75-87-0
Chloranil	$C_6Cl_4O_2$	118-75-2
p-Chloranil potassium	$C_6Cl_4KO_2$	21136-28-7
Chloroacetic acid	$C_2H_3ClO_2$	79-11-8
2-Chloroadamantane	$C_{10}H_{15}Cl$	7346-41-0
m-Chloroaniline	C_6H_6ClN	108-42-9
p-Chloroaniline	C_6H_6ClN	106-47-8
2-Chloroanthraquinone	$C_{14}H_7ClO_2$	131-09-9
Chlorobenzene	C_6H_5Cl	108-90-7
2-Chlorobenzoic acid	$C_7H_5ClO_2$	118-91-2
3-Chlorobenzoic acid	$C_7H_5ClO_2$	535-80-8
4-Chlorobenzoic acid	$C_7H_5ClO_2$	74-11-3
2-Chlorobiphenyl	$C_{12}H_9Cl$	2051-60-7
4-Chlorobiphenyl	$C_{12}H_9Cl$	2051-62-9
Chlorobis(N,N-dimethyldithiocarbamate) iron(III)	$C_6H_{12}ClFeN_2S_4$	14879-21-1
2-Chlorobromobenzene	C_6H_4BrCl	694-80-4
3-Chlorobromobenzene	C_6H_4BrCl	108-37-2
4-Chlorobromobenzene	C_6H_4BrCl	106-39-8
1-Chlorobutane	C_4H_9Cl	109-69-3
2-Chlorobutane	C_4H_9Cl	78-86-4

cis-3-Chloro-2-butenoic acid	$C_4H_5ClO_2$	55831-56-6
trans-3-Chloro-2-butenoic acid	$C_4H_5ClO_2$	6214-28-4
β-Chlorocrotonic acid	$C_4H_5ClO_2$	55831-56-6
Chlorocyclopentane	C_5H_9Cl	930-28-9
Chlorodifluoromethane	$CHClF_2$	75-45-6
7-Chloro-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one	$C_{15}H_{11}ClN_2O$	1088-11-5
2-Chloro-9-(3-dimethylaminopropylidene)-10-thioxanthene(Z)	$C_{18}H_{18}ClNS$	113-59-7
2-Chloro-9-(3-dimethylaminopropyl)-10-phenothiazine hydrochloride	$C_{17}H_{20}Cl_2N_2S$	69-09-0
4-Chloro-1,3-dioxolan-2-one	$C_4H_5ClO_3$	3967-54-2
Chloroethane	C_2H_5Cl	75-00-3
Chloroethyl methacrylate	$C_6H_9ClO_2$	1888-94-4
Chloroform	$CHCl_3$	67-66-3
1-Chloroheptane	$C_7H_{15}Cl$	629-06-1
1-Chlorohexane	$C_6H_{13}Cl$	544-10-5
β-Chloroisocrotonic acid	$C_4H_5ClO_2$	6214-28-4
2-Chloroisonitrosoacetanilide	$C_8H_7ClN_2O_2$	14722-82-8
Chloromethane	CH_3Cl	74-87-3
2-Chloro-4-(methoxymethyl)-6-methyl-5-nitro-3-pyridinecarbonitrile	$C_9H_8ClN_3O_3$	719-48-2
1-Chloro-3-methylbutane	$C_5H_{11}Cl$	107-84-6
4-Chloromethyl-1,3-dioxolan-2-one	$C_5H_7ClO_3$	2463-45-8
1-Chloro-2-methylpropane	C_4H_9Cl	513-36-0
2-Chloro-2-methylpropane	C_4H_9Cl	507-20-0
1-Chloronaphthalene	$C_{10}H_7Cl$	90-13-1
2-Chloronaphthalene	$C_{10}H_7Cl$	91-58-7
1-Chloro-2-nitrobenzene	$C_6H_4ClNO_2$	88-73-3
2-Chloro-2-nitropropane	$C_3H_6ClNO_2$	594-71-8
1-Chlorooctadecane	$C_{18}H_{37}Cl$	3386-33-2
1-Chlorooctane	$C_8H_{17}Cl$	111-85-3
1-Chloro-1,1,3,3,3-pentafluoropropane	$C_3H_2ClF_5$	76-15-3
Chloropentamethylbenzene	$C_{11}H_{15}Cl$	5153-39-9
1-Chloropentane	$C_5H_{11}Cl$	543-59-9
2-Chlorophenol	C_6H_5ClO	95-57-8
3-Chlorophenol	C_6H_5ClO	108-43-0
4-Chlorophenol	C_6H_5ClO	106-48-9
m-Chlorophenylisocyanate	C_7H_4ClNO	2909-38-8
p-Chlorophenylisocyanate	C_7H_4ClNO	104-12-1
17-[6-(4-Chlorophenyl)-1-oxohexyl]oxy-(17*α*)-19-norpregn-4-en-20-yn-3-one	$C_{32}H_{39}ClO_3$	71203-42-4
1-Chloropropane	C_3H_7Cl	540-54-5
3-Chloropropene-1	C_3H_5Cl	107-05-1
2-Chlorothiophene	C_4H_3ClS	96-43-5
α-Chlorotoluene	C_7H_7Cl	100-44-7
2-chloro-6-(trichloromethyl)pyridine	$C_6H_3Cl_4N$	1929-82-4
Chlorotrifluoroethene	C_2ClF_3	79-38-9
Chlorotrifluoroethylene	C_2ClF_3	79-38-9
Chlorotrimethylsilane	C_3H_9ClSi	75-77-4
Chlorpromazine hydrochloride	$C_{17}H_{20}Cl_2N_2S$	69-09-0
Chlorprothixene	$C_{18}H_{18}ClNS$	113-59-7
Cholesterol	$C_{27}H_{46}O$	57-88-5
Cholesteryl myristate	$C_{41}H_{72}O_2$	1989-52-2
Cholesteryl oleate	$C_{45}H_{78}O_2$	303-43-5
Cholesteryl palmitate	$C_{43}H_{76}O_2$	601-34-3
Cholesteryl stearate	$C_{45}H_{80}O_2$	35602-69-8
Chroman	$C_9H_{10}O$	493-08-3
Chromium acetylacetonate	$C_{15}H_{21}CrO_6$	21679-31-2
Chromocene	$C_{10}H_{10}Cr$	1271-24-5
Chromone	$C_9H_6O_2$	491-38-3
Cinnamic acid	$C_9H_8O_2$	140-10-3
Citral	$C_{10}H_{16}O$	55-52-7
Citric acid	$C_6H_8O_7$	77-92-9
Citric acid monohydrate	$C_6H_8O_7 \cdot H_2O$	5949-29-1
Citrulline(DL)	$C_6H_{13}N_3O_3$	627-77-0
Cobaltocene	$C_{10}H_{10}Co$	1277-43-6
2,4,6-Collidine	$C_8H_{11}N$	108-75-8
Congressane	$C_{14}H_{20}$	2292-79-7
Copper acetylacetonate	$C_{10}H_{14}CuO_2$	13395-16-9
Copper benzylacetylenide	C_9H_7Cu	66582-10-3
Copper butylacetylenide	C_6H_9Cu	33589-44-5
Copper (II) formate tetradeuterate	$C_2H_2CuO_4 \cdot 4D_2O$	21774-43-6
Copper (II) formate tetrahydrate	$C_2H_2CuO_4 \cdot 4H_2O$	5893-61-8
Copper phenylacetylenide	C_8H_5Cu	13146-23-1
Copper phenylethynylacetylenide	$C_{10}H_5Cu$	65792-84-9
Copper vinylacetylenide	C_4H_3Cu	5256-77-9
Coriandrol	$C_{10}H_{18}O$	126-90-9
Coriandrol(L)	$C_{10}H_{18}O$	126-90-9
Coronene	$C_{24}H_{12}$	191-07-1
Coumaran	C_8H_8O	496-14-0
Coumarin	$C_9H_6O_2$	91-64-5
Creatine	$C_4H_9N_3O_2$	6020-87-7
Creatine hydrate	$C_4H_9N_3O_2 \cdot H_2O$	57-00-1
Creatinine	$C_4H_7N_3O$	60-27-5
m-Cresol	C_7H_8O	108-39-4
o-Cresol	C_7H_8O	95-48-7
p-Cresol	C_7H_8O	106-44-5
Crotonaldehyde	C_4H_6O	4170-30-3
Cubane	C_8H_8	277-10-1
Cumene	C_9H_{12}	98-82-8
p-*α*-Cumylphenol	$C_{15}H_{16}O$	599-64-4
Cyanamid	CH_2N_2	156-62-7
Cyanoacetamide	$C_3H_4N_2O$	107-91-5
1-Cyanobicyclo[1.1.0]butane	C_5H_5N	16955-35-4
1-Cyanobicyclo[2.2.1]heptane	$C_8H_{11}N$	103434-09-9
2-Cyanobicyclo[2.2.1]heptane(endo)	$C_8H_{11}N$	3211-87-8
2-Cyanobicyclo[2.2.1]heptane(exo)	$C_8H_{11}N$	3211-09-3
1-Cyanobicyclo[3.1.0]hexane	C_7H_9N	31357-72-9
1-Cyanobicyclo[2.1.0]pentane	C_6H_7N	31357-71-8
Cyanocyclobutane	C_5H_7N	4426-11-3
Cyanocyclohexane	$C_7H_{11}N$	766-05-2
Cyanocyclopentane	C_6H_9N	4254-02-8
Cyanocyclopropane	C_4H_5N	5500-21-0
Cyanoethane	C_3H_5N	107-12-0
Cyanoethene	C_3H_3N	107-13-1
Cyanogen	C_2N_2	460-19-5
3-Cyano-4-methoxymethyl-6-methyl-(2-pyridone)	$C_9H_{10}N_2O_2$	6339-38-4
3-Cyano-4-methoxymethyl-5-nitro-6-methyl-(2-pyridone)	$C_9H_9N_3O_4$	6281-75-0
1-Cyano-3-methylenecyclobutane	C_6H_7N	15760-35-7
2-Cyano-2-methylpropane	C_5H_9N	630-18-2
2-Cyanopropane	C_4H_7N	78-82-0
α-Cyanopropionaldehyde	C_4H_5NO	26692-50-2
β-Cyanopropionaldehyde	C_4H_5NO	3515-93-3
Cyanuric acid	$C_3H_3N_3O_3$	108-80-5
Cyclam	$C_{10}H_{24}N_4$	295-37-4
Cyclobutane	C_4H_8	287-23-0
Cyclobutyl cyanide	C_5H_7N	4426-11-3
α-Cyclodextrin	$C_{36}H_{60}O_{30}$	10016-20-3
β-Cyclodextrin	$C_{42}H_{70}O_{35}$	7585-39-9
γ-Cyclodextrin	$C_{48}H_{80}O_{40}$	17465-86-0
β-Cyclodextrin undecahydrate	$C_{42}H_{70}O_{35} \cdot 11H_2O$	85490-99-9
trans,trans,cis-1,5,9-Cyclododecatriene	$C_{12}H_{18}$	706-31-0
Cycloheptaamylose	$C_{42}H_{70}O_{35}$	7585-39-9
Cycloheptaamylose undecahydrate	$C_{42}H_{70}O_{35} \cdot 11H_2O$	85490-99-9
Cycloheptane	C_7H_{14}	291-64-5
Cycloheptane-thiourea adduct	$C_{10}H_{26}N_6S_3$	39822-97-4
Cycloheptanol	$C_7H_{14}O$	502-41-0
Cycloheptatriene	C_7H_8	544-25-2
Cycloheptene	C_7H_{12}	628-92-2
cis-Cycloheptene	C_7H_{12}	45509-99-7
Cyclohexaamylose	$C_{36}H_{60}O_{30}$	10016-20-3
1,3-Cyclohexadiene	C_6H_8	592-57-4
1,4-Cyclohexadiene	C_6H_8	628-41-1
Cyclohexane	C_6H_{12}	110-82-7
Cyclohexane-d_{12}	C_6D_{12}	1735-17-7
cis-Cyclohexane-1,2-dicarboxylic anhydride	$C_8H_{10}O_3$	13149-00-3
1,3-Cyclohexanedione	$C_6H_8O_2$	504-02-9
1,4-Cyclohexanedione	$C_6H_8O_2$	637-88-7

Cyclohexanethiol	$C_6H_{12}S$	1569-69-3
Cyclohexane-thiourea adduct	$C_9H_{24}N_6S_3$	33561-77-2
Cyclohexanol	$C_6H_{12}O$	108-93-0
Cyclohexanone	$C_6H_{10}O$	108-94-1
Cyclohexanone oxime	$C_6H_{11}NO$	100-64-1
(Cyclohexatriene)(cyclopentadienyl) iron(II) hexafluorophosphate	$C_{11}H_{11}F_6FeP$	12176-31-7
Cyclohexene	C_6H_{10}	110-83-8
Cyclohexene oxide	$C_6H_{10}O$	286-20-4
Cyclohexyl alcohol	$C_6H_{12}O$	108-93-0
Cyclohexylbenzene	$C_{12}H_{16}$	827-52-1
17-[(4-Cyclohexylbenzoyl)oxy]-(17α)-19-norpregn-4-en-20-yn-3-one	$C_{33}H_{40}O_3$	71203-41-2
Cyclohexyl bromide	$C_6H_{11}Br$	108-85-0
Cyclohexyl cyanide	$C_7H_{11}N$	766-05-2
Cyclohexyl(ethylcyclohexyl)methane	$C_{15}H_{28}$	66374-71-8
Cyclohexyl(2-ethylcyclohexyl)methane	$C_{15}H_{28}$	66374-71-8
11-Cyclohexylheneicosane	$C_{27}H_{54}$	6703-99-7
Cyclohexyl isocyanide	$C_7H_{11}N$	931-53-3
1-Cyclohexyl-1-isopropylcyclohexylethane	$C_{17}H_{32}$	unavailable
Cyclohexyl(isopropylcyclohexyl)methane	$C_{16}H_{30}$	unavailable
Cyclohexyl mercaptan	$C_6H_{12}S$	1569-69-3
1-Cyclohexyl-3-methylhydroindan	$C_{16}H_{26}$	unavailable
1-Cyclohexyl-1,3,3-trimethylhydroindan	$C_{18}H_{32}$	22236-61-9
Cyclooctaamylose	$C_{48}H_{80}O_{40}$	17465-86-0
Cyclooctadecane	$C_{18}H_{36}$	296-18-4
Cycloocta-1,5-diene	C_8H_{12}	111-78-4
Cyclooctane	C_8H_{16}	292-64-8
Cyclooctane-thiourea adduct	$C_{11}H_{28}N_6S_3$	39822-99-6
Cyclooctatetraene	C_8H_8	629-20-9
Cyclooctene	C_8H_{14}	931-88-4
Cyclopentadiene	C_5H_6	542-92-7
Cyclopentadienyl manganese tricarbonyl	$C_8H_5MnO_3$	12079-65-1
Cyclopentadienyl tricarbonyl manganese	$C_8H_5MnO_3$	120709-65-1
Cyclopentane	C_5H_{10}	287-92-3
Cyclopentanethiol	$C_5H_{10}S$	1679-07-8
Cyclopentanol	$C_5H_{10}O$	96-41-3
Cyclopentene	C_5H_8	142-29-0
Cyclopentylamine	$C_5H_{11}N$	1003-03-8
Cyclopentylbicyclohexyl	$C_{17}H_{30}$	26447-22-3
Cyclopentyl cyanide	C_6H_9N	4254-02-8
Cyclopentyl mercaptan	$C_5H_{10}S$	1679-07-8
Cyclopentyl methyl sulfide	$C_6H_{12}S$	7133-36-0
Cyclopentyl-1-thiaethane	$C_6H_{12}S$	7133-36-0
Cyclopropane	C_3H_6	75-19-4
Cyclopropylamine	C_3H_7N	765-30-0
Cyclopropyl cyanide	C_4H_5N	5500-21-0
Cyclo-di-*p*-xylene	$C_{16}H_{16}$	1633-22-3
Cymantrene	$C_8H_5MnO_3$	12079-65-1
p-Cymene	$C_{10}H_{14}$	99-87-6
Cysteine(L)	$C_3H_7NO_2S$	52-90-4
Cystine(L)	$C_6H_{12}N_2O_4S_2$	56-89-3
Cytosine	$C_4H_5N_3O$	71-30-7

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Decachlorobiphenyl	$C_{12}Cl_{10}$	2051-24-3
Decacyclene	$C_{36}H_{18}$	191-48-0
Decafluorobiphenyl	$C_{12}F_{10}$	434-90-2
Decahydronaphthalene	$C_{10}H_{18}$	91-17-8
cis-Decahydronaphthalene	$C_{10}H_{18}$	91-17-8
trans-Decahydronaphthalene	$C_{10}H_{18}$	493-02-7
Decalin	$C_{10}H_{18}$	91-17-8
cis-Decalin	$C_{10}H_{18}$	493-01-6
trans-Decalin	$C_{10}H_{18}$	493-02-7
Decanal	$C_{10}H_{20}O$	112-31-2
n-Decane	$C_{10}H_{22}$	124-18-5
1-Decanethiol	$C_{10}H_{22}S$	143-10-2
Decanoic acid	$C_{10}H_{20}O_2$	334-48-5
1-Decanol	$C_{10}H_{22}O$	112-30-1
5-Decanol	$C_{10}H_{22}O$	5205-34-5
1-Decene	$C_{10}H_{20}$	872-05-9
1-Decene-urea adduct	$C_{2.3}H_{6.7}N_2O$	24494-58--
n-Decyl alcohol	$C_{10}H_{22}O$	112-30-1
Decylcyanobiphenyl	$C_{23}H_{29}N$	59454-35-7
n-Decylcyclohexane	$C_{16}H_{32}$	1795-16-0
n-Decylcyclopentane	$C_{15}H_{30}$	1795-21-7
11-*n*-Decylheneicosane	$C_{31}H_{64}$	55320-06--
n-Decyl mercaptan	$C_{10}H_{22}S$	143-10-2
Decyl methacrylate	$C_{14}H_{26}O_2$	3179-47-1
Dehydroisophytol	$C_{20}H_{38}O$	29171-23-
Dextrose	$C_6H_{12}O_6$	50-99-7
Diacenaphtho[1,2-j:1′,2′-l]-fluoranthene	$C_{36}H_{18}$	191-48-0
1,2-Diaceto-3-stearin	$C_{25}H_{46}O_6$	26836-44-1
1,7-Diacetoxy-2,4,6-trinitro-2,4,6-triazaheptane	$C_8H_{14}N_6O_{10}$	14173-62-7
p-Diacetylbenzene diethyl ketal	$C_{18}H_{30}O_4$	47189-08-3
1,1′-Diacetylferrocene	$C_{14}H_{14}FeO_2$	1273-94-7
1,1′-Diadamantyl ketone	$C_{21}H_{30}O$	38256-01-8
Diallyl	C_6H_{10}	592-42-7
Diamantane	$C_{14}H_{20}$	2292-79-7
2,4-Diaminoazobenzene	$C_{12}H_{12}N_4$	495-54-5
4,4′-Diaminodiphenyl ether	$C_{12}H_{12}N_2O$	101-80--
4,4′-Diaminodiphenyl oxide	$C_{12}H_{12}N_2O$	101-80--
4,4′-Diaminodiphenyl sulfone	$C_{12}H_{12}N_2O_2S$	80-08-0
1,2-Diaminoethane	$C_2H_8N_2$	107-15-3
N,N′-Di-(2-aminoethyl)piperazine	$C_8H_{20}N_4$	24028-46--
1,2-Diamino-2-methylpropane	$C_4H_{12}N_2$	811-93-8
1,2-Diaminopropane	$C_3H_{10}N_2$	78-90-0
Diamond	C	7782-40-3
4,4′-Dianilino-3,3′-diaminodiphenyl ether	$C_{24}H_{22}N_4O$	18888-98-7
4,4′-Dianilino-3,3′-diaminodiphenyl oxide	$C_{24}H_{22}N_4O$	18888-98-7
Dianisyldiethynylsilane	$C_{18}H_{16}O_2Si$	55986-09-9
1,4-Diazabicyclo[2.2.2]octane	$C_6H_{12}N_2$	280-57-9
2,3-Diazabicyclo[2.2.2]oct-2-ene N-oxide	$C_6H_{10}N_2O$	25926-96-0
6,7-Diazatricyclo[3.2.2.0^{2,4}]non-6-ene N-oxide	$C_7H_{10}N_2O$	25926-99-3
1,2,3,4-Dibenzanthracene-picric acid	$C_{28}H_{17}N_3O_7$	72454-46-7
1,2,5,6-Dibenzanthracene-picric acid	$C_{28}H_{17}N_3O_7$	1951-78-0
Dibenzofuran	$C_{12}H_8O$	132-64-9
Dibenzothiophene	$C_{12}H_8S$	132-65-0
1,2-Dibenzoylethane	$C_{16}H_{14}O_2$	495-71-6
Dibenzoylethylene	$C_{16}H_{12}O_2$	4070-75-
1,1′-Dibenzoylferrocene	$C_{24}H_{18}FeO_2$	12180-80-3
Dibenzyl	$C_{14}H_{14}$	103-29-7
Dibromoacetic acid	$C_2H_2Br_2O_2$	631-64-
1,2-Dibromobenzene	$C_6H_4Br_2$	583-53-9
1,3-Dibromobenzene	$C_6H_4Br_2$	108-36-
1,4-Dibromobenzene	$C_6H_4Br_2$	106-37-6
p-Dibromobenzene	$C_6H_4Br_2$	106-37-6
1′,1‴-Diiodobiferrocenium hexafluoroantimonate	$C_{20}H_{16}F_6Fe_2I_2Sb$	140677-36-7
1,4-Dibromobutane	$C_4H_8Br_2$	110-52-
1,4-Dibromo-2,3-dichlorohexafluorobutane	$C_4Br_2Cl_2F_6$	375-42-5
1,2-Dibromoethane	$C_2H_4Br_2$	106-93--
1,2-Dibromoethane-d_1	$C_2H_3DBr_2$	unavailable
1,2-Dibromoethane-d_2(1,1)	$C_2D_2H_2Br_2$	unavailable
1,2-Dibromoethane-d_2(1,2)	$C_2D_2H_2Br_2$	126266-42-0
1,2-Dibromoethane-d_3	$C_2HD_3Br_2$	117164-17-7
1,2-Dibromoethane-d_4	$C_2D_4Br_2$	22581-63-1
Dibromoethanoic acid	$C_2H_2Br_2O_2$	631-64-1
Dibromomethane	CH_2Br_2	74-95-3
2,4-Dibromophenol	$C_6H_4Br_2O$	615-58-7
1,2-Dibromopropane	$C_3H_6Br_2$	78-75-1
1,3-Dibromopropane	$C_3H_6Br_2$	109-64-8
1,2-Dibromotetrafluoroethane	$C_2Br_2F_4$	124-73-2

1,6-Dibromo-2,3,5-trichlorononafluorohexane	$C_6Br_2Cl_3F_9$	85131-86-8
4,4′-Dibutanoyloxydiphenyldiacetylene	$C_{24}H_{22}O_4$	92341-25-8
5,6-Dibutyl-5,6-bis(4-*tert*-butylphenyl)decane	$C_{38}H_{62}$	85668-76-4
Di-*tert*-butyldiazene-N-oxide	$C_8H_{18}N_2O$	87339-11-5
2,6-Di-*tert*-butyl-4-(3,5-di-*tert*-butyl-4-oxocycloxexa-2,5-dienylidene methyl) phenol	$C_{29}H_{42}O_2$	4534-84-3
2,6-Di-*tert*-butyl-4-(3,5-di-*tert*-butyl-4-oxocyclohexa-2,5-dienylidene methyl phenoxyl	$C_{29}H_{41}O_2$	2370-18-5
Di-*n*-butyl ether	$C_8H_{18}O$	142-96-1
Di-*tert*-butyl ether	$C_8H_{18}O$	6163-66-2
Di-*n*-butyl ketone	$C_9H_{18}O$	502-56-7
4,4′-Di-*n*-butyloxyazoxybenzene	$C_{20}H_{26}N_2O_3$	17051-01-3
Di-*tert*-butyl peroxide	$C_8H_{18}O_2$	110-05-4
Dibutyl *o*-phthalate	$C_{16}H_{22}O_4$	84-74-2
Di-*n*-butyl sebacate	$C_{18}H_{34}O_4$	109-43-3
Dibutyl succinate	$C_{12}H_{22}O_4$	141-03-7
Di-*n*-butyl sulfide	$C_8H_{18}S$	544-40-1
1,3-Dibutylurea	$C_9H_{20}N_2O$	1792-17-2
Dichloroacetic acid	$C_2H_2Cl_2O_2$	79-43-6
1,2-Dichlorobenzene	$C_6H_4Cl_2$	95-50-1
1,3-Dichlorobenzene	$C_6H_4Cl_2$	541-73-1
1,4-Dichlorobenzene	$C_6H_4Cl_2$	106-46-7
m-Dichlorobenzene	$C_6H_4Cl_2$	541-73-1
o-Dichlorobenzene	$C_6H_4Cl_2$	95-50-1
p-Dichlorobenzene	$C_6H_4Cl_2$	106-46-7
p-Dichlorobenzophenone	$C_{13}H_8Cl_2O$	90-98-2
4,4′-Dichlorobenzophenone	$C_{13}H_8Cl_2O$	90-98-2
cis-Dichlorobis(methylamine)platinum	$C_2H_{10}Cl_2N_2Pt$	15273-32-2
trans-Dichlorobis(methylamine)platinum	$C_2H_{10}Cl_2N_2Pt$	15319-09-2
1,2-Dichlorobutane	$C_4H_8Cl_2$	616-21-7
1,4-Dichlorobutane	$C_4H_8Cl_2$	110-56-5
β,β'-Dichlorodiethylether	$C_4H_8Cl_2O$	111-44-4
Dichlorodiethylsilane	$C_4H_{10}Cl_2Si$	1719-53-5
Dichlorodifluoromethane	CCl_2F_2	75-71-8
Dichlorodimethylsilane	$C_2H_6Cl_2Si$	75-78-5
4,5-Dichloro-1,3-dioxolan-2-one	$C_3H_2Cl_2O_3$	3967-55-3
4,4′-Dichlorodiphenyl sulphone	$C_{12}H_8Cl_2O_2S$	80-07-9
1,1-Dichloroethane	$C_2H_4Cl_2$	75-34-3
1,2-Dichloroethane	$C_2H_4Cl_2$	107-06-2
Dichloroethanoic acid	$C_2H_2Cl_2O_2$	79-43-6
1,1-Dichloroethene	$C_2H_2Cl_2$	75-35-4
1,2-Dichloroethene	$C_2H_2Cl_2$	540-59-0
cis-1,2-Dichloroethene	$C_2H_2Cl_2$	156-59-2
trans-1,2-Dichloroethene	$C_2H_2Cl_2$	156-60-5
1,2-Dichloroethylene	$C_2H_2Cl_2$	540-59-0
cis-1,2-Dichloroethylene	$C_2H_2Cl_2$	156-59-2
trans-1,2-Dichloroethylene	$C_2H_2Cl_2$	156-60-5
Dichlorofluoromethane	$CHCl_2F$	75-43-4
1,6-Dichlorohexane	$C_6H_{12}Cl_2$	2163-00-0
Dichloromethane	CH_2Cl_2	75-09-2
Dichloromethylvinylsilane	$C_3H_6Cl_2Si$	124-70-9
2,4-Dichloro-4′-nitrodiphenyl ether	$C_{12}H_7Cl_2NO_3$	1836-75-5
1,5-Dichloro-3-oxapentane	$C_4H_8Cl_2O$	111-44-4
1,5-Dichloropentane	$C_5H_{10}Cl_2$	628-76-2
2,3-Dichlorophenol	$C_6H_4Cl_2O$	576-24-9
2,4-Dichlorophenol	$C_6H_4Cl_2O$	120-83-2
2,5-Dichlorophenol	$C_6H_4Cl_2O$	583-78-8
2,6-Dichlorophenol	$C_6H_4Cl_2O$	87-65-0
3,4-Dichlorophenol	$C_6H_4Cl_2O$	95-77-2
3,5-Dichlorophenol	$C_6H_4Cl_2O$	591-35-5
1,2-Dichloropropane	$C_3H_6Cl_2$	78-87-5
1,3-Dichloropropane	$C_3H_6Cl_2$	142-28-9
2,2-Dichloropropane	$C_3H_6Cl_2$	594-20-7
1,2-Dichloro-1,1,2,2-tetrafluoroethane	$C_2Cl_2F_4$	76-14-2
Di-α-cumyl peroxide	$C_{18}H_{22}O_2$	27137-90-2
Dicyandiamide	$C_2H_4N_4$	461-58-5
1,2-Dicyanobenzene	$C_8H_4N_2$	91-15-6
1,4-Dicyanobenzene	$C_8H_4N_2$	623-26-7
Dicyanomethane	$C_3H_2N_2$	109-77-3
1,3-Dicyanopropane	$C_5H_6N_2$	544-13-8
2,2-Dicyanopropane	$C_5H_6N_2$	7321-55-3
1,3-Dicyclohexylbutane	$C_{16}H_{30}$	41851-35-8
1,1-Dicyclohexyldodecane	$C_{24}H_{46}$	18254-57-4
2,11-Dicyclohexyldodecane	$C_{24}H_{46}$	95746-44-4
1,1-Dicyclohexylethane	$C_{14}H_{26}$	2319-61-1
1,2-Dicyclohexylethane	$C_{14}H_{26}$	3321-50-4
1,1-Dicyclohexylheptane	$C_{19}H_{36}$	2090-15-5
Dicyclohexylmethane	$C_{13}H_{24}$	3178-23-2
1,2-Dicyclohexylpropane	$C_{15}H_{28}$	41851-34-7
endo-Dicyclopentadiene	$C_{10}H_{12}$	1755-01-7
1,3-Dicyclopentylcyclopentane	$C_{15}H_{26}$	6051-40-7
4,4′-Didecanoyloxydiphenyldiacetylene	$C_{36}H_{46}O_4$	92341-28-1
Di-*n*-decylammonium chloride	$C_{20}H_{44}ClN$	2486-84-2
Di-*n*-decyl sebacate	$C_{30}H_{58}O_4$	2432-89-5
4,4′-Didodecanoyloxydiphenyldiacetylene	$C_{40}H_{54}O_4$	92341-29-2
Di-*n*-dodecyl sebacate	$C_{34}H_{64}O_4$	2432-88-4
Diethanolamine	$C_4H_{11}NO_2$	111-42-2
4,4′-Diethanoyloxydiphenyldiacetylene	$C_{20}H_{14}O_4$	92341-23-6
4,4′-Diethoxyazoxybenzene	$C_{16}H_{18}N_2O_3$	4792-83-0
1,1-Diethoxyethane	$C_6H_{14}O_2$	105-57-7
1,2-Diethoxyethane	$C_6H_{14}O_2$	629-14-1
Diethylamine	$C_4H_{11}N$	109-89-7
Diethylaminoethyl methacrylate	$C_{10}H_{19}NO_2$	105-16-8
N,N-Diethylaniline	$C_{10}H_{15}N$	91-66-7
1′,1‴-Diethylbiferrocenium triiodide	$C_{24}H_{26}I_3Fe_2$	78713-00-5
4,5-Diethyl-4,5-bis-(4-*tert*-butylphenyl)octane	$C_{32}H_{50}$	85668-73-1
Diethyl carbonate	$C_5H_{10}O_3$	105-58-8
Diethylcyclohexane	$C_{10}H_{20}$	1331-43-7
1,4-Diethylcyclohexane	$C_{10}H_{20}$	1679-00-1
Diethyl disulfide	$C_4H_{10}S_2$	110-81-6
Diethylene glycol	$C_4H_{10}O_3$	111-46-6
Diethylene glycol-glycerol-adipate polymer	$C_{13}H_{22}O_8$	26760-54-3
Diethylene glycol-trimethylolpropane-adipate polymer	$C_{15}H_{28}O_8$	28183-09-7
Diethyleneimide oxide	C_4H_9NO	110-91-8
Diethylenetriamine	$C_4H_{13}N_3$	111-40-0
Diethyl ethanedioate	$C_6H_{10}O_4$	95-92-1
Diethyl ether	$C_4H_{10}O$	60-29-7
Di(2-ethylhexyl)adipate	$C_{22}H_{42}O_4$	103-23-1
Di-(2-ethylhexyl) *o*-phthalate	$C_{24}H_{38}O_4$	117-81-7
Diethylhydropyrene	$C_{20}H_{34}$	unavailable
N,N-Diethylhydroxylamine	$C_4H_{11}NO$	3710-84-7
Diethyl ketone	$C_5H_{10}O$	96-22-0
Diethyl malonate	$C_7H_{12}O_4$	105-53-3
Diethyl mercury	$C_4H_{10}Hg$	627-44-1
Diethylmethylamine	$C_5H_{13}N$	616-39-7
Diethyl oxalate	$C_6H_{10}O_4$	95-92-1
3,3-Diethylpentane	C_9H_{20}	1067-20-5
Diethyl *o*-phthalate	$C_{12}H_{14}O_4$	84-66-2
Diethyl *p*-phthalate	$C_{12}H_{14}O_4$	636-09-9
Diethyl succinate	$C_8H_{14}O_4$	123-25-1
Diethyl sulfide	$C_4H_{10}S$	352-93-2
Diethyl terephthalate	$C_{12}H_{14}O_4$	636-09-9
1,1-Diethylurea	$C_5H_{12}N_2O$	634-95-7
1,3-Diethylurea	$C_5H_{12}N_2O$	623-76-7
N,N-Diethylurea	$C_5H_{12}N_2O$	634-95-7
Diethyl zinc	$C_4H_{10}Zn$	557-20-0
Diethylzinc diethyltellurim complex	$C_8H_{20}TeZn$	132851-15-1
1,1-Diethynyl-2,3,4,5-tetraphenyl-1-germacyclo-pentadiene	$C_{32}H_{22}Ge$	57863-11-3
Diethynyldiphenylgermane	$C_{16}H_{12}Ge$	1675-59-8
1,2-Difluorobenzene	$C_6H_4F_2$	367-11-3
1,3-Difluorobenzene	$C_6H_4F_2$	372-18-9
1,4-Difluorobenzene	$C_6H_4F_2$	540-36-3
4,4′-Difluorobiphenyl	$C_{12}H_8F_2$	398-23-2
1,1-Difluoro-1-chloroethane	$C_2H_3ClF_2$	75-68-3
1,2-Difluoro-2,2-dichloroethane	$C_2H_2Cl_2F_2$	431-06-1
1,1-Difluoroethane	$C_2H_4F_2$	75-37-6
2,2-Difluorotetrachloroethane	$C_2Cl_4F_2$	76-11-9
1,2-Difluoro-1,2,2-trichloroethane	$C_2HCl_3F_2$	354-21-2

Diformylhydrazine	$C_2H_4N_2O_2$	628-36-4
Diglycine nitrate	$C_4H_{11}N_3O_7$	6845-92-7
Diglycylglycine	$C_6H_{11}N_3O_4$	556-33-2
Diglyme	$C_6H_{14}O_3$	111-96-6
4,4′-Diheptanoyloxydiphenyldiacetylene	$C_{30}H_{34}O_4$	92341-27-0
Di-*n*-hexadecyl sebacate	$C_{42}H_{82}O_4$	26719-48-2
4,4′-Dihexanoyloxydiphenyldiacetylene	$C_{28}H_{30}O_4$	92341-26-9
N,N′-Di-*n*-hexyladipamide	$C_{18}H_{36}N_2O_2$	21150-82-3
Di-*n*-hexylammonium chloride	$C_{12}H_{28}ClN$	2296-13-1
Dihexyl bis(hexamethylene-1,6-)-trisebacate	$C_{54}H_{98}O_{12}$	55205-82-8
Dihexyl hexamethylene-1,6-disebacate	$C_{38}H_{70}O_8$	55205-81-7
N,N′-Di-*n*-hexylsebacamide	$C_{22}H_{44}N_2O_2$	31827-03-9
Di-*n*-hexyl sebacate	$C_{22}H_{42}O_4$	2449-10-7
4,4′-Dihydrazinodiphenyl oxide	$C_{12}H_{14}N_4O$	51033-02-4
9,10-Dihydroanthracene	$C_{14}H_{12}$	613-31-0
2,5-Dihydro-3,4-benzofuran	C_8H_8O	496-14-0
4,5-Dihydro-2,3-benzofuran	C_8H_8O	496-16-2
2,3-Dihydrofuran	C_4H_6O	1191-99-7
2,5-Dihydrofuran clathrate hydrate	$C_4H_6O \cdot 17H_2O$	14306-51-5
1,2-Dihydro-4-(methoxymethyl)-6-methyl-2-oxo-3-pyridinecarbonitrile	$C_9H_{10}N_2O_2$	6339-38-4
9,10-Dihydrophenanthrene	$C_{14}H_{12}$	776-35-2
Dihydrosulfide carbon sulfide	CH_2S_3	594-08-1
3,4-Dihydroxybenzaldehyde	$C_7H_6O_3$	139-85-5
1,2-Dihydroxybenzene	$C_6H_6O_2$	120-80-9
1,3-Dihydroxybenzene	$C_6H_6O_2$	108-46-3
1,4-Dihydroxybenzene	$C_6H_6O_2$	123-31-9
4,4′-Dihydroxybiphenyl	$C_{12}H_{10}O_2$	92-88-6
1,3-Dihydroxybutane	$C_4H_{10}O_2$	107-88-0
1,4-Dihydroxybutane	$C_4H_{10}O_2$	110-63-4
2,3-Dihydroxybutane	$C_4H_{10}O_2$	513-85-9
1,8-Dihydroxy-3,6-dioxaoctane	$C_6H_{14}O_4$	112-27-6
4,4′-Dihydroxydiphenyl-2,2-propane	$C_{15}H_{16}O_2$	80-05-7
1,2-Dihydroxyethane	$C_2H_6O_2$	107-21-1
1,2-Dihydroxyethane-d_2	$C_2H_4D_2O_2$	2219-52-5
1,5-Dihydroxy-3-oxapentane	$C_4H_{10}O_3$	111-46-6
1,2-Dihydroxypropane	$C_3H_8O_2$	57-55-6
1,14-Dihydroxy-3,6,9,12-tetraoxatetradecane	$C_{10}H_{22}O_6$	4792-15-8
2,5-Dihydroxytoluene	$C_7H_8O_2$	95-71-6
3,5-Dihydroxytoluene monohydrate	$C_7H_8O_2 \cdot H_2O$	6153-39-5
1,11-Dihydroxy-3,6,9-trioxaundecane	$C_8H_{18}O_5$	112-60-7
1,2-Diiodobenzene	$C_6H_4I_2$	615-42-9
1,3-Diiodobenzene	$C_6H_4I_2$	626-00-6
1,4-Diiodobenzene	$C_6H_4I_2$	624-38-4
Diiodomethane	CH_2I_2	75-11-6
1,3-Diiodopropane	$C_3H_6I_2$	627-31-6
Diisobutylaluminum hydride	$C_8H_{19}Al$	1191-15-7
Diisobutyl amine	$C_8H_{19}N$	110-96-3
Diisobutylketone	$C_9H_{18}O$	108-83-8
1,4-Diisocyanatobenzene	$C_8H_4N_2O_2$	104-49-4
1,6-Diisocyanatohexane	$C_8H_{12}N_2O_2$	822-06-0
1,5-Diisocyanatonaphthalene	$C_{12}H_6N_2O_2$	3173-72-6
Diisododecyl phthalate	$C_{32}H_{54}O_4$	27554-06-9
p,*p*′-Diisopropylbiphenyl	$C_{18}H_{22}$	18970-30-4
Diisopropyl ketone	$C_7H_{14}O$	565-80-0
Diisopropyl sulfide	$C_6H_{14}S$	625-80-9
1,4:5,8-Dimethanodecalin	$C_{12}H_{18}$	538-33-2
Dimethanolurea	$C_3H_8N_2O_3$	140-95-4
4,4′-Dimethoxyazoxybenzene	$C_{14}H_{14}N_2O_3$	1562-94-3
1,1-Dimethoxy-3-cyanopropane	$C_6H_{11}NO_2$	14618-78-1
meso-2,3-Dimethoxy-2,3-diphenylsuccinonitrile	$C_{18}H_{16}N_2O_2$	61502-57-6
1,2-Dimethoxyethane	$C_4H_{10}O_2$	110-71-4
Dimethoxymethane	$C_3H_8O_2$	109-87-5
Di(*p*-methoxyphenyl)-*trans*-cyclohexane-1,4-dicarboxylate	$C_{22}H_{24}O_6$	26379-55-5
2,2-Dimethoxypropane	$C_5H_{12}O_2$	77-76-9
Dimethyl acetal of β-cyanopropionaldehyde	$C_6H_{11}NO_2$	14618-78-
N,N-Dimethylacetamide	C_4H_9NO	127-19-
Dimethylacetylene	C_4H_6	503-17-
N,N-Dimethyl-L-alanine methyl ester	$C_6H_{13}NO_2$	42293-86-
Dimethylamine	C_2H_7N	124-40-
N,N-Dimethylaminodiborane	$C_2H_{11}B_2N$	22580-01-
Dimethylaminoethyl methacrylate	$C_8H_{15}NO_2$	2867-47-
3-Dimethylaminomethyl indole	$C_{11}H_{14}N_2$	87-52-
Dimethylaminopropylenediamine	$C_5H_{15}N_3$	unavailabl
3-(Dimethylamino)propionitrile	$C_5H_{10}N_2$	1738-25-
β-Dimethylaminopropionitrile	$C_5H_{10}N_2$	1738-25-
Dimethylammonium tetrafluoroborate	$C_2H_8BF_4N$	16970-97-
2,6-Dimethylaniline	$C_8H_{11}N$	87-62-
N,N-Dimethylaniline	$C_8H_{11}N$	121-69-
1,1-Dimethylazoethane	$C_8H_{18}N_2$	927-83-
1,1-Dimethylazoxyethane	$C_8H_{18}N_2O$	16649-52-
1,2-Dimethylbenzene	C_8H_{10}	95-47-
1,3-Dimethylbenzene	C_8H_{10}	108-38-
1,4-Dimethylbenzene	C_8H_{10}	106-42-
2,3-Dimethylbenzoic acid	$C_9H_{10}O_2$	603-79-
2,4-Dimethylbenzoic acid	$C_9H_{10}O_2$	611-01-
2,5-Dimethylbenzoic acid	$C_9H_{10}O_2$	610-72-
2,6-Dimethylbenzoic acid	$C_9H_{10}O_2$	632-46-
3,4-Dimethylbenzoic acid	$C_9H_{10}O_2$	619-04-
3,5-Dimethylbenzoic acid	$C_9H_{10}O_2$	499-06-
2,2′-Dimethylbiphenyl	$C_{14}H_{14}$	605-39-
2,3-Dimethyl-2,3-bis(4-*tert*-butylphenyl)butane	$C_{26}H_{38}$	5171-91-
3,4-Dimethyl-3,4-bis(4-*tert*-butylphenyl)hexane	$C_{30}H_{46}$	85668-74-
2,2-Dimethylbutane	C_6H_{14}	75-83-
2,3-Dimethylbutane	C_6H_{14}	79-29-
2,2-Dimethylbutane-thiourea adduct	$C_9H_{26}N_6S_3$	39822-98-
3,3-Dimethyl-1-butanol	$C_6H_{14}O$	624-95-
3,3-Dimethyl-2-butanone	$C_6H_{12}O$	75-97-
2,3-Dimethyl-2-butene	C_6H_{12}	563-79-
3,3-Dimethyl-1-butene	C_6H_{12}	558-37-
Dimethyl cadmium	C_2H_6Cd	506-82-
Dimethylcadmium·dimethylselenium	$C_4H_{12}CdSe$	143481-65-
Dimethylcadmium·dimethyltellurium	$C_4H_{12}CdTe$	143481-66-
1,4-Dimethylcubane dicarboxylate	$C_{12}H_{12}O_4$	2941-62-
1,1-Dimethylcyclohexane	C_8H_{16}	590-66-
1,2-Dimethylcyclohexane	C_8H_{16}	583-57-
1-*cis*-2-Dimethylcyclohexane	C_8H_{16}	2207-01-
1-*trans*-2-Dimethylcyclohexane	C_8H_{16}	6876-23-
1-*cis*-3-Dimethylcyclohexane	C_8H_{16}	638-04-
1-*trans*-3-Dimethylcyclohexane	C_8H_{16}	2207-03-
1-*cis*-4-Dimethylcyclohexane	C_8H_{16}	624-29-
1-*trans*-4-Dimethylcyclohexane	C_8H_{16}	2207-04-
1,1-Dimethylcyclopentane	C_7H_{14}	1638-26-
1,2-Dimethylcyclopentane	C_7H_{14}	2452-99-
1-*cis*-2-Dimethylcyclopentane	C_7H_{14}	1192-18-
1-*trans*-3-Dimethylcyclopentane	C_7H_{14}	1759-58-
Dimethyldecalin	$C_{12}H_{22}$	unavailabl
3,6-Dimethyl-1,4-dioxane-2,5-dione	$C_6H_8O_4$	95-96-
2,3-Dimethyl-2,3-diphenylbutane	$C_{18}H_{22}$	1889-67-
Dimethyl diselenium	$C_2H_6Se_2$	7101-31-
Dimethyl disulfide	$C_2H_6S_2$	624-92-
Dimethyl ether	C_2H_6O	115-10-
N,N-Dimethylformamide	C_3H_7NO	68-12-
Dimethyl fumarate	$C_6H_8O_4$	624-49-
N,N-Dimethylglycine ethyl ester	$C_6H_{13}NO_2$	33229-89-
N,N-Dimethylglycine methyl ester	$C_5H_{11}NO_2$	7148-06-
2,6-Dimethyl-4-heptanone	$C_9H_{18}O$	108-83-
2,5-Dimethylhexa-2,4-diene	C_8H_{14}	764-13-
2,5-Dimethylhexane	C_8H_{18}	592-13-
3,3-Dimethylhexane	C_8H_{18}	563-16-
N,N-Dimethylhydrazine	$C_2H_8N_2$	57-14-

N,N′-Dimethylhydrazine	$C_2H_8N_2$	540-73-8
1,1-Dimethylhydrazinium tetrafluoroborate	$C_2H_9BF_4N_2$	811-64-3
1,1-Dimethylindan	$C_{11}H_{14}$	4912-92-9
4,6-Dimethylindan	$C_{11}H_{14}$	1685-82-1
4,7-Dimethylindan	$C_{11}H_{14}$	6682-71-9
Dimethyl ketone	C_3H_6O	67-64-1
Dimethyl ketone clathrate hydrate	$C_3H_6O\cdot17H_2O$	18879-06-6
Dimethyl maleate	$C_6H_8O_4$	624-48-6
Dimethylmalonic acid dimethyl ester	$C_7H_{12}O_4$	6065-54-9
Dimethylmalononitrile	$C_5H_6N_2$	7321-55-3
N,N-Dimethylmethanamide	C_3H_7NO	68-12-2
1,8-Dimethylnaphthalene	$C_{12}H_{12}$	569-41-5
2,3-Dimethylnaphthalene	$C_{12}H_{12}$	581-40-8
2,6-Dimethylnaphthalene	$C_{12}H_{12}$	581-42-0
2,7-Dimethylnaphthalene	$C_{12}H_{12}$	582-16-1
2,6-Dimethylocta-2,7-dien-6-ol	$C_{10}H_{18}O$	78-70-6
2,7-Dimethyloctane	$C_{10}H_{22}$	1072-16-8
3,7-Dimethyl-1-octanol	$C_{10}H_{22}O$	106-21-8
3,7-Dimethyl-6-octen-1-yn-3-ol	$C_{10}H_{16}O$	2917-20-8
3,3-Dimethyl-2-oxabutane	$C_5H_{12}O$	1634-04-4
4,4-Dimethyl-3-oxahexane	$C_7H_{16}O$	919-94-8
2,4-Dimethyl-3-oxapentane	$C_6H_{14}O$	108-20-3
3,3-Dimethyl-2-oxapentane	$C_6H_{14}O$	994-05-8
4,4-Dimethyl-3-oxapentane	$C_6H_{14}O$	637-92-3
17-(2,2-Dimethyl-1-oxopropoxy)-(17α)-19-norpregn-4-en-20-yn-3-one	$C_{25}H_{34}O_3$	65445-09-2
3,4-Dimethylpentanal	$C_7H_{14}O$	19353-21-0
2,2-Dimethylpentane	C_7H_{16}	590-35-2
2,3-Dimethylpentane	C_7H_{16}	565-59-3
2,4-Dimethylpentane	C_7H_{16}	108-08-7
3,3-Dimethylpentane	C_7H_{16}	562-49-2
2,4-Dimethyl-3-pentanone	$C_7H_{14}O$	565-80-0
N,N-Dimethyl-2-pentylnonylamine	$C_{16}H_{35}N$	99916-30-0
2,3-Dimethylphenol	$C_8H_{10}O$	526-75-0
2,4-Dimethylphenol	$C_8H_{10}O$	105-67-9
2,5-Dimethylphenol	$C_8H_{10}O$	95-87-4
2,6-Dimethylphenol	$C_8H_{10}O$	576-26-1
3,4-Dimethylphenol	$C_8H_{10}O$	95-65-8
3,5-Dimethylphenol	$C_8H_{10}O$	108-68-9
Dimethyl-3,4-phosphacymantrene	$C_9H_8MnO_3P$	56993-57-8
3,4-Dimethylphospholyl manganese tricarbonyl	$C_9H_8MnO_3P$	56993-57-8
Dimethyl *o*-phthalate	$C_{10}H_{10}O_4$	131-11-3
Dimethyl *p*-phthalate	$C_{10}H_{10}O_4$	120-61-6
2,2-Dimethylpropanal	$C_5H_{10}O$	630-19-3
2,2-Dimethylpropanamide	$C_5H_{11}NO$	754-10-9
N,N-Dimethylpropanamide	$C_5H_{11}NO$	758-96-3
2,2-Dimethylpropane	C_5H_{12}	463-82-1
N,N-Dimethyl-1,3-propanediamine	$C_5H_{14}N_2$	109-55-7
2,2-Dimethyl-1,3-propanediol	$C_5H_{12}O_2$	126-30-7
2,2-Dimethylpropanoic acid	$C_5H_{10}O_2$	75-98-9
2,2-Dimethyl-1-propanol	$C_5H_{12}O$	75-84-3
2,2-Dimethylpropionitrile	C_5H_9N	630-18-2
2-(1,2-Dimethylpropyl)-5,6-dimethylheptenal	$C_{14}H_{26}O$	99914-84-8
2,3-Dimethylpyridine	C_7H_9N	583-61-9
2,4-Dimethylpyridine	C_7H_9N	108-47-4
2,5-Dimethylpyridine	C_7H_9N	589-93-5
2,6-Dimethylpyridine	C_7H_9N	108-48-5
3,4-Dimethylpyridine	C_7H_9N	583-58-4
3,5-Dimethylpyridine	C_7H_9N	591-22-0
2,4-Dimethylpyrrole	C_6H_9N	625-82-1
2,5-Dimethylpyrrole	C_6H_9N	625-84-3
Dimethyl selenium	C_2H_6Se	593-79-3
1,1-Dimethyl-1-silacyclobutane	$C_5H_{12}Si$	2295-12-7
Dimethyl sulfide	C_2H_6S	75-18-3
Dimethyl sulfone	$C_2H_6O_2S$	67-71-0
Dimethyl sulfoxide	C_2H_6OS	67-68-5
Dimethyl terephthalate	$C_{10}H_{10}O_4$	120-61-6
Dimethyltetraphenylcyclotrisiloxane	$C_{26}H_{26}O_3Si_3$	1438-86-4
2,2-Dimethyl-4,4,6,6-tetraphenylcyclotrisiloxane	$C_{26}H_{26}O_3Si_3$	1438-86-4
1,3-Dimethyl-1,1,3,3-tetraphenyldisiloxane	$C_{26}H_{26}OSi_2$	807-28-3
3,3-Dimethyl-2-thiabutane	$C_5H_{12}S$	6163-64-0
2,4-Dimethyl-3-thiapentane	$C_6H_{14}S$	625-80-9
2,5-Dimethylthiophene	C_6H_8S	638-02-8
Dimethyl-2,2,2-trichloro-1-hydroxyethylphosphonate	$C_4H_8Cl_3O_4P$	52-68-6
6,10-Dimethyl-2-undecanone	$C_{13}H_{26}O$	1604-34-8
6,10-Dimethyl-3,5,9-undecatrien-2-one	$C_{13}H_{20}O$	141-10-6
6,10-Dimethyl-4,5,9-undecatrien-2-one	$C_{13}H_{20}O$	16647-05-5
1,3-Dimethyluracil	$C_6H_8N_2O_2$	874-14-6
1,1-Dimethylurea	$C_3H_8N_2O$	598-94-7
1,3-Dimethylurea	$C_3H_8N_2O$	96-31-1
Dimethyl zinc	C_2H_6Zn	544-97-8
Dimethylzinc dimethylselenium complex	$C_4H_{12}SeZn$	108430-95-1
Dimethylzinc dimethylsulfide complex	$C_4H_{12}SZn$	91071-61-3
Dimethylzinc dimethyltellerium complex	$C_4H_{12}TeZn$	127283-03-8
1,2′-Dinaphthylmethane	$C_{21}H_{16}$	611-48-3
Dinitrile-2,2′-azodiisobutyric acid	$C_8H_{12}N_4$	78-67-1
1,2-Dinitrobenzene	$C_6H_4N_2O_4$	528-29-0
1,3-Dinitrobenzene	$C_6H_4N_2O_4$	99-65-0
1,4-Dinitrobenzene	$C_6H_4N_2O_4$	100-25-4
1,3-Dinitro-1,3-diazacycloheptane	$C_5H_{10}N_4O_4$	5754-90-5
1,3-Dinitro-1,3-diazacyclohexane	$C_4H_8N_4O_4$	5754-89-2
1,3-Dinitro-1,3-diazacyclopentane	$C_3H_6N_4O_4$	5754-91-6
4,4′-Dinitrodiphenyl ether	$C_{12}H_8N_2O_5$	101-63-3
1,5-Dinitronaphthalene	$C_{10}H_6N_2O_4$	605-71-0
1,8-Dinitronaphthalene	$C_{10}H_6N_2O_4$	602-38-0
2,3-Dinitrophenol	$C_6H_4N_2O_5$	66-56-8
2,4-Dinitrophenol	$C_6H_4N_2O_5$	51-28-5
2,5-Dinitrophenol	$C_6H_4N_2O_5$	329-71-5
2,6-Dinitrophenol	$C_6H_4N_2O_5$	573-56-8
3,4-Dinitrophenol	$C_6H_4N_2O_5$	577-71-9
3,5-Dinitrophenol	$C_6H_4N_2O_5$	586-11-8
2,2-Dinitropropane	$C_3H_6N_2O_4$	595-49-3
2,4-Dinitrotoluene	$C_7H_6N_2O_4$	121-14-2
2,6-Dinitrotoluene	$C_7H_6N_2O_4$	606-20-2
4,4′-Dinonanoyloxydiphenyldiacetylene	$C_{34}H_{42}O_4$	71332-85-9
Di-*n*-octadecyl sebacate	$C_{46}H_{90}O_4$	3072-03-5
4,4′-Dioctanoyloxydiphenyldiacetylene	$C_{32}H_{38}O_4$	71332-84-8
Di-*n*-octylamine	$C_{16}H_{35}N$	1120-48-5
Di-*n*-octylammonium chloride	$C_{16}H_{36}ClN$	2296-14-2
Dioctyl phthalate	$C_{24}H_{38}O_4$	117-84-0
Dioctyl *o*-phthalate	$C_{24}H_{38}O_4$	117-84-0
Di-*n*-octyl sebacate	$C_{26}H_{50}O_4$	2432-87-3
4,7-Dioxadecane	$C_8H_{18}O_2$	18854-56-3
2,5-Dioxaheptane	$C_5H_{12}O_2$	500005-27-6
2,5-Dioxahexane	$C_4H_{10}O_2$	110-71-4
1,3-Dioxane	$C_4H_8O_2$	505-22-6
1,4-Dioxane	$C_4H_8O_2$	123-91-1
1,3-Dioxane clathrate hydrate	$C_4H_8O_2\cdot17H_2O$	51105-19-2
1,4-Dioxane-2,5-dione	$C_4H_4O_4$	502-97-6
2,5-Dioxanonane	$C_7H_{16}O_2$	500005-29-8
2,5-Dioxaoctane	$C_6H_{14}O_2$	500005-28-7
3,6-Dioxaoctane	$C_6H_{14}O_2$	629-14-1
2,4-Dioxapentane	$C_3H_8O_2$	109-87-5
1,3-Dioxepane	$C_5H_{10}O_2$	505-65-7
1,3-Dioxolane	$C_3H_6O_2$	646-06-0
1,3-Dioxolane clathrate hydrate	$C_3H_6O_2\cdot17H_2O$	34776-95-9
2,5-Dioxopiperazine	$C_4H_6N_2O_2$	106-57-0
4,4′-Dipentanoyloxydiphenyldiacetylene	$C_{26}H_{26}O_4$	71332-83-7
Di-*n*-pentylammonium chloride	$C_{10}H_{24}ClN$	23307-02-0
Diphenyl	$C_{12}H_{10}$	92-52-4
Diphenylacetic acid	$C_{14}H_{12}O_2$	117-34-0
Diphenylacetylene	$C_{14}H_{10}$	501-65-5
1,2-Diphenylbenzimidazole	$C_{19}H_{14}N_2$	2622-67-5

1,1′-Diphenyl-1,1′-bicyclohexane	$C_{24}H_{30}$	59358-71-3
1,1′-Diphenyl-1,1′-bicyclooctane	$C_{28}H_{38}$	59358-73-5
1,1′-Diphenyl-1,1′-bicyclopentane	$C_{22}H_{26}$	59358-70-2
Diphenylcarbinol	$C_{13}H_{12}O$	91-01-0
Diphenylcarbodiimide	$C_{13}H_{10}N_2$	622-16-2
Diphenyl carbonate	$C_{13}H_{10}O_3$	102-09-0
Diphenylchloromethane	$C_{13}H_{11}Cl$	90-99-3
Diphenyldiethynylsilane	$C_{16}H_{12}Si$	1675-57-6
Diphenyl diketone	$C_{14}H_{10}O_2$	134-81-6
1,1-Diphenyldodecane	$C_{24}H_{34}$	1603-53-8
Diphenylene-2,2′-disulfide-S-oxide	$C_{12}H_8OS_2$	49833-13-8
Diphenylenemethane	$C_{13}H_{10}$	86-73-7
Diphenylene oxide	$C_{12}H_8O$	132-64-9
4′,4‴-Diphenylenephthalidodicarboxylic acid dihydrazide	$C_{22}H_{18}N_4O_4$	19261-73-5
1,1-Diphenylethane	$C_{14}H_{14}$	612-00-0
1,2-Diphenylethane	$C_{14}H_{14}$	103-29-7
Diphenyl ether	$C_{12}H_{10}O$	101-84-8
1,1-Diphenylethylene	$C_{14}H_{12}$	530-48-3
Diphenylethyne	$C_{14}H_{10}$	501-65-5
Diphenylgermane	$C_{12}H_{12}Ge$	1675-58-7
Diphenylmercury	$C_{12}H_{10}Hg$	587-85-9
Diphenylmethane	$C_{13}H_{12}$	101-81-5
4,4′-Diphenylmethane diisocyanate	$C_{15}H_{10}N_2O_2$	101-68-8
Diphenyl oxide	$C_{12}H_{10}O$	101-84-8
Diphenylsilane-diethynyldiphenylgermane vitreous copolymer	$(C_{28}H_{24}GeSi)_n$	1693-51-2
Diphenyl sulfide	$C_{12}H_{10}S$	139-66-2
Diphenyl sulfone	$C_{12}H_{10}O_2S$	127-63-9
Diphenyl sulfoxide	$C_{12}H_{10}OS$	945-51-7
Diphenyltetramethylcyclotrisiloxane	$C_{16}H_{22}O_3Si_3$	1693-51-2
1,3-Diphenylurea	$C_{13}H_{12}N_2O$	102-07-8
Dipiperazinylethane	$C_{10}H_{22}N_4$	19479-83-5
4,4′-Dipropanoyloxydiphenyldiacetylene	$C_{22}H_{18}O_4$	92341-24-7
1,2-Di-*n*-propoxyethane	$C_8H_{18}O_2$	18854-56-3
N,N′-Di-*n*-propyladipamide	$C_{12}H_{24}N_2O_2$	85668-72-0
Dipropylamine	$C_6H_{15}N$	142-84-7
4,5-Dipropyl-4,5-bis(4-*tert*-butylphenyl)octane	$C_{34}H_{54}$	85668-72-0
Dipropyl disulfide	$C_6H_{14}S_2$	629-19-6
Dipropylene glycol	$C_6H_{14}O_3$	106-62-7
Di-*n*-propyl ether	$C_6H_{14}O$	111-43-3
Dipropyl sulfide	$C_6H_{14}S$	111-47-7
Di-*n*-tetradecylsebacate	$C_{38}H_{74}O_4$	26719-47-1
2,3-Dithiabutane	$C_2H_6S_2$	624-92-0
3,4-Dithiahexane	$C_4H_{10}S_2$	110-81-6
1,3-Dithiane	$C_4H_8S_2$	505-23-7
1,4-Dithiane	$C_4H_8S_2$	505-29-3
4,5-Dithiaoctane	$C_6H_{14}S_2$	629-19-6
4,5-Dithia-1,8-octanedioic acid	$C_6H_{10}O_4S_2$	4775-93-3
β,β'-Dithiodilactic acid	$C_6H_{10}O_4S_2$	4775-93-3
Di(*p*-tolyl)mercury	$C_{14}H_{14}Hg$	537-64-4
4,4′-Diundecanoyloxydiphenyldiacetylene	$C_{38}H_{50}O_4$	71332-86-0
DMF	C_3H_7NO	68-12-2
Docosafluorobicyclohexyl	$C_{12}F_{22}$	558-64-5
n-Docosane	$C_{22}H_{46}$	629-97-0
Dodecacarbonyl triiron	$C_{12}Fe_3O_{12}$	17685-52-8
n-Dodecane	$C_{12}H_{26}$	112-40-3
Dodecanedioic acid	$C_{12}H_{22}O_4$	693-23-2
1-Dodecanethiol	$C_{12}H_{26}S$	112-55-0
Dodecanoic acid	$C_{12}H_{24}O_2$	143-07-7
1-Dodecanol	$C_{12}H_{26}O$	112-53-8
1-Dodecene	$C_{12}H_{24}$	112-41-4
1-Dodecene-urea adduct	$C_{2.2}H_{6.5}N_2O$	1191-66-8
n-Dodecyl alcohol	$C_{12}H_{26}O$	112-53-8
n-Dodecylcyclohexane	$C_{18}H_{36}$	1795-17-1
n-Dodecyl mercaptan	$C_{12}H_{26}S$	112-55-0
n-Dodecyl methyl ketone	$C_{14}H_{28}O$	2345-27-9
n-Dotetracontane	$C_{42}H_{86}$	7098-20-6
n-Dotriacontane	$C_{32}H_{66}$	544-85-4
Dulcite	$C_6H_{14}O_6$	608-66-2
Dulcitol	$C_6H_{14}O_6$	608-66-2
Durene	$C_{10}H_{14}$	95-93-

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n-Eicosane	$C_{20}H_{42}$	112-95-
1-Eicosanethiol	$C_{20}H_{42}S$	13373-97-
Eicosanoic acid	$C_{20}H_{40}O_2$	506-30-
n-Eicosanyl mercaptan	$C_{20}H_{42}S$	13373-97-
1-Eicosene-urea adduct	$C_{2.4}H_{6.8}N_2O$	24494-56-
Enanthal	$C_7H_{14}O$	111-71-
{zeta}-Enantholactam	$C_7H_{13}NO$	673-66-
Erbium ethylsulfate	$C_6H_{15}ErO_{12}S_3 \cdot 9H_2O$	unavailab
Erythritol	$C_4H_{10}O_4$	149-32-
Ethanal	C_2H_4O	75-07-
Ethanamide	C_2H_5NO	60-35-
Ethane	C_2H_6	74-84-
Ethanedioic acid	$C_2H_2O_4$	144-62-
1,2-Ethanediol	$C_2H_6O_2$	107-21-
1,2-Ethanediol-d_2	$C_2H_4D_2O_2$	2219-52-
Ethanenitrile	C_2H_3N	75-05-
Ethanethiol	C_2H_6S	75-08-
Ethanoic acid	$C_2H_4O_2$	64-19-
Ethanoic anhydride	$C_4H_6O_3$	108-24-
Ethanol	C_2H_6O	64-17-
Ethanol-d_1	C_2H_5DO	1624-36-
N-Ethanol isatoxime	$C_{10}H_{10}N_2O_2$	unavailab
Ethenyl ethanoate	$C_4H_6O_2$	108-05-
N-*p*-Ethoxybenzylidene-*p*′-butylaniline	$C_{19}H_{23}NO$	29743-08-
4-Ethoxy-4′-butylazobenzene	$C_{18}H_{22}N_2O$	31401-34-
2-Ethoxyethanol	$C_4H_{10}O_2$	110-80-
2-Ethoxyethanol acetate	$C_6H_{12}O_3$	111-15-
2-Ethoxyisonitrosoacetanilide	$C_{10}H_{12}N_2O_3$	38423-62-
4-Ethoxyisonitrosoacetanilide	$C_{10}H_{12}N_2O_3$	17122-74-
1-Ethoxy-2-methoxyethane	$C_5H_{12}O_2$	500005-27-
N-Ethylacetamide	C_4H_9NO	627-45-
Ethyl acetate	$C_4H_8O_2$	141-78-
Ethyl acetoacetate	$C_6H_{10}O_3$	141-97-
Ethyl alcohol	C_2H_6O	64-17-
Ethyl alcohol-d_1	C_2H_5DO	1624-36-
Ethylammoniumbromide	C_2H_8BrN	593-55-
Ethylammonium dicyanochloromercurate (II)	$C_4H_5ClHgN_3$	13491-58-
Ethylammonium nitrate	$C_2H_9N_2O_3$	22113-86-
Ethyl azoxybenzenedicarboxylate	$C_{18}H_{18}N_2O_5$	6421-04-
Ethyl behenate	$C_{24}H_{48}O_2$	5908-87-
Ethylbenzene	C_8H_{10}	100-41-
Ethyl benzoate	$C_9H_{10}O_2$	93-89-
m-Ethylbenzoic acid	$C_9H_{10}O_2$	619-20-
o-Ethylbenzoic acid	$C_9H_{10}O_2$	612-19-
p-Ethylbenzoic acid	$C_9H_{10}O_2$	619-64-
2-Ethylbicyclohexyl	$C_{14}H_{26}$	66826-94-
2-Ethylbicyclohexylmethane	$C_{15}H_{28}$	66374-71-
2-Ethylbiphenyl	$C_{14}H_{14}$	1812-51-
Ethyl bromide	C_2H_5Br	74-96-
Ethyl butanoate	$C_6H_{12}O_2$	105-54-
2-Ethyl-1-butanol	$C_6H_{14}O$	97-95-
Ethyl butyrate	$C_6H_{12}O_2$	105-54-
Ethyl carbamate	$C_3H_7NO_2$	51-79-
N-Ethylcarbazole	$C_{14}H_{13}N$	86-28-
Ethyl cellulose	$(C_{12}H_{22}O_5)_n$	9004-57-
Ethyl chloride	C_2H_5Cl	75-00-
Ethyl 2-chloropropanoate	$C_5H_9ClO_2$	535-13-
Ethyl α-chloropropionate	$C_5H_9ClO_2$	535-13-
24-β-Ethylcholesterol	$C_{29}H_{50}O$	83-46-
trans-Ethyl cinnamate	$C_{11}H_{12}O_2$	103-36-
Ethyl cyanide	C_3H_5N	107-12-
Ethyl cyanoacetate	$C_5H_7NO_2$	105-56-
Ethylcyclohexane	C_8H_{16}	1678-91-
Ethyl cyclohexanecarboxylate	$C_9H_{16}O_2$	3289-28-
Ethylcyclopentane	C_7H_{14}	1640-89-
1-Ethylcyclopentene	C_7H_{12}	2146-38-
Ethyl cyclopropanecarboxylate	$C_6H_{10}O_2$	4606-07-

Ethyldecalin	$C_{12}H_{22}$	unavailable
α-Ethyldecalin	$C_{12}H_{22}$	1008-17-9
β-Ethyldecalin	$C_{12}H_{22}$	1618-23-1
Ethyl dichloroacetate	$C_4H_6Cl_2O_2$	535-15-9
Ethyl 2,3-dichloropropanoate	$C_5H_8Cl_2O_2$	6628-21-3
Ethyl α,β-dichloropropionate	$C_5H_8Cl_2O_2$	6628-21-3
Ethyl-2,2-dimethylpropanoate	$C_7H_{14}O_2$	3938-95-2
Ethyl docosanate	$C_{24}H_{48}O_2$	5908-87-2
Ethyl dodecanoate	$C_{14}H_{28}O_2$	106-33-2
Ethyl eicosanoate	$C_{22}H_{44}O_2$	18281-05-5
Ethylene	C_2H_4	74-85-1
Ethylene-butadiene copolymer	$(C_6H_{10})_n$	25068-01-3
Ethylene carbonate	$C_3H_4O_3$	96-49-1
Ethylene diamine	$C_2H_8N_2$	107-15-3
Ethylene dibromide	$C_2H_4Br_2$	106-93-4
Ethylene dibromide-d_1	$C_2H_3DBr_2$	unavailable
Ethylene dibromide-d_2(1,1)	$C_2D_2H_2Br_2$	unavailable
Ethylene dibromide-d_2(1,2)	$C_2D_2H_2Br_2$	126266-42-0
Ethylene dibromide-d_3	$C_2HD_3Br_2$	117164-17-7
Ethylene dibromide-d_4	$C_2D_4Br_2$	22581-63-1
Ethylene dichloride	$C_2H_4Cl_2$	107-06-2
Ethylene dinitramine	$C_2H_6N_4O_4$	505-71-5
Ethylene glycol	$C_2H_6O_2$	107-21-1
Ethylene glycol-d_2	$C_2H_4D_2O_2$	2219-52-5
Ethylene glycol acetate	$C_4H_8O_3$	111-55-7
Ethylene glycol diacetate	$C_6H_{10}O_4$	111-55-7
Ethyleneglycoldibutanoate	$C_{10}H_{18}O_4$	105-72-6
Ethyleneglycoldipropanoate	$C_8H_{14}O_4$	123-80-8
Ethylene oxalate	$C_4H_4O_4$	3524-70-7
Ethylene oxide	C_2H_4O	75-21-8
Ethylene oxide hydrate	$C_2H_4O\cdot 7H_2O$	16002-48-5
N-Ethylethanamide	C_4H_9NO	627-45-2
Ethyl ethanoate	$C_4H_8O_2$	141-78-6
Ethyl formate	$C_3H_6O_2$	109-94-4
Ethyl heptadecanoate	$C_{19}H_{38}O_2$	14010-23-2
Ethyl hexacosanate	$C_{28}H_{56}O_2$	29030-81-7
Ethyl hexadecanoate	$C_{18}H_{36}O_2$	628-97-7
2-Ethylhexanol	$C_8H_{18}O$	104-76-7
9-(2′-Ethylhexyl)perhydrofluorene	$C_{21}H_{38}$	unavailable
Ethyl hydrocinnamate	$C_{11}H_{14}O_2$	2021-28-5
Ethylhydroindan	$C_{11}H_{20}$	unavailable
Ethylidene chloride	$C_2H_4Cl_2$	75-34-3
Ethylidenecyclohexane	C_8H_{14}	1003-64-1
Ethylidenecyclopentane	C_7H_{12}	2146-37-4
Ethylidene difluoride	$C_2H_4F_2$	75-37-6
2-Ethylimidazole	$C_5H_8N_2$	1072-62-4
Ethyl iodide	C_2H_5I	75-03-6
Ethyl isothiocyanate	C_3H_5NS	542-85-8
Ethyl laurate	$C_{14}H_{28}O_2$	106-33-2
Ethyl margarate	$C_{19}H_{38}O_2$	14010-23-2
Ethyl mercaptan	C_2H_6S	75-08-1
Ethyl methanoate	$C_3H_6O_2$	109-94-4
Ethyl methyl sulfide	C_3H_8S	624-89-5
Ethyl nitrate	$C_2H_5NO_3$	625-58-1
Ethyl nonadecanoate	$C_{21}H_{42}O_2$	18281-04-4
Ethyl octadecanoate	$C_{20}H_{40}O_2$	111-61-5
Ethyl palmitate	$C_{18}H_{36}O_2$	628-97-7
3-Ethylpentane	C_7H_{16}	617-78-7
3-Ethyl-3-pentanol	$C_7H_{14}O$	597-49-9
2-Ethylperhydrophenanthrene	$C_{16}H_{28}$	unavailable
3-Ethylperhydropyrene	$C_{18}H_{30}$	unavailable
4-Ethylphenol	$C_8H_{10}O$	123-07-9
Ethyl N-phenylcarbamate	$C_9H_{11}NO_2$	101-99-5
Ethyl phenyl ether	$C_8H_{10}O$	103-73-1
Ethyl propanoate	$C_5H_{10}O_2$	105-37-3
Ethyl propionate	$C_5H_{10}O_2$	105-37-3
Ethyl n-propyl ether	$C_5H_{12}O$	628-32-0
Ethyl n-propyl ketone	$C_6H_{12}O$	589-38-8
Ethyl n-propyl sulfide	$C_5H_{12}S$	4110-50-3
Ethyl silicate	$C_8H_{20}O_4Si$	78-10-4
Ethyl stearate	$C_{20}H_{40}O_2$	111-61-5
Ethyl tetracosanate	$C_{26}H_{52}O_2$	24634-95-5
Ethyltetryl	$C_8H_7N_5O_8$	6052-13-7
Ethyl triacontanate	$C_{32}H_{64}O_2$	7505-12-6
Ethyltrichloroacetate	$C_4H_5Cl_3O_2$	515-84-4
Ethyltrichlorosilane	$C_2H_5Cl_3Si$	115-21-9
Ethylurea	$C_3H_8N_2O$	625-52-5
17α-Ethynyl-17β-hydroxy-19-nor-4-androsten-3-one	$C_{20}H_{26}O_2$	68-22-4
17α-Ethynyl-17β-hydroxy-19-nor-4-androsten-3-one acetate	$C_{22}H_{28}O_3$	51-98-9
Eugenol	$C_{10}H_{12}O_2$	97-53-0

F

Ferrocene	$C_{10}H_{10}Fe$	102-54-5
Ferrocene-d_{10}	$C_{10}D_{10}Fe$	12082-87-0
Ferrocene-d_{10} thiourea clathrate (1:3)	$C_{13}H_{12}D_{10}FeN_6S_3$	108339-57-7
Ferrocenium hexafluorophosphate	$C_{10}H_{10}F_6FeP$	11077-24-0
Fluoranthene	$C_{16}H_{10}$	206-44-0
Fluoranthene-picric acid	$C_{22}H_{13}N_3O_7$	34532-28-0
Fluorene	$C_{13}H_{10}$	86-73-7
Fluorene-picric acid	$C_{19}H_{13}N_3O_7$	64580-92-3
1-Fluoroadamantane	$C_{10}H_{15}F$	768-92-3
p-Fluoroaniline	C_6H_6FN	371-40-4
Fluorobenzene	C_6H_5F	462-06-6
Fluoroform	CHF_3	75-46-7
2-Fluoronaphthalene	$C_{10}H_7F$	323-09-1
p-Fluorophenol	C_6H_5FO	371-41-5
2-Fluorotoluene	C_7H_7F	95-52-3
3-Fluorotoluene	C_7H_7F	352-70-5
4-Fluorotoluene	C_7H_7F	352-32-9
Fluorotrichloromethane	CCl_3F	75-69-4
Formaldehyde,dimethylacetal	$C_3H_8O_2$	109-87-5
Formamide	CH_3NO	75-12-7
Formic acid	CH_2O_2	64-18-6
Freon 11	CCl_3F	75-69-4
Freon 12	CCl_2F_2	75-71-8
Freon 14	CF_4	75-73-0
Freon 21	$CHCl_2F$	75-43-4
Freon 22	$CHClF_2$	75-45-6
Freon 23	CHF_3	75-46-7
Freon 113	$C_2Cl_3F_3$	76-13-1
Freon 114	$C_2Cl_2F_4$	76-14-2
Freon-122	$C_2HCl_3F_2$	354-21-2
Freon-132	$C_2H_2Cl_2F_2$	431-06-1
Freon 143	$C_2H_3F_3$	420-46-2
Freon 152a	$C_2H_4F_2$	75-37-6
Freon C318	C_4F_8	115-25-3
Fructose	$C_6H_{12}O_6$	7660-25-5
Fullerene	C_{60}	99685-96-8
Fullerene epoxide	$C_{60}O$	135105-53-2
Fumaric acid	$C_4H_4O_4$	110-17-8
Furan	C_4H_4O	110-00-9
Furfural	$C_5H_4O_2$	98-01-1
Furfuraldehyde	$C_5H_4O_2$	98-01-1
Furfuryl alcohol	$C_5H_6O_2$	98-00-0

G

Gadolinium isothiocyanate hexahydrate	$C_3GdN_3S_3\cdot 6H_2O$	94007-91-7
Galactitol	$C_6H_{14}O_6$	608-66-2
Galactose	$C_6H_{12}O_6$	59-23-4
α-Galactose(D)	$C_6H_{12}O_6$	59-23-4
Gallium triethyl	$C_6H_{15}Ga$	1115-99-7
Galvinoxyl hydrogalvinoxyl (6:1) radical	$C_{203}H_{288}O_{14}$	120660-76-6
Galvinoxyl hydrogalvinoxyl (9:1) radical	$C_{290}H_{411}O_{20}$	120660-77-7
Galvinoxyl radical	$C_{29}H_{41}O_2$	2370-18-5
Geranial	$C_{10}H_{16}O$	141-27-5
Germanium tetraethyl	$C_8H_{20}Ge$	597-63-7
Glassy carbon	C	7440-44-0

α-Glucose(D)	$C_6H_{12}O_6$	492-62-6
α-Glucose pentaacetate(D)	$C_{16}H_{22}O_{22}$	604-68-2
β-Glucose pentaacetate(D)	$C_{16}H_{22}O_{22}$	604-69-3
Glutamic acid	$C_5H_9NO_4$	56-86-0
Glutamic acid(D)	$C_5H_9NO_4$	6893-26-1
Glutamic acid(L)	$C_5H_9NO_4$	56-86-0
Glutamic acid hydrochloride	$C_5H_{10}ClNO_4$	138-15-8
Glutamine(L)	$C_5H_{10}N_2O_3$	56-85-9
Glutaric acid	$C_5H_8O_4$	110-94-1
Glutaronitrile	$C_5H_6N_2$	544-13-8
Glycerol	$C_3H_8O_3$	56-81-5
Glycerol-d_3	$C_3H_5D_3O_3$	7325-16-8
Glyceryl triacetate	$C_9H_{14}O_6$	102-76-1
Glyceryl tributyrate	$C_{15}H_{26}O_6$	60-01-5
Glyceryl tricaproate	$C_{21}H_{38}O_6$	621-70-5
Glyceryl tridecanoate	$C_{33}H_{62}O_6$	621-71-6
Glyceryl trilaurate	$C_{39}H_{74}O_6$	538-24-9
Glyceryl trimargarate	$C_{54}H_{104}O_6$	2438-40-6
Glyceryl trimyristate	$C_{45}H_{86}O_6$	555-45-3
Glyceryl trioctanoate	$C_{27}H_{50}O_6$	538-23-8
Glyceryl tripalmitate	$C_{51}H_{98}O_6$	555-44-2
Glyceryl tristearate	$C_{57}H_{110}O_6$	555-43-1
Glycine	$C_2H_5NO_2$	56-40-6
Glycolide	$C_4H_4O_4$	502-97-6
Glycylglycine	$C_4H_8N_2O_3$	556-50-3
Gramine	$C_{11}H_{14}N_2$	87-52-5
Graphite	C	7782-42-5
Graphite, Acheson	C	7782-42-5
Graphite, Acheson, irradiated	C	7782-42-5
Graphite, natural Taiguinsk	C	7782-42-5
Graphite, pyrolytic	C	7782-42-5
Guanidine carbonate	$C_2H_7N_3O_3$	593-85-1
Guanine	$C_5H_5N_5O$	73-40-5

H

n-Heneicosane	$C_{21}H_{44}$	629-94-7
n-Hentriacontane	$C_{31}H_{64}$	630-04-6
n-Heptacosane	$C_{27}H_{56}$	593-49-7
n-Heptadecane	$C_{17}H_{36}$	629-78-7
Heptadecanoic acid	$C_{17}H_{34}O_2$	506-12-7
1-Heptadecanol	$C_{17}H_{36}O$	1454-85-9
n-Heptadecyl alcohol	$C_{17}H_{36}O$	123-24-0
1,1,1,2,3,3,3-Heptafluoropropane	C_3HF_7	431-89-0
n-Heptaldehyde	$C_7H_{14}O$	111-71-7
2,2,4,4,6,8,8-Heptamethylnonane	$C_{16}H_{34}$	4390-04-9
1,1,1,3,5,5,5-Heptamethyl-3-phenyltrisiloxane	$C_{13}H_{26}O_2Si_3$	546-44-1
Heptanal	$C_7H_{14}O$	111-71-7
n-Heptane	C_7H_{16}	142-82-5
1-Heptanethiol	$C_7H_{16}S$	1639-09-4
Heptanoic acid	$C_7H_{14}O_2$	111-14-8
1-Heptanol	$C_7H_{16}O$	111-70-6
4-Heptanol	$C_7H_{16}O$	589-55-9
1-Heptene	C_7H_{14}	592-76-7
4-*n*-Heptoxyphenyl-4′-*n*-butylbenzoate	$C_{24}H_{32}O_3$	38454-35-2
n-Heptyl alcohol	$C_7H_{16}O$	111-70-6
n-Heptylbenzene	$C_{13}H_{20}$	1078-71-3
4-*n*-Heptylbicyclohexyl	$C_{19}H_{36}$	96667-88-8
n-Heptyl bromide	$C_7H_{15}Br$	629-04-9
n-Heptyl chloride	$C_7H_{15}Cl$	629-06-1
n-Heptylcyclohexane	$C_{13}H_{26}$	5617-41-4
n-Heptyl iodide	$C_7H_{15}I$	4282-40-0
n-Heptyl mercaptan	$C_7H_{16}S$	1639-09-4
4-*n*-Heptyltercyclohexyl	$C_{25}H_{46}$	unavailable
4′-*n*-Heptyl-*m*-tercyclohexyl	$C_{25}H_{46}$	unavailable
Hexachlorobenzene	C_6Cl_6	118-74-1
γ-Hexachlorocyclohexane	$C_6H_6Cl_6$	58-89-9
Hexachlorocyclopropane	C_3Cl_6	2065-35-2
Hexachloroethane	C_2Cl_6	67-72-1
n-Hexacosane	$C_{26}H_{54}$	630-01-3
Hexacyclopropylethane	$C_{20}H_{30}$	26902-55-6
Hexadecafluoro-3-butyltetrahydrofuran	$C_8F_{16}O$	500005-57-
Hexadecafluorodimethylcyclohexane	C_8F_{16}	26637-68-
Hexadecafluoroheptane	C_7F_{16}	335-57-
n-Hexadecane	$C_{16}H_{34}$	544-76-
1-Hexadecanethiol	$C_{16}H_{34}S$	2917-26-
Hexadecanoic acid	$C_{16}H_{32}O_2$	57-10-
1-Hexadecanol	$C_{16}H_{34}O$	36653-82-
Hexa-*o*-decanoyl-scyllo-inositol	$C_{66}H_{120}O_{12}$	99409-67-
1-Hexadecene	$C_{16}H_{32}$	629-73-
1-Hexadecene-urea adduct	$C_{2.3}H_{6.7}N_2O$	24494-57-
n-Hexadecyl mercaptan	$C_{16}H_{34}S$	2917-26-
1,5-Hexadiene	C_6H_{10}	592-42-
2,4-Hexadiyne	C_6H_6	2809-69-
Hexaethylbenzene	$C_{18}H_{30}$	604-88-
Hexaethylcyclohexane	$C_{18}H_{36}$	98803-61-
1,1,3,3,5,5-Hexaethylcyclotrisiloxane	$C_{12}H_{30}O_3Si_3$	2031-79-
Hexaethyldisiloxane	$C_{12}H_{30}OSi_2$	994-49-
Hexaethylene glycol	$C_{12}H_{26}O_7$	2615-15-
Hexafluoroacetone	C_3F_6O	684-16-
Hexafluorobenzene	C_6F_6	392-56-
Hexafluoroethane	C_2F_6	76-16-
Hexafluoropropanone	C_3F_6O	684-16-
Hexa-*o*-hexanoyl-scyllo-inositol	$C_{42}H_{72}O_{12}$	88269-10-
2,3,6,7,10,11-Hexa-*n*-hexyloxytriphenylene	$C_{54}H_{84}O_6$	70351-86-
4bα,4cβ,5,9bβ,9cα,10-Hexahydrocyclabuta-[1,2-a:3,4-a′]diindene	$C_{18}H_{16}$	25456-55-
4bβ,4cα,9,9aα,9bβ,10-Hexahydrocyclobuta-[1,2-a:4,3-a′]diindene	$C_{18}H_{16}$	23358-17-
Hexahydroindan	C_9H_{16}	496-10-
cis-Hexahydroindan	C_9H_{16}	4551-51-
trans-Hexahydroindan	C_9H_{16}	3296-50-
1,2,3,6,7,8-Hexahydropyrene	$C_{16}H_{16}$	1732-13-
Hexahydroxyhexaethylenediamine chromium sulfate decahydrate	$C_{12}H_{54}Cr_4N_{12}O_{18}S_3 \cdot 10H_2O$	35705-97-
Hexakis(μ-acetato)(μ$_3$-oxo)tris(pyridine) iron(II)diiron(III) chloroform	$C_{28}H_{34}Cl_3Fe_3N_3O_{13}$	117799-61-
Hexakis(μ-acetato)(μ$_3$-oxo)tris(pyridine) trimanganese·pyridine	$C_{32}H_{38}Mn_3N_4O_{13}$	109839-55-
2,3,6,7,10,11-Hexakis(1-decynyl)triphenylene	$C_{78}H_{108}$	125594-11-
2,3,6,7,10,11-Hexakis[(4-heptylphenyl) ethynyl]triphenylene	$C_{108}H_{120}$	125594-09-
Hexakis[(4-hexylphenyl)ethynyl]benzene	$C_{90}H_{102}$	125594-06-
Hexakis[(4-pentylphenyl)ethynyl]benzene	$C_{84}H_{90}$	125594-05-
2,3,6,7,10,11-Hexakis[(4-pentylphenyl) ethynyl]triphenylene	$C_{96}H_{96}$	125594-08-
Hexamethylbenzene	$C_{12}H_{18}$	87-85-
Hexamethylbenzene, deuterated	$C_{12}D_{18}$	4342-40-
Hexamethylcyclotrisilazane	$C_6H_{21}N_3Si_3$	1009-93-
Hexamethylcyclotrisiloxane	$C_6H_{18}O_3Si_3$	541-05-
1,1,3,3,5,5-Hexamethyl-7,7-diphenylcyclotetrasiloxane	$C_{18}H_{28}O_4Si_4$	1693-44-
1,1,1,5,5,5-Hexamethyl-3,3-diphenyltrisiloxane	$C_{24}H_{28}O_2Si_3$	797-77-
Hexamethyldisilane	$C_6H_{18}Si_2$	1450-14-
Hexamethyldisiloxane	$C_6H_{18}OSi_2$	107-46-
Hexamethyldisilylmethane	$C_7H_{20}Si_2$	2117-28-
1,6-Hexamethylene diisocyanate	$C_8H_{12}N_2O_2$	822-06-
1,6-Hexamethylene diisocyanate polycyclotrimer	$(C_8H_{12}N_2O_2)_n$	28182-81-
Hexamethyleneimine	$C_6H_{13}N$	111-49-
Hexamethylenetetramine	$C_6H_{12}N_4$	100-97-
Hexamethylphosphoramide	$C_6H_{18}N_3OP$	680-31-
Hexamethylphosphoric triamide	$C_6H_{18}N_3OP$	680-31-
cis-(5,12)-7,7,14,14-Hexamethyl-1,4,8,11-tetraazacyclotetradecane	$C_{16}H_{36}N_4$	56144-66-
2,6,10,15,19,23-Hexamethyltetracosane	$C_{30}H_{62}$	111-01-
1,1,3,3,5,5-Hexamethyl-1,3,5-trisilacyclohexane	$C_9H_{24}Si_3$	1627-99-
1-Hexanal	$C_6H_{12}O$	66-25-
n-Hexane	C_6H_{14}	110-54-
1,6-Hexanedioic acid	$C_6H_{10}O_4$	124-04-

1,6-Hexanediol	$C_6H_{14}O_2$	629-11-8
1-Hexanethiol	$C_6H_{14}S$	111-31-9
Hexanitroethane	$C_2N_6O_{12}$	918-37-6
Hexanoic acid	$C_6H_{12}O_2$	142-62-1
1-Hexanol	$C_6H_{14}O$	111-27-3
2-Hexanol	$C_6H_{14}O$	626-93-7
3-Hexanol	$C_6H_{14}O$	623-37-0
2-Hexanone	$C_6H_{12}O$	591-78-6
3-Hexanone	$C_6H_{12}O$	107-87-9
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene	$C_{66}H_{96}O_{12}$	70351-94-9
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid I)	$C_{66}H_{96}O_{12}$	70351-94-9
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid II)	$C_{66}H_{96}O_{12}$	70351-94-9
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid III)	$C_{66}H_{96}O_{12}$	70351-94-9
Hexa-*o*-octanoyl-scyllo-inositol	$C_{54}H_{96}O_{12}$	98566-49-5
Hexaphenylcyclotrisiloxane	$C_{36}H_{30}O_3Si_3$	512-63-0
1,1,3,3,5,5-Hexaphenyl-7,7-dimethylcyclotetrasiloxane	$C_{38}H_{36}O_4Si_4$	1693-46-5
Hexaphenyldisiloxane	$C_{36}H_{30}OSi_2$	1829-40-9
Hexaphenylisomelamine	$C_{39}H_{30}N_6$	604-45-5
Hexaphenylmelamine	$C_{39}H_{30}N_6$	18343-40-3
Hexapropylene glycol	$C_{18}H_{38}O_7$	52794-80-6
n-Hexatriacontane	$C_{36}H_{74}$	630-06-8
1-Hexene	C_6H_{12}	592-41-6
cis-2-Hexene	C_6H_{12}	7688-21-3
1-Hexene polysulfone	$(C_6H_{12}O_2S)_n$	34903-07-6
Hexogen	$C_3H_6N_6O_6$	121-82-4
4-*n*-Hexoxyphenyl-4′-*n*-decyloxybenzoate	$C_{29}H_{42}O_4$	68162-09-4
n-Hexyl alcohol	$C_6H_{14}O$	11-27-3
n-Hexylamine	$C_6H_{15}N$	111-26-2
n-Hexylbenzene	$C_{12}H_{18}$	1077-16-3
n-Hexyl bromide	$C_6H_{13}Br$	111-25-1
n-Hexyl chloride	$C_6H_{13}Cl$	544-10-5
17-[[(4-Hexylcyclohexyl)carbonyl]oxy]-[17α,17(*trans*)]-19-norpregn-4-en-20-yn-3-one	$C_{33}H_{48}O_3$	71203-37-7
Hexyl ethanoate	$C_8H_{16}O_2$	142-92-7
n-Hexyl iodide	$C_6H_{13}I$	638-45-9
n-Hexyl mercaptan	$C_6H_{14}S$	111-31-9
p-*n*-Hexyloxybenzylideneamino-*p*′-benzonitrile	$C_{20}H_{22}N_2O$	35280-78-5
p-*n*-Hexyloxybenzylideneamino-*p*′-chlorobenzene	$C_{19}H_{22}ClNO$	5219-48-7
p-*n*-Hexyloxybenzylideneamino-*p*′-fluorobenzene	$C_{19}H_{22}FNO$	56544-26-4
p-*n*-Hexyloxybenzylideneaniline	$C_{19}H_{23}NO$	5219-49-8
N-*p*-*n*-Hexyloxybenzylidene-*p*′-*n*-butylaniline	$C_{23}H_{31}NO$	29743-11-1
p-*n*-Hexyloxybenzylidene-*p*′-toluidine	$C_{20}H_{25}NO$	25959-51-7
Hexyl N-phenylcarbamate	$C_{13}H_{19}NO_2$	unavailable
1-Hexynylcopper	C_6H_9Cu	33589-44-5
Hippuric acid	$C_9H_9NO_3$	495-69-2
Hippurylglycine	$C_{11}H_{12}N_2O_4$	1145-32-0
Histidine hydrochloride(L)	$C_6H_{10}ClN_3O_2$	1007-42-7
HMX	$C_4H_8N_8O_8$	2691-41-0
Homocubane-4-carboxylic acid	$C_{10}H_{10}O_2$	15844-05-0
Hydrazinium hydrogen oxalate	$C_2H_6N_2O_4$	20321-02-2
Hydrogen cyanide	CHN	74-90-8
Hydroquinone	$C_6H_6O_2$	123-31-9
o-Hydroxyacetanilide	$C_8H_9NO_2$	614-80-2
1-Hydroxyadamantane	$C_{10}H_{16}O$	768-95-6
2-Hydroxyadamantane	$C_{10}H_{16}O$	700-57-2
2-Hydroxybenzaldehyde	$C_7H_6O_2$	90-02-8
Hydroxybenzene	C_6H_6O	108-95-2
m-Hydroxybenzoic acid	$C_7H_6O_3$	99-06-9
o-Hydroxybenzoic acid	$C_7H_6O_3$	69-72-7
p-Hydroxybenzoic acid	$C_7H_6O_3$	99-96-7
o-Hydroxybiphenyl	$C_{12}H_{10}O$	90-43-7
Hydroxybutanedioic acid	$C_4H_6O_5$	6915-15-7
2-(2′-Hydroxyethoxy)ethyl pivalate	$C_9H_{18}O_4$	20267-21-4
2-Hydroxyethyl-2′,2′-dimethylpropionate	$C_7H_{14}O_3$	20267-19-0
2-Hydroxyethyl pivalate	$C_7H_{14}O_3$	20267-19-0
N-(2-Hydroxy-4-methoxybenzylidene)-*p*-butylaniline	$C_{18}H_{21}NO_2$	30633-94-4
2-Hydroxy-4-(methoxymethyl)-6-methyl-5-nitro-3-pyridinecarbonitrile	$C_9H_9N_3O_4$	6281-75-0
5-Hydroxy-4-(methoxymethyl)-6-methyl-3-pyridinemethanol	$C_9H_{13}NO_3$	1464-33-1
2-Hydroxymethyl-2-methyl-1,3-propanediol	$C_5H_{12}O_3$	77-85-0
2-Hydroxymethyl-2-methyl-1,3-propanediol tetrahydrate	$C_5H_{12}O_3{\cdot}4H_2O$	142381-76-8
5-Hydroxy-6-methyl-3,4-pyridinedimethanol	$C_8H_{11}NO_3$	65-23-6
1-Hydroxynaphthalene	$C_{10}H_8O$	90-15-3
2-Hydroxynaphthalene	$C_{10}H_8O$	135-19-3
17-Hydroxy-(17α)-19-norpregn-4-en-20-yn-3-one	$C_{20}H_{26}O_2$	68-22-4
2-Hydroxymethyl-2-nitro-1,3-propanediol	$C_4H_9NO_5$	126-11-4
2,3-Hydroxynaphthalene	$C_{10}H_8O_2$	92-44-4
4-*p*-Hydroxyphenyl-2,2,4-trimethylchroman	$C_{18}H_{20}O_2$	472-41-3
2-Hydroxypropanoic acid(D)	$C_3H_6O_3$	10326-41-7
2-Hydroxypropanoic acid(DL)	$C_3H_6O_3$	50-21-5
2-Hydroxypropanoic acid(L)	$C_3H_6O_3$	79-33-4
m-Hydroxytoluene	C_7H_8O	108-39-4
o-Hydroxytoluene	C_7H_8O	95-48-7
p-Hydroxytoluene	C_7H_8O	106-44-5
anti^{9,10}-10-endo-Hydroxytricyclo[4.2.1.1^{2,5}]deca-3,7-dien-9-one	$C_{10}H_{10}O_2$	65181-88-6
Hypoxanthine	$C_5H_4N_4O$	68-94-0
I		
Idryl	$C_{16}H_{10}$	206-44-0
Imidazole	$C_3H_4N_2$	288-32-4
2-Imino-4-thiazolidinone	$C_3H_4N_2S$	556-90-1
Indane	C_9H_{10}	496-11-7
Indazole	$C_7H_6N_2$	271-44-3
Indene	C_9H_8	95-13-6
Indene picric acid	$C_{15}H_{11}N_3O_7$	72454-47-8
Indole	C_8H_7N	120-72-9
3-Indole aldehyde	C_9H_7NO	487-89-8
meso-Inositol	$C_6H_{12}O_6$	87-89-8
myo-Inositol	$C_6H_{12}O_6$	87-89-8
Iodobenzene	C_6H_5I	591-50-4
4-Iodobenzoic acid	$C_7H_5IO_2$	619-58-9
Iodobis(N,N-diethyldithioearbamato) iron(III)	$C_{10}H_{20}FeIN_2S_4$	38246-70-7
Iodobis(N,N-dimethyldithiocarbamato) iron(III)	$C_6H_{12}FeIN_2S_4$	23672-38-0
1-Iodobutane	C_4H_9I	542-69-8
2-Iodobutane	C_4H_9I	513-48-4
Iodoethane	C_2H_5I	75-03-6
Iodoform	CHI_3	75-47-8
1-Iodoheptane	$C_7H_{15}I$	4282-40-0
1-Iodohexane	$C_6H_{13}I$	638-45-9
Iodomethane	CH_3I	74-88-9
1-Iodo-3-methylbutane	$C_5H_{11}I$	541-28-6
1-Iodo-2-methylpropane	C_4H_9I	513-38-2
1-Iodopentane	$C_5H_{11}I$	628-17-1
1-Iodopropane	C_3H_7I	107-08-4
2-Iodopropane	C_3H_7I	75-30-9
Iron (III) acetylacetonate	$C_{15}H_{21}FeO_6$	14024-18-1
Isoamyl alcohol	$C_5H_{12}O$	123-51-3
Isoamyl bromide	$C_5H_{11}Br$	107-82-4
Isoamyl chloride	$C_5H_{11}Cl$	107-84-6
Isoamyl iodide	$C_5H_{11}I$	541-28-6
Isoamyl mercaptan	$C_5H_{12}S$	541-31-1
Isoamyl propionate	$C_8H_{16}O_2$	105-68-0
Isobutane	C_4H_{10}	75-28-5
Isobutene	C_4H_8	115-11-7

Isobutylamine	$C_4H_{11}N$	78-81-9
Isobutyl acetate	$C_6H_{12}O_2$	110-19-0
Isobutyl alcohol	$C_4H_{10}O$	78-83-1
Isobutyl bromide	C_4H_9Br	78-77-3
Isobutyl chloride	C_4H_9Cl	513-36-0
α-Isobutyldecalin	$C_{14}H_{26}$	92369-83-0
Isobutyl formate	$C_5H_{10}O_2$	542-55-2
Isobutyl iodide	C_4H_9I	513-38-2
Isobutyl mercaptan	$C_4H_{10}S$	513-44-0
Isobutylmethylketone	$C_6H_{12}O$	108-10-1
Isobutyric acid	$C_4H_8O_2$	79-31-2
Isobutyryl chloride	C_4H_7ClO	79-30-1
Isochroman	$C_9H_{10}O$	493-05-0
1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl) benzene	$C_{13}H_{15}NO$	2094-99-7
1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl) benzene	$C_{13}H_{15}NO$	2889-58-9
1-Isocyanobicyclo[2.2.1]heptane	$C_8H_{11}N$	88523-51-7
Isocyanocyclohexane	$C_7H_{11}N$	931-53-3
Isodurene	$C_{10}H_{14}$	527-53-7
Isoleucine(L)	$C_6H_{13}NO_2$	73-32-5
Isonicotinic acid	$C_6H_5NO_2$	55-22-1
Isonitrosoacetanilide	$C_8H_8N_2O_2$	1769-41-1
Isooctane	C_8H_{18}	540-84-1
Isooctyl alcohol	$C_8H_{18}O$	26952-21-6
Isopentane	C_5H_{12}	78-78-4
Isophthalic acid	$C_8H_6O_4$	88-99-3
Isophthalyl dichloride	$C_8H_4Cl_2O_2$	99-63-8
Isophytol	$C_{20}H_{38}O$	60046-87-9
Isoprene	C_5H_8	78-79-5
2-Isopropoxyethanol	$C_5H_{12}O_2$	2167-39-7
N-Isopropylacetamide	$C_5H_{11}NO$	1118-69-0
Isopropyl acetate	$C_5H_{10}O_2$	108-21-4
Isopropyl alcohol	C_3H_8O	67-63-0
Isopropylamine	C_3H_9N	75-31-0
Isopropylamine nitrate	$C_3H_{10}N_2O_3$	87478-71-5
Isopropylbenzene	C_9H_{12}	98-82-8
Isopropylbicyclohexyl	$C_{15}H_{28}$	unavailable
2-Isopropylbicyclohexyl	$C_{15}H_{28}$	66374-73-0
Isopropylbiphenyl	$C_{15}H_{16}$	7116-95-2
p-Isopropylbiphenyl	$C_{15}H_{16}$	7116-95-2
Isopropyl bromide	C_3H_7Br	75-26-3
Isopropyl cyanide	C_4H_7N	78-82-0
Isopropyldecalin	$C_{13}H_{24}$	27193-29-9
α-Isopropyldecalin	$C_{13}H_{24}$	1010-74-8
Isopropyl ether	$C_6H_{14}O$	108-20-3
Isopropylhydroindan	$C_{12}H_{22}$	unavailable
Isopropyl iodide	C_3H_7I	75-30-9
Isopropyl mercaptan	C_3H_8S	75-33-2
1-Isopropyl-4-methylbenzene	$C_{10}H_{14}$	99-87-6
Isopropyl methyl ketone	$C_5H_{10}O$	563-80-4
Isopropyl methyl sulfide	$C_4H_{10}S$	1551-21-9
Isopropyl nitrate	$C_3H_7NO_3$	1712-64-7
Isopropylurea	$C_4H_{10}N_2O$	691-60-1
Isoquinoline	C_9H_7N	119-65-3
Isovaleric acid	$C_5H_{10}O_2$	503-74-2
Isoxazole	C_3H_3NO	288-14-2

L

Lactic acid(D)	$C_3H_6O_3$	10326-41-7
Lactic acid(DL)	$C_3H_6O_3$	50-21-5
Lactic acid(L)	$C_3H_6O_3$	79-33-4
Lactide(DL)	$C_6H_8O_4$	615-95-2
Lactose	$C_{12}H_{22}O_{11}$	63-42-3
β-Lactose	$C_{12}H_{22}O_{11}$	5965-66-2
α-Lactose monohydrate	$C_{12}H_{22}O_{11}\cdot H_2O$	5989-81-1
β-Lactose monohydrate	$C_{12}H_{22}O_{11}\cdot H_2O$	5989-81-1
Lanthanum isothiocyanate heptahydrate	$C_3LaN_3S_3\cdot 7H_2O$	113614-87-2
Latex	$(C_5H_8)_n$	9016-00-6
Lauric acid	$C_{12}H_{24}O_2$	143-07-7
Lead(II) decanoate	$C_{20}H_{38}O_4Pb$	15773-52-
Lead dicalcium propionate	$C_{18}H_{30}Ca_2O_{12}Pb$	17203-66-
Lead(II) n-dodecanoate	$C_{24}H_{46}O_4Pb$	15773-55-
Lead(II) enanthate	$C_{14}H_{26}O_4Pb$	21180-26-
Lead(II) heptadecanoate	$C_{34}H_{66}O_4Pb$	63399-94-
Lead(II) heptanoate	$C_{14}H_{26}O_4Pb$	21180-26-
Lead(II) n-hexadecanoate	$C_{32}H_{62}O_4Pb$	15773-56-
Lead(II) n-hexanoate	$C_{12}H_{22}O_4Pb$	15773-53-
Lead(II) nonadecanoate	$C_{38}H_{74}O_4Pb$	69065-37-
Lead(II) nonanoate	$C_{18}H_{34}O_4Pb$	63400-08-
Lead(II) n-octadecanoate	$C_{36}H_{70}O_4Pb$	1072-35-
Lead(II) n-octanoate	$C_{16}H_{30}O_4Pb$	7319-86-
Lead(II) oenanthate	$C_{14}H_{26}O_4Pb$	21180-26-
Lead(II) oxalate	C_2O_4Pb	21180-26-
Lead(II) pelargonate	$C_{18}H_{34}O_4Pb$	63400-08-
Lead(II) pentadecanoate	$C_{30}H_{58}O_4Pb$	63400-06-
Lead(II) n-tetradecanoate	$C_{28}H_{54}O_4Pb$	32112-52-
Lead(II) tridecanoate	$C_{26}H_{50}O_4Pb$	50354-80-
Lead(II) undecanoate	$C_{22}H_{42}O_4Pb$	63400-07-
Leucine(DL)	$C_6H_{13}NO_2$	328-39-
Leucine(L)	$C_6H_{13}NO_2$	61-90-
Leucylglycine(DL)	$C_8H_{16}N_2O_3$	615-82-
Lexan polycarbonate	$(C_{16}H_{14}O_3)_n$	24936-68-
Limonene	$C_{10}H_{16}$	138-86-
Linalool	$C_{10}H_{18}O$	78-70-
Lindane	$C_6H_6Cl_6$	58-89-
Lithium acetate	$C_2H_3LiO_2$	546-89-
Lithium acetate dihydrate	$C_2H_3LiO_2\cdot 2H_2O$	6108-17-
Lithium butyrate	$C_4H_7LiO_2$	21303-03-
Lithium formate	$CHLiO_2$	556-63-
Lithium heptanoate	$C_7H_{13}LiO_2$	16761-13-
Lithium n-hexanoate	$C_6H_{11}LiO_2$	16577-51-
Lithium 2-methylpropanoate	$C_4H_7LiO_2$	25179-23-
Lithium n-pentanoate	$C_5H_9LiO_2$	38869-19-
Lithium propionate	$C_3H_5LiO_2$	6531-45-
Lutetium ethylsulfate	$C_6H_{15}LuO_{12}S_3\cdot 9H_2O$	unavailab
2,3-Lutidine	C_7H_9N	583-61-

M

Magnesium acetate	$C_4H_6O_4Mg$	142-72-
Magnesium diacetate tetrahydrate	$C_4H_6O_4Mg\cdot 4H_2O$	16674-78-
Magnesium diethanoate tetrahydrate	$C_4H_6O_4Mg\cdot 4H_2O$	16674-78-
Maleic acid	$C_4H_4O_4$	110-16-
Maleic anhydride	$C_4H_2O_3$	108-31-
Malic acid(DL)	$C_4H_6O_5$	617-48-
Malonamide	$C_3H_6N_2O_2$	108-13-
Malonic acid	$C_3H_4O_4$	141-82-
Malonic acid-d_4	$C_3D_4O_4$	813-56-
Malonic acid dimethyl ester	$C_5H_8O_4$	108-59-
Malononitrile	$C_3H_2N_2$	109-77-
Maltose	$C_{12}H_{22}O_{11}$	69-79-
Mandelic acid	$C_8H_8O_3$	90-64-
Manganese squarate clathrate	$C_{13.5}H_{15}O_{19.5}Mn\cdot 0.19H_2O$	129828-88-
Manganocene	$C_{10}H_{10}Mn$	73138-26-
Mannitol	$C_6H_{14}O_6$	69-65-
Mannitol(D)	$C_6H_{14}O_6$	69-65-
Mannose	$C_6H_{12}O_6$	3458-28-
Mannose(D)	$C_6H_{12}O_6$	3458-28-
Manxane	$C_{11}H_{20}$	29415-95-
Marlex 50 polymer	$(CH_2)_n$	9002-88-
Melamine	$C_3H_6N_6$	108-78-
Mercuric caprate	$C_{20}H_{38}HgO_4$	27394-49-
Mercuric caprylate	$C_{16}H_{30}HgO_4$	28043-54-
Mercuric decanoate	$C_{20}H_{38}HgO_4$	27394-49-
Mercuric dodecanoate	$C_{24}H_{46}HgO_4$	23186-25-
Mercuric hexadecanoate	$C_{32}H_{64}HgO_4$	16888-60-
Mercuric laurate	$C_{24}H_{46}HgO_4$	23186-25-
Mercuric myristate	$C_{28}H_{54}HgO_4$	36215-49-
Mercuric octadecanoate	$C_{36}H_{70}HgO_4$	645-99-
Mercuric octanoate	$C_{16}H_{30}HgO_4$	28043-54-

Mercuric palmitate	$C_{32}H_{64}HgO_4$	16888-60-1
Mercuric stearate	$C_{36}H_{70}HgO_4$	645-99-8
Mercuric tetradecanoate	$C_{28}H_{54}HgO_4$	36215-49-3
Mercury diphenyl	$C_{12}H_{10}Hg$	587-85-9
Mercury di(*p*-tolyl)	$C_{14}H_{14}Hg$	537-64-4
Mesitol	$C_9H_{12}O$	527-60-6
Mesitylene	C_9H_{12}	108-67-8
Mesityl oxide	$C_6H_{10}O$	141-79-7
2,2-Metacyclophane	$C_{16}H_{16}$	2319-27-3
Methacrylamide	C_4H_7NO	79-39-0
Methacrylic acid	$C_4H_6O_2$	79-41-4
Methacrylonitrile	C_4H_5N	126-98-7
p-Methacryloyloxybenzoic acid	$C_{11}H_{10}O_4$	15721-10-5
Methanamide	CH_3NO	75-12-7
Methane	CH_4	74-82-8
Methanethiol	CH_4S	74-15-0
Methanetricarboxylic acid triethyl ester	$C_{10}H_{16}O_6$	6279-86-3
Methanoic acid	CH_2O_2	64-18-6
Methanol	CH_4O	67-56-1
Methanol-d_1	CH_3DO	1455-13-6
Methanol-d_3	CHD_3O	1849-29-2
Methanol-d_4	CD_4O	811-98-3
Methionine	$C_5H_{11}NO_2S$	59-51-8
Methionine(L)	$C_5H_{11}NO_2S$	63-68-3
Methoxybenzene	C_7H_8O	100-66-3
4-Methoxybenzoic acid	$C_8H_8O_3$	100-09-4
α-Methoxybenzyl cyanide	C_9H_9NO	13031-13-5
N-(4-Methoxybenzylidene)-*p*-*n*-butylaniline	$C_{18}H_{21}NO$	26227-73-6
4-Methoxy-4′-butoxy-trans-stilbene	$C_{19}H_{22}O_2$	35135-42-3
4-Methoxy-4′-dodecoxy-trans-stilbene	$C_{27}H_{38}O_2$	35135-49-0
2-Methoxyethanol	$C_3H_8O_2$	109-86-4
2-Methoxyethanol acetate	$C_5H_{10}O_3$	110-49-6
4-Methoxy-4′-heptoxy-trans-stilbene	$C_{22}H_{28}O_2$	35135-45-6
4-Methoxy-4′-hexoxy-trans-stilbene	$C_{21}H_{26}O_2$	35135-44-5
2-Methoxyisonitrosoacetanilide	$C_9H_{10}N_2O_3$	6335-42-8
4-Methoxyisonitrosoacetanilide	$C_9H_{10}N_2O_3$	6335-41-7
Methoxymethane	C_2H_6O	115-10-6
4-Methoxy-4′-octoxy-trans-stilbene	$C_{23}H_{30}O_2$	35135-46-7
2-Methoxy-4′-pentoxy-trans-stilbene	$C_{20}H_{24}O_2$	35135-43-4
2-Methoxy-1-propene	C_4H_8O	116-11-0
3-Methoxypropionitrile	C_4H_7NO	110-67-8
3-Methoxypropylamine	$C_4H_{11}NO$	5332-73-0
Methyl acetate	$C_3H_6O_2$	79-20-9
Methyl acrylate	$C_4H_6O_2$	96-33-3
α-Methyl acrylic acid	$C_4H_6O_2$	79-41-4
Methylal	$C_3H_8O_2$	109-87-5
Methyl alcohol	CH_4O	67-56-1
Methyl alcohol-d_1	CH_3DO	1455-13-6
Methyl alchohol-d_3	CHD_3O	1849-29-2
Methyl alcohol-d_4	CD_4O	811-98-3
Methylamine	CH_5N	74-89-5
4-Methyl-7-aminocoumarin	$C_{10}H_9NO_2$	26093-31-2
2-Methyl-3-amino-4-methoxymethyl-5-aminomethylpyridine	$C_9H_{15}N_3O$	35623-09-7
2-Methyl-1-aminopropane	$C_4H_{11}N$	78-81-9
2-Methyl-2-aminopropane	$C_4H_{11}N$	75-64-9
Methyl ammonium aluminum alum	$CH_6AlNO_8S_2\cdot 12H_2O$	15243-18-2
Methylammonium bismuth bromide	$C_5H_{30}Bi_2Br_{11}N_5$	119931-90-7
Methylammonium bromide	CH_6BrN	6876-37-5
Methylammonium chloride	CH_5ClN	593-51-1
Methylammonium iodide	CH_6IN	14965-49-2
Methylammonium iodide-d_5	CD_5IN	14779-57-8
Methylammonium tin bromide	CH_6Br_3NSn	67908-85-4
Methylammonium tribromoplumbate(II)	CH_6Br_3NPb	69276-13-7
Methylammonium tribromostannate	CH_6Br_3NSn	67908-85-4
Methylammonium trichloroplumbate(II)	CH_6Cl_3NPb	69276-12-6
Methylammonium triiodoplumbate(II)	CH_6I_3NPb	69507-98-8
2-Methylaniline	C_7H_9N	95-53-4
3-Methylaniline	C_7H_9N	108-44-1
4-Methylaniline	C_7H_9N	106-49-0
N-Methylaniline	C_7H_9N	100-61-8
Methyl behenate	$C_{23}H_{46}O_2$	929-77-1
Methyl benzoate	$C_8H_8O_2$	93-58-3
2-Methylbenzoic acid	$C_8H_8O_2$	118-90-1
3-Methylbenzoic acid	$C_8H_8O_2$	99-04-7
4-Methylbenzoic acid	$C_8H_8O_2$	99-94-5
Methylbicyclo[1.1.0]butane-1-carboxylate	$C_6H_8O_2$	4935-01-7
2-Methylbicyclo[2.2.1]heptane(*exo*)	C_8H_{14}	872-78-6
2-Methylbicyclo[2.2.1]heptane(*endo*)	C_8H_{14}	765-90-2
2-Methylbicyclohexyl	$C_{13}H_{24}$	66324-47-8
2-Methylbicyclohexylmethane	$C_{14}H_{26}$	66826-96-8
Methyl bromide	CH_3Br	74-83-9
3-Methyl-1,2-butadiene	C_5H_8	598-25-4
2-Methyl-1,3-butadiene	C_5H_8	78-79-5
N-Methylbutanamide	$C_5H_{11}NO$	17794-44-4
2-Methylbutane	C_5H_{12}	78-78-4
2-Methyl-2-butanethiol	$C_5H_{12}S$	1679-09-0
3-Methyl-1-butanethiol	$C_5H_{12}S$	541-31-1
3-Methyl-2-butanethiol	$C_5H_{12}S$	2084-18-6
Methyl butanoate	$C_5H_{10}O_2$	623-42-7
3-Methylbutanoic acid	$C_5H_{10}O_2$	503-74-2
2-Methylbutanoic acid ethyl ester	$C_7H_{14}O_2$	7452-79-1
2-Methyl-2-butanol	$C_5H_{12}O$	75-85-4
3-Methyl-1-butanol	$C_5H_{12}O$	123-51-3
3-Methyl-2-butanol	$C_5H_{12}O$	598-75-4
3-Methyl-2-butanone	$C_5H_{10}O$	563-80-4
2-Methyl-1-butene	C_5H_{10}	563-46-2
2-Methyl-2-butene	C_5H_{10}	513-35-9
3-Methyl-1-butene	C_5H_{10}	563-45-1
2-Methyl-3-buten-2-ol	$C_5H_{10}O$	115-18-4
4-(2-Methylbutoxy)phenyl ester of 4-*n*-(decycloxybenzoic) acid (D)	$C_{28}H_{40}O_4$	74438-86-1
Methyl *n*-butyl ether	$C_5H_{12}O$	628-28-4
Methyl *tert*-butyl ether	$C_5H_{12}O$	1634-04-4
Methyl *n*-butyl ketone	$C_6H_{12}O$	591-78-6
Methyl *tert*-butyl ketone	$C_6H_{12}O$	75-97-8
Methyl *tert*-butyl sulfide	$C_5H_{12}S$	6163-64-0
Methyl butyrate	$C_5H_{10}O_2$	623-42-7
Methyl caprate	$C_{11}H_{22}O_2$	110-42-9
Methyl carbamate	$C_2H_5NO_2$	598-55-0
N-Methylcarbazole	$C_{13}H_{11}N$	1484-12-4
Methyl chloride	CH_3Cl	74-87-3
Methyl chloroform	$C_2H_3Cl_3$	71-55-6
Methyl cyanide	C_2H_3N	75-05-8
Methyl cyclobutanecarboxylate	$C_6H_{10}O_2$	765-85-5
Methylcyclohexane	C_7H_{14}	108-87-2
1-Methylcyclohexanol	$C_7H_{14}O$	590-67-0
2-Methylcyclohexanol	$C_7H_{14}O$	583-59-5
3-Methylcyclohexanol	$C_7H_{14}O$	591-23-1
4-Methylcyclohexanol	$C_7H_{14}O$	589-91-3
2-Methylcyclohexanone	$C_7H_{12}O$	583-60-8
3-Methylcyclohexanone	$C_7H_{12}O$	591-24-2
4-Methylcyclohexanone	$C_7H_{12}O$	589-92-4
4-Methylcyclohexene	C_7H_{12}	591-47-9
Methylcyclopentane	C_6H_{12}	96-37-7
1-Methylcyclopentene	C_6H_{10}	693-89-0
3-Methylcyclopentene	C_6H_{10}	1120-62-3
2-Methylcyclothiapentane	$C_5H_{10}S$	1795-09-1
3-Methylcyclothiapentane	$C_5H_{10}S$	1795-09-1
α-Methyldecalin	$C_{11}H_{20}$	2958-75-0
β-Methyldecalin	$C_{11}H_{20}$	2958-75-0
2-Methyldecane	$C_{11}H_{24}$	6975-98-0
Methyldecanoate	$C_{11}H_{22}O_2$	110-42-9
Methyl *n*-decyl ether	$C_{11}H_{24}O$	7289-52-3
4-Methyl-7-diethylaminocoumarin	$C_{14}H_{17}NO_2$	91-44-1
1-Methyl-2,4-diisocyanatobenzene	$C_9H_6N_2O_2$	584-84-9

4-Methyl-7-dimethylaminocoumarin	$C_{12}H_{13}NO_2$	87-01-4
Methyl 2,2-dimethylpropanoate	$C_6H_{12}O_2$	598-98-1
4-Methyl-3,5-dioxaheptane	$C_6H_{14}O_2$	105-57-7
6-Methyl-5,7-dioxaundecane	$C_{10}H_{22}O_2$	871-22-7
4-Methyl-1,3-dioxolan-2-one	$C_5H_{10}O_3$	108-32-7
Methyldiphenylamine	$C_{13}H_{13}N$	552-82-9
Methyl eicosanoate	$C_{21}H_{42}O_2$	1120-28-1
Methyl enanthoate	$C_8H_{16}O_2$	106-73-0
3,3′-Methylene bis(6-aminophenol)	$C_{13}H_{14}N_2O_2$	22428-30-4
Methylene bromide	CH_2Br_2	74-95-3
Methylenecyclobutane	C_5H_8	1120-56-5
3-Methylenecyclobutyl cyanide	C_6H_7N	15760-35-7
Methylenecyclohexane	C_7H_{12}	1192-37-6
Methylene dichloride	CH_2Cl_2	75-09-2
Methylene glycol acetate	$C_3H_6O_3$	628-51-3
Methylene glycol diacetate	$C_3H_6O_3$	628-51-3
Methylene iodide	CH_2I_2	75-11-6
Methyl ester of nitroacetic acid	$C_3H_5NO_4$	2483-57-0
Methyl ethanoate	$C_3H_6O_2$	79-20-9
N-(1-Methylethyl)ethanamide	$C_5H_{11}NO$	1118-69-0
1-Methylethyl ethanoate	$C_5H_{10}O_2$	108-21-4
Methylethylethanolamine	$C_5H_{13}NO$	2893-43-8
Methyl ethyl ketone	C_4H_8O	78-93-3
Methyl ethyl ketoxime	C_4H_9NO	96-29-7
N-Methylformamide	C_2H_5NO	123-39-7
Methyl formate	$C_2H_4O_2$	107-31-3
2-Methylfuran	C_5H_6O	534-22-5
N-Methylglycine	$C_3H_7NO_2$	107-97-1
2-Methylheptane	C_8H_{18}	592-27-8
3-Methylheptane	C_8H_{18}	111002-96-1
4-Methylheptane	C_8H_{18}	589-53-7
Methyl heptanoate	$C_8H_{16}O_2$	106-73-0
2-Methyl-1-heptanol	$C_8H_{18}O$	60435-70-3
2-Methyl-2-heptanol	$C_8H_{18}O$	625-25-2
2-Methyl-4-heptanol	$C_8H_{18}O$	21570-35-4
3-Methyl-2-heptanol	$C_8H_{18}O$	31367-46-1
4-Methyl-2-heptanol	$C_8H_{18}O$	56298-90-9
4-Methyl-3-heptanol	$C_8H_{18}O$	14979-39-6
4-Methyl-4-heptanol	$C_8H_{18}O$	598-01-6
5-Methyl-1-heptanol	$C_8H_{18}O$	7212-53-5
5-Methyl-2-heptanol	$C_8H_{18}O$	54630-50-1
6-Methyl-2-heptanol	$C_8H_{18}O$	4730-22-7
6-Methyl-3-heptanol	$C_8H_{18}O$	18720-66-6
6-Methyl-5-hepten-2-one	$C_8H_{14}O$	110-93-0
Methyl hexadecanoate	$C_{17}H_{34}O_2$	112-39-0
3-Methylhexanal	$C_7H_{14}O$	19269-28-4
2-Methylhexane	C_7H_{16}	591-76-4
3-Methylhexane	C_7H_{16}	589-34-4
Methyl hexyl ketone	$C_8H_{16}O$	111-13-7
Methylhydrazine	CH_6N_2	60-34-4
Methylhydroindan	$C_{10}H_{18}$	unavailable
4-Methyl-7-hydroxycoumarin	$C_{10}H_8O_3$	90-33-5
2-Methyl-3-hydroxy-4,5-dihydroxymethylpyridine	$C_8H_{11}NO_3$	65-23-6
2-Methyl-3-hydroxy-4-methoxymethyl-5-hydroxymethylpyridine	$C_9H_{13}NO_3$	1464-33-1
2-Methylimidazole	$C_4H_6N_2$	693-98-1
Methyl iodide	CH_3I	74-88-9
Methyl isopropyl ether	$C_4H_{10}O$	598-53-8
1-Methyl-7-isopropylphenanthrene	$C_{18}H_{18}$	483-65-8
Methylmalonic acid dimethyl ester	$C_6H_{10}O_4$	609-02-9
Methyl mercaptan	CH_4S	74-93-1
Methyl methacrylate	$C_5H_8O_2$	80-62-6
N-Methylmethanamide	C_2H_5NO	123-39-7
Methyl methanoate	$C_2H_4O_2$	107-31-3
Methyl 2-methylpropenoate	$C_5H_8O_2$	80-62-6
Methyl myristate	$C_{15}H_{30}O_2$	124-10-7
1-Methylnaphthalene	$C_{11}H_{10}$	90-12-0
2-Methylnaphthalene	$C_{11}H_{10}$	91-57-6
Methyl nitrate	CH_3NO_3	598-58-3
Methyl nitroacetate	$C_3H_5NO_4$	2483-57-
2-Methyl-3-nitro-4-methoxymethyl-5-cyano-6-chloropyridine	$C_9H_8ClN_3O_3$	719-48-
2-Methyl-2-nitro-1,3-propanediol	$C_4H_9NO_4$	77-49-
2-Methyl-2-nitro-1-propanol	$C_4H_9NO_3$	76-39-
Methyl nonadecanoate	$C_{20}H_{40}O_2$	1731-94-
2-Methylnonane	$C_{10}H_{22}$	871-83-
3-Methylnonane(DL)	$C_{10}H_{22}$	5911-04-
4-Methylnonane(DL)	$C_{10}H_{22}$	17301-94-
5-Methylnonane	$C_{10}H_{22}$	15869-85-
Methyl octadecanoate	$C_{19}H_{38}O_2$	112-61-
Methyl octanoate	$C_9H_{18}O_2$	111-11-
Methyl oenanthoate	$C_8H_{16}O_2$	106-73-
5-Methyl-3-oxahex-1-ene	$C_6H_{12}O$	109-53-
4-Methyl-3-oxa-1-pentanol	$C_5H_{12}O_2$	2167-39-
2-Methyloxirane	C_3H_6O	75-56-
2-Methyl-3-oxo-propanenitrile	C_4H_5NO	26692-50-
Methyl palmitate	$C_{17}H_{34}O_2$	112-39-
N-Methylpentanamide	$C_6H_{13}NO$	6225-10-
2-Methylpentane	C_6H_{14}	107-83-
3-Methylpentane	C_6H_{14}	96-14-
Methyl pentanoate	$C_6H_{12}O_2$	624-24-
2-Methyl-1-pentanol	$C_6H_{14}O$	105-30-
2-Methyl-2-pentanol	$C_6H_{14}O$	590-36-
3-Methyl-2-pentanol	$C_6H_{14}O$	565-60-
3-Methyl-3-pentanol	$C_6H_{14}O$	77-74-
4-Methyl-2-pentanol	$C_6H_{14}O$	108-11-
4-Methyl-2-pentanone	$C_6H_{12}O$	108-10-
4-Methyl-3-penten-2-one	$C_6H_{10}O$	141-79-
Methyl N-perfluorobutanoate	$C_5H_3F_7O_2$	356-24-
9-Methylperhydrofluorene	$C_{14}H_{34}$	unavailab
4-Methylphenanthrene	$C_{15}H_{12}$	832-64-
2-Methylphenol	C_7H_8O	95-48-
3-Methylphenol	C_7H_8O	108-39-
4-Methylphenol	C_7H_8O	106-44-
Methyl phenylcarbamate	$C_8H_9NO_2$	2603-10-
Methyl phenyl ether	C_7H_8O	100-66-
Methyl phenyl ketone	C_8H_8O	98-86-
Methyl phenyl sulfide	C_7H_8S	100-68-
Methylphosphonyl chlorofluoride	CH_3ClFOP	753-71-
Methylphosphonyl dichloride	CH_3Cl_2OP	676-83-
Methylphosphonyl difluoride	CH_3F_2OP	676-99-
2-Methylpiperidine	$C_6H_{13}N$	109-05-
4-Methylpiperidine	$C_6H_{13}N$	626-58-
N-Methylpiperidine	$C_6H_{13}N$	626-67-
Methyl pivalate	$C_6H_{12}O_2$	598-98-
2-Methylpropanamide	C_4H_9NO	563-83-
N-Methylpropanamide	C_4H_9NO	1187-58-
2-Methylpropane	C_4H_{10}	75-28-
2-Methyl-1-propanethiol	$C_4H_{10}S$	513-44-
2-Methyl-2-propanethiol	$C_4H_{10}S$	75-66-
Methyl propanoate	$C_4H_8O_2$	554-12-
2-Methylpropanoic acid	$C_4H_8O_2$	79-31-
2-Methyl-1-propanol	$C_4H_{10}O$	78-83-
2-Methyl-2-propanol	$C_4H_{10}O$	75-65-
2-Methylpropanoyl chloride	C_4H_7ClO	79-30-
2-Methylpropene	C_4H_8	115-11-
2-Methylpropenenitrile	C_4H_5N	126-98-
Methyl propenoate	$C_4H_6O_2$	96-33-
Methyl propionate	$C_4H_8O_2$	554-12-
2-Methylpropionitrile	C_4H_7N	78-82-
N-(2-Methyl-2-propyl)ethanamide	$C_6H_{13}NO$	1540-94-
2-Methyl-1-propyl ethanoate	$C_6H_{12}O_2$	110-19-
2-Methyl-2-propyl ethanoate	$C_6H_{12}O_2$	540-88-
Methyl n-propyl ether	$C_4H_{10}O$	557-17-
2-Methylpropyl methanoate	$C_5H_{10}O_2$	542-55-
Methyl n-propyl sulfide	$C_4H_{10}S$	3877-15-
2-Methylpyridine	C_6H_7N	109-06-
3-Methylpyridine	C_6H_7N	108-99-
4-Methylpyridine	C_6H_7N	108-89-
N-Methylpyrrole	C_5H_7N	96-54-

1-Methylpyrrolidine	$C_5H_{11}N$	120-94-5
3-Methylpyrrolidine	$C_5H_{11}N$	34375-89-8
1-Methyl-2-pyrrolidone	C_5H_9NO	872-50-4
Methyl salicylate	$C_8H_8O_3$	119-36-8
Methyl silicate	$C_4H_{12}O_4Si$	681-84-5
Methyl stearate	$C_{19}H_{38}O_2$	112-61-8
α-Methylstyrene	C_9H_{10}	98-83-9
2-Methylsuccinic acid	$C_5H_8O_4$	498-21-5
Methyl tetradecanoate	$C_{15}H_{30}O_2$	124-10-7
3-Methyltetrahydrophthalic anhydride	$C_9H_{10}O_3$	5333-84-6
N-Methyl-2,4,6,N-tetranitroaniline	$C_7H_5N_5O_8$	479-45-8
Methyltetryl	$C_8H_7N_5O_8$	43072-20-4
3-Methyl-2-thiabutane	$C_4H_{10}S$	1551-21-9
2-Methylthiacyclopentane	$C_5H_{10}S$	1795-09-1
3-Methylthiacyclopentane	$C_5H_{10}S$	4740-00-5
2-Methylthiazole	C_4H_5NS	3581-87-1
2-Methylthiolane	$C_5H_{10}S$	1795-09-1
3-Methylthiolane	$C_5H_{10}S$	4740-00-5
2-Methylthiophene	C_5H_6S	554-14-3
Methyl trichlorothioacrylate	$C_4H_3Cl_3OS$	76619-91-5
Methyltriphenylarsonium bis[7,7,8,8-tetracyanoquino-dimethanide]	$C_{43}H_{26}AsN_8$	1284-18-0
Methyltriphenylphosphonium bis(7,7,8,8-tetracyano-quinodimethanide)	$C_{43}H_{26}N_8P$	11133-40-7
Methylurea	$C_2H_6N_2O$	598-50-5
N-Methylvaleramide	$C_6H_{13}NO$	6225-10-1
Methyl valerate	$C_6H_{12}O_2$	624-24-8
4-Methyoxy-4′-heptanoylazobenzene	$C_{20}H_{24}N_2O_3$	97402-83-0
Milk sugar	$C_{12}H_{22}O_{11}$	63-42-3
Mixed valence iron oxo-centered complex with acetate and 3-methyl pyridine	$C_{36}H_{46}Fe_3N_4O_{13}$	105943-92-8
1-Monobenzoylglycerol	$C_{10}H_{12}O_4$	3376-59-8
2-Monobenzoylglycerol	$C_{10}H_{12}O_4$	26699-73-0
Monobutylurea	$C_5H_{12}N_2O$	592-31-4
Mono-*tert*-butylurea	$C_5H_{12}N_2O$	1118-12-3
1-Monocaprin	$C_{13}H_{26}O_4$	2277-23-8
Monochloroacetic acid	$C_2H_3ClO_2$	79-11-8
Monoethylurea	$C_3H_8N_2O$	625-52-5
Monoisopropylurea	$C_4H_{10}N_2O$	691-60-1
1-Monolaurin	$C_{15}H_{30}O_4$	142-18-7
2-Monolaurin	$C_{15}H_{30}O_4$	1678-45-1
Monomethylurea	$C_2H_6N_2O$	598-50-5
1-Monomyristin	$C_{17}H_{34}O_4$	589-68-4
2-Monomyristin	$C_{17}H_{34}O_4$	27214-38-6
1-Monopalmitin	$C_{19}H_{38}O_4$	542-44-9
2-Monopalmitin	$C_{19}H_{38}O_4$	23470-00-0
Monophenylurea	$C_7H_8N_2O$	64-10-8
Monopropylurea	$C_4H_{10}N_2O$	627-06-5
1-Monostearin	$C_{21}H_{42}O_4$	123-94-4
2-Monostearin	$C_{21}H_{42}O_4$	621-61-4
Morniflumate	$C_{19}H_{20}F_3N_3O_3$	65847-85-0
Morpholine	C_4H_9NO	110-91-8
Murexide	$C_8H_8N_6O_6$	3051-09-0
Myristic acid	$C_{14}H_{28}O_2$	544-63-8

N

NAD	$C_{21}H_{27}N_7O_{14}P_2\cdot 3H_2O$	53-84-9
Naphthacene	$C_{18}H_{12}$	92-24-0
Naphthalene	$C_{10}H_8$	91-20-3
Naphthalene-2,6-dicarboxylic acid	$C_{12}H_8O_4$	1141-38-4
Naphthalene-2,6-dicarboxylic acid dimethyl ester	$C_{14}H_{12}O_4$	840-65-3
2,3-Naphthalenediol	$C_{10}H_8O_2$	92-44-4
Naphthalene-1,8-disulfide-S-oxide	$C_{10}H_6OS_2$	49833-12-7
Naphthalene picric acid	$C_{16}H_{11}N_3O_7$	29972-02-9
Naphthalene-pyromellitic dianhydride adduct	$C_{20}H_{10}O_6$	3470-19-7
Naphthalene-1,2,4,5-tetracyanobenzene	$C_{20}H_{10}N_4$	740-98-7
Naphthalene-tetracyanoethylene adduct	$C_{16}H_8N_4$	1223-66-1
Naphthalene-1,3,5-trinitrobenzene adduct	$C_{16}H_{11}N_3O_6$	1787-27-5
α-Naphthol	$C_{10}H_8O$	90-15-3
β-Naphthol	$C_{10}H_8O$	135-19-3
β-Naphthylamine	$C_{10}H_9N$	91-59-8
β-Naphthylamine-*p*-nitrosodimethylaniline complex	$C_{46}H_{47}N_7O_2$	unavailable
1,5-Naphthylenediisocyanate	$C_{12}H_6N_2O_2$	3173-72-6
Natural ricinoleic acid	$C_{18}H_{34}O_3$	141-22-0
Natural Rubber	$(C_5H_8)_n$	9003-31-0
Neodymium isothiocyanate heptahydrate	$C_3N_3NdS_3\cdot 7H_2O$	113614-85-0
Neopentane	C_5H_{12}	463-82-1
Nickelocene	$C_{10}H_{10}Ni$	1271-28-9
Nicotinamide adenine dinucleotide trihydrate	$C_{21}H_{27}N_7O_{14}P_2\cdot 3H_2O$	54-84-9
Nicotinic acid	$C_6H_5NO_2$	59-67-6
Niflumic acid	$C_{13}H_9F_3N_2O_2$	4394-00-7
p-Nitroacetanilide	$C_8H_9N_2O_3$	104-04-1
3-Nitro-4-aminotoluene	$C_7H_8N_2O_2$	89-62-3
5-Nitro-2-aminotoluene	$C_7H_8N_2O_2$	99-52-5
2-Nitroaniline	$C_6H_6N_2O_2$	88-74-4
3-Nitroaniline	$C_6H_6N_2O_2$	99-09-2
4-Nitroaniline	$C_6H_6N_2O_2$	100-01-6
4-Nitroanisole	$C_7H_7NO_3$	100-17-4
p-Nitroanisole	$C_7H_7NO_3$	100-17-4
Nitrobenzene	$C_6H_5NO_2$	98-95-3
2-Nitrobenzoic acid	$C_7H_5NO_4$	552-16-9
3-Nitrobenzoic acid	$C_7H_5NO_4$	121-92-6
4-Nitrobenzoic acid	$C_7H_5NO_4$	62-23-7
4-Nitrochlorobenzene	$C_6H_4ClNO_2$	100-00-5
m-Nitrocinnamic acid	$C_9H_7NO_4$	555-68-0
o-Nitrocinnamic acid	$C_9H_7NO_4$	612-41-9
p-Nitrocinnamic acid	$C_9H_7NO_4$	619-89-6
Nitroethane	$C_2H_5NO_2$	79-24-3
4-Nitroethoxybenzene	$C_8H_9NO_3$	100-29-8
p-Nitroethoxybenzene	$C_8H_9NO_3$	100-29-8
Nitroguanidine	$CH_4N_4O_2$	556-88-7
Nitromethane	CH_3NO_2	75-52-5
4-Nitromethoxybenzene	$C_7H_7NO_3$	100-17-4
4-Nitrophenetole	$C_8H_9NO_3$	100-29-8
p-Nitrophenetole	$C_8H_9NO_3$	100-29-8
2-Nitrophenol	$C_6H_5NO_3$	88-75-5
3-Nitrophenol	$C_6H_5NO_3$	554-84-7
4-Nitrophenol	$C_6H_5NO_3$	100-02-7
4-Nitrophenyl-4′-*n*-octyloxybenzoate	$C_{21}H_{25}NO_5$	52910-78-8
p-Nitrosodimethylaniline	$C_8H_{10}N_2O$	138-89-6
p-Nitrosodimethylaniline-β-naphthylamine complex	$C_{46}H_{47}N_7O_2$	unavailable
2-Nitrotoluene	$C_7H_7NO_2$	88-72-2
3-Nitrotoluene	$C_7H_7NO_2$	99-08-1
4-Nitrotoluene	$C_7H_7NO_2$	99-99-0
3-Nitro-1,2,4-triazol-5-one	$C_2H_2N_4O_3$	932-64-9
n-Nonacosane	$C_{29}H_{60}$	630-03-5
Nonadecacarbonyl diiron	$C_9Fe_2O_9$	15321-51-4
n-Nonadecane	$C_{19}H_{40}$	629-92-5
Nonadecanoic acid	$C_{19}H_{38}O_2$	646-30-0
Nonanal	$C_9H_{18}O$	124-19-6
1-Nonanol	$C_9H_{20}O$	143-08-8
n-Nonane	C_9H_{20}	111-84-2
Nonanoic acid	$C_9H_{18}O_2$	112-05-0
5-Nonanone	$C_9H_{18}O$	502-56-7
1-Nonene	C_9H_{18}	124-11-8
Nonyl acrylate	$C_{12}H_{22}O_2$	2664-55-3
n-Nonyl alcohol	$C_9H_{20}O$	143-08-8
4-*n*-Nonylbicyclohexyl	$C_{21}H_{40}$	95135-87-8
4-Nonyl-4′-cyanobiphenyl	$C_{22}H_{27}N$	52709-85-0
Nonyl methacrylate	$C_{13}H_{24}O_2$	2696-43-7
Nonyl N-phenylcarbamate	$C_{16}H_{25}NO_2$	33689-71-3
4-*n*-Nonyltercyclohexyl	$C_{27}H_{50}$	unavailable

Norbornadiene	C_7H_8	121-46-0
Norbornane	C_7H_{12}	279-23-2
Norbornene	C_7H_{10}	498-66-8
1-Norbornyl cyanide	$C_8H_{11}N$	103434-09-9
1-Norbornyl isonitrile	$C_8H_{11}N$	88523-51-7
Norcarnane	C_7H_{12}	286-08-8
Nordazepam	$C_{15}H_{11}ClN_2O$	1088-11-5
Norethindrone	$C_{20}H_{26}O_2$	68-22-4
Norethindrone acetate	$C_{22}H_{28}O_3$	51-98-9
Norethindrone benzoate	$C_{27}H_{30}O_3$	71203-39-9
Norethindrone biphenyl-4-carboxylate	$C_{33}H_{34}O_3$	71203-40-2
Norethindrone *trans*-3-(4-butylclohexyl)propionate	$C_{33}H_{48}O_3$	71203-38-8
Norethindrone-6-(4-chlorophenyl)-hexanoate	$C_{32}H_{39}ClO_3$	71203-42-4
Norethindrone 4-cyclohexylbenzoate	$C_{33}H_{40}O_3$	71203-41-3
Norethindrone dimethylpropionate	$C_{25}H_{34}O_3$	65445-09-2
Norethindrone heptanoate	$C_{27}H_{38}O_3$	3836-23-5
Norethindrone *trans*-4-hexylcyclohexylcarboxylate	$C_{33}H_{48}O_3$	71203-37-7
Norethindrone pentamethyldisiloxyl ether	$C_{25}H_{40}O_3Si_2$	71203-43-5
Norleucine(DL)	$C_6H_{13}NO_2$	616-06-8
Norleucine(L)	$C_6H_{13}NO_2$	327-57-1
Nortricyclene	C_7H_{10}	279-19-6
Norvaline(L)	$C_5H_{11}NO_2$	6600-40-4
Nylon 6	$(C_6H_{11}NO)_n$	25038-54-4

O

n-Octacosane	$C_{28}H_{58}$	630-02-4
n-Octadecane	$C_{18}H_{38}$	593-45-3
1-Octadecanethiol	$C_{18}H_{38}S$	2885-00-9
Octadecanoic acid	$C_{18}H_{36}O_2$	57-11-4
cis-ω-12,δ-6-Octadecenoic acid	$C_{18}H_{34}O_2$	593-39-5
1-Octadecanol	$C_{18}H_{38}O$	112-92-5
1-Octadecene-urea adduct	$C_{2.4}H_{6.8}N_2O$	38588-35-1
cis-9-Octadecenoic acid	$C_{18}H_{34}O_2$	112-80-1
n-Octadecyl alcohol	$C_{18}H_{38}O$	112-92-5
n-Octadecyl chloride	$C_{18}H_{37}Cl$	3386-33-2
n-Octadecyl mercaptan	$C_{18}H_{38}S$	2885-00-9
p-*n*-Octadecyloxybenzoic acid	$C_{25}H_{42}O_3$	15872-50-1
p-*n*-Octadecyloxybenzoic acid	$C_{25}H_{41}DO_3$	unavailable
Octaethylcyclotetrasiloxane	$C_{16}H_{40}D_4Si_4$	1451-99-6
Octafluorocyclobutane	C_4F_8	115-25-3
Octafluoropropane	C_3F_8	76-19-7
Octafluorotoluene	C_7F_8	434-64-0
1,2,3,4,5,6,7,8-Octahydroanthracene	$C_{14}H_{18}$	1079-71-6
Octahydroazocine	$C_7H_{15}N$	1121-92-2
5,6,6a,6b,11,12,12a,12b-Octahydrodibenzo-[a,g]biphenylene	$C_{20}H_{20}$	42182-87-6
5,6,6a,6b,7,8,12b,12c-Octahydrodibenzo-[a,i]biphenylene	$C_{20}H_{20}$	42182-84-3
1,1,4,4,10,10,13,13-Octamethyl-cyclooctadecane	$C_{26}H_{52}$	23014-57-5
Octamethyldiphenylcyclopentasiloxane	$C_{20}H_{34}O_5Si_5$	13438-48-7
Octamethylcyclotetrasilazane	$C_8H_{28}N_4Si_4$	1020-84-4
Octamethylcyclotetrasiloxane	$C_8H_{24}O_4Si_4$	556-67-2
Octanal	$C_8H_{16}O$	124-13-0
n-Octane	C_8H_{18}	111-65-9
1-Octanethiol	$C_8H_{18}S$	111-88-6
Octanoic acid	$C_8H_{16}O_2$	124-07-2
1-Octanol	$C_8H_{18}O$	111-87-5
2-Octanol	$C_8H_{18}O$	123-96-6
3-Octanol	$C_8H_{18}O$	589-98-0
4-Octanol	$C_8H_{18}O$	589-62-8
2-Octanone	$C_8H_{16}O$	111-13-7
Octaphenylcyclotetrasiloxane	$C_{48}H_{40}O_4Si_4$	546-56-5
n-Octatetracontane	$C_{48}H_{98}$	7098-26-2
Octa(vinylsilasesquioxane)	$C_{16}H_{24}O_{12}Si_8$	69655-76-1
1-Octene	C_8H_{16}	111-66-0
2-Octene	C_8H_{16}	111-67-1
Octogen	$C_4H_8N_8O_8$	2691-41-0
Octogen(α)	$C_4H_8N_8O_8$	2691-41-0
Octogen(β)	$C_4H_8N_8O_8$	2691-41-0
Octogen(δ)	$C_4H_8N_8O_8$	2691-41-0
Octogen(γ)	$C_4H_8N_8O_8$	2691-41-0
n-Octyl alcohol	$C_8H_{18}O$	111-87-5
n-Octylamine	$C_8H_{19}N$	111-86-4
n-Octylbenzene	$C_{14}H_{22}$	2189-60-8
n-Octyl chloride	$C_8H_{17}Cl$	111-85-3
4-Octyl-4′-cyanobiphenyl	$C_{21}H_{25}N$	52709-84-9
4-Octyloxy-4′-heptyl-α-cyanostilbene	$C_{30}H_{41}NO$	66414-48-0
n-Octyl mercaptan	$C_8H_{16}S$	111-88-6
Octyl methacrylate	$C_{12}H_{22}O_2$	688-84-6
Octyloxycyanobiphenyl	$C_{21}H_{25}NO$	52709-84-9
Oenanthal	$C_7H_{14}O$	111-71-7
Oleic acid	$C_{18}H_{34}O_2$	112-80-1
Oligoethylene butylene glycol adipate	$C_{12}H_{22}O_6$	26570-73-0
Orcinol monohydrate	$C_7H_8O_2 \cdot H_2O$	6153-39-5
Ornithine(DL)	$C_5H_{12}N_2O_2$	616-07-9
Ornithine dihydrochloride	$C_5H_{14}Cl_2N_2O_2$	16682-12-5
Orthoformic acid	CH_4O_3	unavailable
3-Oxabicyclo[3.2.2]nonane	$C_8H_{14}O$	283-27-2
3-Oxa-1-butanol	$C_3H_8O_2$	109-86-4
2-Oxadodecane	$C_{11}H_{24}O$	7289-52-3
4-Oxaheptane	$C_6H_{14}O$	111-43-3
3-Oxa-1-heptanol	$C_6H_{14}O_2$	111-76-2
3-Oxahept-1-ene	$C_6H_{12}O$	111-34-2
2-Oxahexane	$C_5H_{12}O$	628-28-4
3-Oxahexane	$C_5H_{12}O$	628-32-0
3-Oxa-1-hexanol	$C_5H_{12}O_2$	2807-30-9
Oxalic acid	$C_2H_2O_4$	144-62-7
Oxalyl fluoride	$C_2F_2O_2$	359-40-0
2-Oxa-3-methylbutane	$C_4H_{10}O$	598-53-8
Oxamide	$C_2H_4N_2O_2$	471-46-5
Oxane	$C_5H_{10}O$	142-68-7
2-Oxapentane	$C_4H_{10}O$	557-17-5
3-Oxapentane	$C_4H_{10}O$	60-29-7
3-Oxa-1-pentanol	$C_4H_{10}O_2$	110-80-5
2-Oxapropane	C_2H_6O	115-10-6
9-Oxatetracyclo[5.4.0.0^{3,10}.0^{4,8}]undec-5-en-2-one	$C_{10}H_{10}O_2$	65181-92-2
Oxetane	C_3H_6O	503-30-0
Oxirane	C_2H_4O	75-21-8
4-Oxobutanenitrile	C_4H_5NO	3515-93-3
17-[(Oxoheptyl)oxy]-(17α)-19-norpregn-4-en-20-yn-3-one	$C_{27}H_{38}O_3$	3836-23-5
μ_3-Oxo-tris(pyridine)hexakis(acetato) iron(II) diiron pyridine	$C_{32}H_{38}Fe_3N_4O_{13}$	99582-28-2
Oxolane	C_4H_8O	109-99-9
4,4′-Oxybis-1,2-benzenediamine	$C_{12}H_{14}N_4O$	2676-59-7
Oxy-*p*,*p*′-dibenzoyl chloride	$C_{14}H_8Cl_2O_3$	50975-64-9

P

Palmitic acid	$C_{16}H_{32}O_2$	57-10-3
2,2-Paracyclophane	$C_{16}H_{16}$	1633-22-3
3,3-Paracyclophane	$C_{18}H_{20}$	2913-24-8
Paraldehyde	$C_6H_{12}O_3$	123-63-7
Pelargonaldehyde	$C_9H_{18}O$	124-19-6
Pelargonic acid	$C_9H_{18}O_2$	112-05-0
Pentachlorobenzene	C_6HCl_5	608-93-5
Pentachloroethane	C_2HCl_5	76-01-7
Pentachlorophenol	C_6HCl_5O	87-86-5
n-Pentacosane	$C_{25}H_{52}$	629-99-2
Pentacycloformaldehyde	$C_5H_{10}O_5$	16528-92-0
Pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane	C_8H_8	277-10-1
Pentacyclo[7.3.1.1^{4,12}.0^{2,7}.0^{6,11}] tetradecane	$C_{14}H_{20}$	2292-79-7

n-Pentadecane	$C_{15}H_{32}$	629-62-9
Pentadecanoic acid	$C_{15}H_{30}O_2$	1002-84-2
1-Pentadecanol	$C_{15}H_{32}O$	629-76-5
Pentadecanolactone	$C_{15}H_{28}O_2$	106-02-5
2-Pentadecanone	$C_{15}H_{30}O$	2345-28-0
n-Pentadecyl alcohol	$C_{15}H_{32}O$	629-76-5
1,2-Pentadiene	C_5H_8	591-95-7
1-*cis*-3-Pentadiene	C_5H_8	1574-41-0
1-*trans*-3-Pentadiene	C_5H_8	2004-70-8
1,4-Pentadiene	C_5H_8	591-93-5
2,3-Pentadiene	C_5H_8	591-96-8
Pentaerythritol	$C_5H_{12}O_4$	115-77-5
Pentaerythritol tetranitrate	$C_5H_8N_4O_{12}$	78-11-5
Pentaerythrityl tetrabromide	$C_5H_8Br_4$	3229-00-3
Pentaerythrityl tetrachloride	$C_5H_8Cl_4$	3228-99-7
Pentaerythrityl tetrafluoride	$C_5H_8F_4$	338-23-8
Pentaerythrityl tetraiodide	$C_5H_8I_4$	1522-88-9
Pentaethylene glycol	$C_{10}H_{22}O_6$	4792-15-8
Pentafluoroaniline	$C_6H_2F_5N$	771-60-8
Pentafluorobenzene	C_6HF_5	363-72-4
Pentafluorochlorobenzene	C_6ClF_5	344-07-0
Pentafluorochloroethane	C_2ClF_5	76-15-3
Pentafluoronitrobenzene	$C_6F_5NO_2$	880-78-4
Pentafluorophenol	C_6HF_5O	771-61-9
2,3,4,5,6-Pentafluorotoluene	$C_7H_3F_5$	771-56-2
1,2,3,4,5-Pentahydroxypentane	$C_5H_{12}O_5$	488-81-3
Pentakis(methylammonium) undecabromodibismuthate	$C_5H_{30}Bi_2Br_{11}N_5$	119931-90-7
Pentamethylbenzene	$C_{11}H_{16}$	700-12-9
Pentamethylbenzoic acid	$C_{12}H_{16}O_2$	2243-32-5
17-[(Pentamethyldisiloxanyl)oxy]-(17α)-19-norpregn-4-en-20-yn-3-one	$C_{20}H_{26}O_2$	71203-43-5
2,2,4,6,6-Pentamethylheptane	$C_{12}H_{26}$	13475-82-6
n-Pentanal	$C_5H_{10}O$	110-62-3
n-Pentane	C_5H_{12}	109-66-0
1,5-Pentanediol	$C_5H_{12}O_2$	111-29-5
1,2,3,4,5-Pentanepentol	$C_5H_{12}O_5$	488-81-3
xylo-1,2,3,4,5-Pentanepentol	$C_5H_{12}O_5$	87-99-0
1-Pentanethiol	$C_5H_{12}S$	110-66-7
Pentanoic acid	$C_5H_{10}O_2$	109-52-4
1-Pentanol	$C_5H_{12}O$	71-41-0
3-Pentanol	$C_5H_{12}O$	584-02-1
2-Pentanone	$C_5H_{10}O$	107-87-9
3-Pentanone	$C_5H_{10}O$	96-22-0
4-*n*-Pentanoyl-4-*n*'-butanoyloxyazobenzene	$C_{21}H_{24}N_2O_3$	120122-98-7
Pentanoyl chloride	C_5H_9ClO	638-29-9
4-*n*-Pentanoyl-4-*n*'-decanoyloxyazobenzene	$C_{27}H_{36}N_2O_3$	120103-03-9
4-*n*-Pentanoyl-4-*n*'-dodecanoyloxyazobenzene	$C_{29}H_{40}N_2O_3$	120103-05-1
4-*n*-Pentanoyl-4-*n*'-ethanoyloxyazobenzene	$C_{19}H_{20}N_2O_3$	120102-96-7
4-*n*-Pentanoyl-4-*n*'-heptadecanoyloxyazobenzene	$C_{34}H_{50}N_2O_3$	120103-10-8
4-*n*-Pentanoyl-4-*n*'-heptanoyloxyazobenzene	$C_{24}H_{30}N_2O_3$	120103-00-6
4-*n*-Pentanoyl-4-*n*'-hexadecanoyloxyazobenzene	$C_{33}H_{48}N_2O_3$	120103-09-5
4-*n*-Pentanoyl-4-*n*'-hexanoyloxyazobenzene	$C_{23}H_{28}N_2O_3$	120102-99-0
4-*n*-Pentanoyl-4-*n*'*n*-nonanoyloxyazobenzene	$C_{26}H_{34}N_2O_3$	120103-02-8
4-*n*-Pentanoyl-4-*n*-'-octadecanoyloxyazobenzene	$C_{35}H_{52}N_2O_3$	120103-11-9
4-*n*-Pentanoyl-4-*n*'-octanoyloxyazobenzene	$C_{25}H_{32}N_2O_3$	120103-01-7
4-*n*-Pentanoyl-4-*n*'-pentadecanoyloxyazobenzene	$C_{32}H_{46}N_2O_3$	120103-08-4
4-*n*-Pentanoyl-4-*n*'-pentanoyloxyazobenzene	$C_{22}H_{26}N_2O_3$	120102-98-9
4-*n*-Pentanoyl-4-*n*'-propanoyloxyazobenzene	$C_{20}H_{22}N_2O_3$	120102-97-8
4-*n*-Pentanoyl-4-*n*-'-tetradecanoyloxyazobenzene	$C_{31}H_{44}N_2O_3$	120103-07-3
4-*n*-Pentanoyl-4-*n*'-tridecanoyloxyazobenzene	$C_{30}H_{42}N_2O_3$	120103-06-2
4-*n*-Pentanoyl-4-*n*'-undecanoyloxyazobenzene	$C_{28}H_{38}N_2O_3$	120103-04-0
2,5,8,11,14-Pentaoxapentadecane	$C_{10}H_{22}O_5$	143-24-8
Pentaphenylethane	$C_{32}H_{26}$	19112-42-6
Pentapropylene glycol	$C_{15}H_{32}O_6$	21482-12-2
n-Pentatriacotane	$C_{35}H_{72}$	630-07-9
1-Pentene	C_5H_{10}	109-67-1
2-Pentene	C_5H_{10}	109-68-2
cis-2-Pentene	C_5H_{10}	627-20-3
trans-2-Pentene	C_5H_{10}	646-04-8
Penton	$(C_5H_8Cl_2O)_n$	25323-58-4
Pentoxane	$C_5H_{10}O_5$	16528-92-0
n-Pentyl alcohol	$C_5H_{12}O$	71-41-0
tert-Pentyl alcohol	$C_5H_{12}O$	75-85-4
n-Pentylamine	$C_5H_{13}N$	110-58-7
n-Pentylammonium chloride	$C_5H_{14}ClN$	142-65-4
n-Pentyl bromide	$C_5H_{11}Br$	110-53-2
Pentyl butanoate	$C_9H_{18}O_2$	540-18-1
n-Pentyl chloride	$C_5H_{11}Cl$	543-59-9
Pentyldiamine manganese tetrachloride	$C_5H_{16}Cl_4MnN_2$	59890-70-9
Pentyl ethanoate	$C_7H_{14}O_2$	628-63-7
n-Pentyl ethanoate	$C_7H_{14}O_2$	628-63-7
n-Pentyl iodide	$C_5H_{11}I$	628-17-1
2-Pentylnonenal	$C_{14}H_{26}O$	3021-89-4
N-[*p*-(*n*-Pentyloxy)benzylidene]-*p*'-*n*-butylaniline	$C_{22}H_{29}NO$	29743-10-0
4-*n*-Pentylphenyl-4'-heptyloxythiobenzoate	$C_{25}H_{34}O_2S$	61519-00-4
Pentyl propionate	$C_8H_{16}O_2$	624-54-4
Perchlorobenzene	C_6Cl_6	118-74-1
Perchlorobiphenyl	$C_{12}Cl_{10}$	2051-24-3
Perchlorophenol	C_6HCl_5O	87-86-5
Perfluorobenzene	C_6F_6	392-56-3
Perfluorobicyclo[4.4.0]dec-1,6-diene	$C_{10}F_{16}$	54939-04-7
Perfluorobicyclohexyl	$C_{12}F_{22}$	558-64-5
Perfluorobiphenyl	$C_{12}F_{10}$	434-90-2
n-Perfluorobutane	C_4F_{10}	355-25-9
Perfluoro-3-butyltetrahydrofuran	$C_8F_{16}O$	500005-57-2
Perfluorodecalin	$C_{10}F_{18}$	306-94-5
cis-Perfluorodecalin	$C_{10}F_{18}$	60433-11-6
trans-Perfluorodecalin	$C_{10}F_{18}$	60433-12-7
Perfluorodimethylcyclohexane	C_8F_{16}	unavailable
Perfluoroheptane	C_7F_{16}	335-57-9
n-Perfluorohexane	C_6F_{14}	355-42-0
Perfluoromethylcyclohexane	C_7F_{14}	355-02-2
Perfluoromethyldiethylamine	$C_5F_{13}N$	758-48-5
n-Perfluorooctane	C_8F_{18}	307-34-6
n-Perfluoropentane	C_5F_{12}	678-26-2
Perfluoropiperidine	$C_5F_{11}N$	836-77-1
Perfluoropropane	C_3F_8	76-19-7
Perfluorotoluene	C_7F_8	434-64-0
Perfluorotriethylamine	$C_6F_{15}N$	359-70-6
Perhydroazepine	$C_6H_{13}N$	111-49-9
Perhydromethylcyclopentadiene dimer	$C_{12}H_{20}$	unavailable
Perhydrophenanthrene	$C_{14}H_{24}$	5743-97-5
Perylene	$C_{20}H_{12}$	198-55-0
Perylene picric acid	$C_{26}H_{15}N_3O_7$	42462-61-3
PETN	$C_5H_8N_4O_{12}$	78-11-5
Petroselinic acid	$C_{18}H_{34}O_2$	593-39-5
Phenanthrene	$C_{14}H_{10}$	85-01-8
Phenanthridine	$C_{13}H_9N$	229-87-8
Phenazine	$C_{12}H_8N_2$	92-82-0
Phenol	C_6H_6O	108-95-2

Phenolphthalein	$C_{20}H_{14}O_4$	77-09-8
Phenol-*p*-toluidine complex	$C_{13}H_{15}NO$	14489-32-8
Phenol-urea complex	$C_{13}H_{16}N_2O_3$	5168-44-5
Phenothiazine	$C_{12}H_9NS$	92-84-2
Phenoxathiin	$C_{12}H_8SO$	262-20-4
2-Phenoxyethanol	$C_8H_{10}O_2$	122-99-6
Phenylacetylene	C_8H_6	536-74-3
Phenylalanine(L)	$C_9H_{11}NO_2$	63-91-2
Phenylaminoethyl methacrylate	$C_{12}H_{15}NO_2$	19288-59-6
4-Phenylbutylammonium bromide	$C_{10}H_{16}BrN$	120375-52-2
4-Phenylbutylammonium chloride	$C_{10}H_{16}ClN$	30684-06-1
4-Phenylbutylammonium nitrate	$C_{10}H_{16}N_2O_3$	120375-45-3
Phenylchloromethane	C_7H_7Cl	100-44-7
1-Phenyl-1-cyclohexyldodecane	$C_{24}H_{40}$	unavailable
10-Phenyldecylammonium bromide	$C_{16}H_{28}BrN$	120396-92-1
10-Phenyldecylammonium chloride	$C_{16}H_{28}ClN$	120375-54-4
1,2-Phenylenediamine	$C_6H_8N_2$	95-54-5
1,3-Phenylenediamine	$C_6H_8N_2$	108-45-2
1,4-Phenylenediamine	$C_6H_8N_2$	106-50-3
1,4-Phenylenediisocyanate	$C_8H_4N_2O_2$	104-49-4
o-Phenylenepyrene picric acid	$C_{28}H_{15}N_3O_7$	72497-58-6
2-Phenylethanol	$C_8H_{10}O$	60-12-8
2-Phenylethylamine	$C_8H_{11}N$	64-04-0
2-Phenylethylammonium bromide	$C_8H_{12}BrN$	53916-94-2
2-Phenylethylammonium chloride	$C_8H_{12}ClN$	156-28-5
2-Phenylethylammonium nitrate	$C_8H_{12}N_2O_3$	120375-47-5
Phenylglycine	$C_8H_9NO_2$	103-01-5
α-Phenylglycine	$C_8H_9NO_2$	69-91-0
α-Phenylglycine(D)	$C_8H_9NO_2$	69-91-0
Phenyl glycidyl ether	$C_9H_{10}O_2$	122-60-1
N-Phenylglycine	$C_8H_9NO_2$	103-01-5
11-Phenylheneicosane	$C_{27}H_{48}$	6703-80-6
7-Phenylheptylammonium bromide	$C_{13}H_{22}BrN$	120375-50-0
7-Phenylheptylammonium chloride	$C_{13}H_{22}ClN$	120375-56-6
6-Phenylhexylammonium bromide	$C_{12}H_{20}BrN$	120375-49-7
6-Phenylhexylammonium chloride	$C_{12}H_{20}ClN$	120375-57-7
6-Phenylhexylammonium nitrate	$C_{12}H_{20}N_2O_3$	120375-43-1
Phenylhydrazine	$C_6H_8N_2$	100-63-0
Phenyl isocyanate	C_7H_5NO	103-71-9
4-(2-Phenylisopropyl)phenol	$C_{15}H_{16}O$	599-64-4
Phenyl isothiocyanate	C_7H_5NS	103-72-0
Phenyl mercaptan	C_6H_6S	108-98-5
Phenylmethylamine	C_7H_9N	100-46-9
Phenylmethylammonium chloride	$C_7H_{10}ClN$	3287-99-8
Phenylmethylammonium nitrate	$C_7H_{10}N_2O_3$	49580-44-1
1-Phenyl-1-methyl-1-silacyclobutane	$C_{10}H_{14}Si$	3944-08-9
9-Phenylnonylammonium bromide	$C_{15}H_{26}BrN$	120375-48-6
9-Phenylnonylammonium chloride	$C_{15}H_{26}ClN$	120375-55-5
8-Phenyloctylammonium bromide	$C_{14}H_{24}BrN$	120396-93-2
8-Phenyloctylammonium chloride	$C_{14}H_{24}ClN$	17734-26-8
8-Phenyloctylammonium nitrate	$C_{14}H_{24}N_2O_3$	120375-41-9
5-Phenylpentylammonim chloride	$C_{11}H_{18}ClN$	120375-51-1
5-Phenylpentylammonium bromide	$C_{11}H_{18}BrN$	53429-15-5
3-Phenyl-5-phenoxymethyl-2-oxazolidinone	$C_{16}H_{15}NO_3$	1226-26-2
3-Phenyl-5-phenoxymethyl-2-N-phenyliminooxazolidine	$C_{22}H_{20}N_2O_2$	34028-37-0
N-Phenylphthalimide	$C_{14}H_9NO_2$	520-03-6
3-Phenylpropanol	$C_9H_{12}O$	122-97-4
Phenylpropionic acid	$C_9H_{10}O_2$	501-52-0
3-Phenylpropylamine	$C_9H_{13}N$	2038-57-5
3-Phenylpropylammonium bromide	$C_9H_{14}BrN$	120375-53-3
3-Phenylpropylammonium chloride	$C_9H_{14}ClN$	30684-05-0
Phenyltin trichloride	$C_6H_5Cl_3Sn$	1124-19-2
Phenyl-*o*-tolylmethane	$C_{14}H_{14}$	713-36-0
Phenyltrichlorogermane	$C_6H_5Cl_3Ge$	1074-29-9
Phenyltrichlorosilane	$C_6H_5Cl_3Si$	98-13-5
Phenyltrichlorostannane	$C_6H_5Cl_3Sn$	1124-19-2
Phenylurea	$C_7H_8N_2O$	64-10-8
Phosgene	CCl_2O	75-44-5
Phosphaferrocene	C_9H_9FeP	63287-55-8
Phthalan	C_8H_8O	496-14-0
Phthalanilic acid	$C_{14}H_{11}NO_3$	4727-29-1
Phthalic acid	$C_8H_6O_4$	100-21-0
m-Phthalic acid	$C_8H_6O_4$	121-91-5
o-Phthalic acid	$C_8H_6O_4$	88-99-3
p-Phthalic acid	$C_8H_6O_4$	100-21-0
m-Phthalic acid dichloride	$C_8H_4Cl_2O_2$	99-63-8
p-Phthalic acid dichloride	$C_8H_4Cl_2O_2$	100-20-9
Phthalic anhydride	$C_8H_4O_3$	85-44-9
o-Phthalonitrile	$C_8H_4N_2$	91-15-6
Phthalonitrile and *m*-phenylene diamine condensation product	$C_{28}H_{18}N_6$	246-42-4
Phthaloyl dichloride	$C_8H_4Cl_2O_2$	88-95-9
o-Phthalyl dichloride	$C_8H_4Cl_2O_2$	88-95-9
p-Phthalyl dichloride	$C_8H_4Cl_2O_2$	100-20-9
Phytone	$C_{18}H_{36}O$	502-69-2
Picene-picric acid	$C_{28}H_{17}N_3O_7$	72454-48-9
α-Picoline	C_6H_7N	109-06-8
β-Picoline	C_6H_7N	108-99-6
Picolinic acid	$C_6H_5NO_2$	98-98-6
Picric acid	$C_6H_3N_3O_7$	88-89-1
Pimelic acid	$C_7H_{12}O_4$	111-16-0
Pinane	$C_{10}H_{18}$	473-55-2
Piperazine	$C_4H_{10}N_2$	110-85-0
Piperidine	$C_5H_{11}N$	110-89-4
α-Piperidone	C_5H_9NO	675-20-7
Pivalaldehyde	$C_5H_{10}O$	630-19-3
Pivalic acid	$C_5H_{10}O_2$	75-98-9
Polyacetylene	$(CH)_n$	26571-64-2
cis-Polyacetylene	$(CH)_n$	74373-36-7
trans-Polyacetylene	$(CH)_n$	73589-68-1
Poly-L-alanine	$(C_3H_5NO)_n$	25191-17-7
Poly-L-alanine, α-helix	$(C_3H_5NO)_n$	25191-17-7
Poly-L-alanine, β-sheet	$(C_3H_5NO)_n$	25191-17-7
Poly(amido-1,2,4-triazole)	$(C_{30}H_{20}N_8O_2)_n$	31742-70-8
Poly-L-arginine hydrochloride	$(C_6H_{12}N_4O\cdot HCl)_n$	26982-20-7
Poly-L-asparagine	$(C_4H_6N_2O_2)_n$	28088-48--
Poly-L-aspartic acid, sodium salt	$(C_4H_4NNaO_3)_n$	34345-47-6
Poly(azomethine) with one EG	$(C_{24}H_{22}N_2O_2)_n$	120885-14-5
Poly(azomethine) with two EG	$(C_{26}H_{26}N_2O_3)_n$	120885-15-6
Poly(azomethine) with three EG	$(C_{28}H_{30}N_2O_4)_n$	120885-16-7
Poly(azomethine) with four EG	$(C_{30}H_{34}N_2O_5)_n$	120885-17-8
Polybenzimidazoloquinazoline	$(C_{34}H_{18}N_6O)_n$	89190-45--
Poly[2,2-bis-(4-phenoxypropane)] 2,4,6-triazine	$(C_{17}H_{14}N_2O_2)_n$	25722-66-1
Poly-1,4-bis-(2,2,6,6-tetramethyl-4-oxy-1-oxylpiperidyl)butadiyne	$(C_{22}H_{36}N_2O_4)_n$	102386-72-1
cis-1,4-Polybutadiene	$(C_4H_6)_n$	40022-03-5
trans-1,4-Polybutadiene	$(C_4H_6)_n$	25038-44-2
1,4-Polybutadiene, GL-657	$(C_4H_6)_n$	9003-17-2
1,4-Polybutadiene, MS-1045	$(C_4H_6)_n$	9003-17-2
Poly(1-butene)	$(C_4H_8)_n$	9003-28-5
Poly(1-butene), isotactic	$(C_4H_8)_n$	9003-28-5

Polybutylene glycol adipate	$(C_{10}H_{16}O_4)_n$	25103-87-1
Poly(butylene terephthalate)	$(C_{12}H_{12}O_4)_n$	26062-94-2
Poly-γ-butyrolactone	$(C_4H_6O_2)_n$	31213-03-3
Poly-ϵ-caprolactam	$(C_6H_{11}NO)_n$	25038-54-4
Poly-ϵ-caprolactone	$(C_6H_{10}O_2)_n$	24980-41-1
Polycyanate	$(C_{17}H_{14}N_2O_2)_n$	25722-66-1
Poly(diethylsiloxane)	$(C_4H_{10}OSi)_n$	28323-47-9
Poly-1,1-diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene	$(C_{32}H_{22}Ge)_n$	57863-12-4
Poly-4,4′-dihydroxy-3,3′-isophthalamidodiphenylmethane	$(C_{21}H_{16}N_2O_4)_n$	38332-83-1
Poly-1,1-dimethyl-1-silatrimethylene	$(C_5H_{12}Si)_n$	25722-29-6
Polydimethylsilamethylene	$(C_3H_8Si)_n$	25722-25-2
Poly(dimethylsiloxane)	$(C_2H_6OSi)_n$	9016-00-6
Poly-1,3-dioxolane	$(C_3H_6O_2)_n$	25067-64-5
Poly(4,4′-dioxyphenyl-2,2′-propane carbonate)	$(C_{16}H_{14}O_3)_n$	24936-68-3
Polydiphenyldiethynylgermanium	$(C_{16}H_{10}Ge)_n$	30137-53-2
Polydiphenyldiethynylsilane	$(C_{16}H_{10}Si)_n$	31693-69-3
Poly-(p,p'-diphenylene oxide)-pyromellitimide	$(C_{22}H_{14}N_2O_7)_n$	25036-53-7
Poly-(p,p'-diphenylenephthalido)-hydrazide	$(C_{30}H_{20}N_4O_6)_n$	40902-22-5
Poly-(p,p'-diphenylenephthalido)-1,3,4-oxadiazole	$(C_{30}H_{16}N_4O_4)_n$	28702-26-3
Polyethylene	$(CH_2)_n$	9002-88-4
Polyethylene, branched	$(CH_2)_n$	9002-88-4
Polyethylene, branched, annealed	$(CH_2)_n$	9002-88-4
Polyethylene, branched, DYNH CT-1660	$(CH_2)_n$	9002-88-4
Polyethylene glycol	$(C_2H_4O)_n$	25322-68-3
Polyethylene, linear	$(CH_2)_n$	9002-88-4
Polyethylene, linear high density	$(CH_2)_n$	9002-88-4
Polyethylene, linear high molecular weight	$(CH_2)_n$	9002-88-4
Polyethylene, linear, Marlex 50 polymer	$(CH_2)_n$	9002-88-4
Polyethylene oxalate	$(C_4H_4O_4)_n$	52224-87-0
Poly(ethylenesebacate)	$(C_{12}H_{20}O_4)_n$	25037-32-5
Poly-L-glutamic acid, sodium salt	$(C_5H_6NNaO_3)_n$	28826-18-8
Polyglycine	$(C_2H_3NO)_n$	25734-27-4
Polyglycine I	$(C_2H_3NO)_n$	25734-27-4
Polyglycine II	$(C_2H_3NO)_n$	25734-27-4
Polyglycolide	$(C_4H_4O_4)_n$	26009-03-0
1-Polyhexene	$(C_6H_{12})_n$	25067-06-5
Poly-L-histidine	$(C_6H_7N_3O)_n$	26062-48-6
Poly L histidine hydrochloride	$(C_6H_7N_3O{\cdot}HCl)_n$	61857-39-1
Polyisobutylene	$(C_4H_8)_n$	9003-27-4
Polyisocyanurate	$(C_{15}H_{10}N_2O_2)_n$	25686-28-6
Polylactide(DL)	$(C_6H_8O_4)_n$	26969-66-4
Poly-L-leucine	$(C_6H_{11}NO)_n$	25322-63-8
Poly-L-lysine hydrobromide	$(C_6H_{12}N_2O{\cdot}HBr)_n$	25988-63-0
Poly-L-lysine hyydrobromide·alanine copolymer	$(C_9H_{17}N_3O_2{\cdot}HBr)_n$	61257-62-3
Poly-L-lysine hydrobromide·phenylalanine copolymer	$(C_{15}H_{21}N_3O{\cdot}HBr)_n$	26700-39-0
Polymethacrylic acid	$(C_4H_6O_2)_n$	25087-26-7
Poly-L-methionine	$(C_5H_9NOS)_n$	26062-47-5
Poly-p-methacryloyloxybenzoic acid	$(C_{11}H_{10}O_4)_n$	25853-28-5
Poly(methyl methacrylate)	$(C_5H_8O_2)_n$	87210-32-0
Poly(4-methyl-1-pentene)	$(C_6H_{12})_n$	24979-98-4
Poly(α-methylstyrene)	$(C_9H_{10})_n$	25014-31-7
Polyoctadiene	$(C_8H_{12})_n$	26353-15-1
Polyoctenylene	$(C_8H_{14})_n$	25267-51-0
Poly(oxacyclobutane)	$(C_3H_6O)_n$	25722-06-9
Polyoxymethylene	$(CH_2O)_n$	110-88-3
Poly(oxy-1,4-phenylene sulfonyl-1,4-phenylene)	$(C_{12}H_8O_3S)_n$	25667-42-9
Poly[oxy-1,4-phenylene-sulfonyl-1,4-phenylene-oxy-1,4-phenylene-(1-methylidene)-1,4-phenylene]	$(C_{25}H_{18}O_3S)_n$	31694-05-0
Polypentadecanolactone	$(C_{15}H_{28}O_2)_n$	36486-90-5
Polypentenamer	$(C_5H_8)_n$	28702-43-4
cis-Polypentenamer	$(C_5H_8)_n$	38439-19-9
trans-Polypentenamer	$(C_5H_8)_n$	29300-20-7
Poly-L-phenylalanine	$(C_9H_9NO)_n$	25191-15-5
Poly-p-phenylene	$(C_6H_4)_n$	25190-62-9
Poly-2,2′-(m-phenylene)-5,5′-dibenzoxazole methane	$(C_{21}H_{12}N_2O_2)_n$	28726-71-8
Poly-[2,2′-(p-phenylene-1,1-diphenyl-5,5′-dibenzimidazole]	$(C_{32}H_{20}N_4)_n$	28576-60-5
Poly[2,2′-(1,4-phenylene)-7,7′-oxy-bis(3-phenylquinoxaline)]	$(C_{34}H_{20}N_4O)_n$	52276-31-0
Polyphenylene PP-1 (linear)	$C_{20.84}H_{16.66}O_{0.62}$	39527-38-3
Polyphenylene PP-2 (crosslinked)	$C_{20.84}H_{16.66}O_{0.62}$	39527-38-3
Poly-1-phenyl-1-methyl-1-silatrimethylene	$(C_{10}H_{14}Si)_n$	unavailable
Poly-L-proline	$(C_5H_7NO)_n$	25191-13-3
Polypropanal	$(C_3H_6O)_n$	25722-18-3
Poly-β-propiolactone	$(C_3H_4O_2)_n$	25037-58-5
Polypropylene	$(C_3H_6)_n$	9003-07-0
Polypropylene, atactic	$(C_3H_6)_n$	9003-07-0
Polypropylene, isotatic	$(C_3H_6)_n$	25085-53-4
Polypropylene, isotatic, amorphous	$(C_3H_6)_n$	25085-53-4
Polypropylene, isotatic, crystalline	$(C_3H_6)_n$	25085-53-4
Polypropylene, syndiotatic	$(C_3H_6)_n$	26063-22-9
Poly-L-proline·glycine·proline copolymer	$(C_{11}H_{17}N_3O_3)_n$	unavailable
Poly-L-serine	$(C_3H_5NO_2)_n$	25821-52-7
Poly-L-sodium glutamate·tyrosine copolymer	$(C_{14}H_{15}N_2NaO_3)_n$	97105-00-5
Polystyrene	$(C_8H_8)_n$	9003-53-6
Polystyrene-d_3	$(C_8H_5D_3)_n$	84741-01-5
Polystyrene-d_5	$(C_8H_3D_5)_n$	30209-80-4
Polystyrene-d_8	$(C_8D_8)_n$	27732-42-9
Polystyrene, atactic	$(C_8H_8)_n$	9003-53-6
Polystyrene, isotatic	$(C_8H_8)_n$	25086-18-4
Polystyrene, isotatic, annealed	$(C_8H_8)_n$	25086-18-4
Polystyrene-polystyrene-d_8 copolymer	$(C_{16}H_8D_8)_n$	70285-56-2
Poly(sulfonyl-1,4-phenylene)	$(C_6H_4O_2S)_n$	31833-61-1
Poly-[N-terphthalyl-bis-(N′-phenyl-o-diphenylamine)]	$(C_{32}H_{24}N_4O_2)_n$	39820-26-3
Polytetrafluoroethylene, annealed	$(C_2F_4)_n$	9002-84-0
Polytetrafluoroethylene, drawn	$(C_2F_4)_n$	9002-84-0
Polytetrafluoroethylene, molded	$(C_2F_4)_n$	9002-84-0
Polytetrafluoroethylene, powder	$(C_2F_4)_n$	9002-84-0
Polytetrafluoroethylene, quenched	$(C_2F_4)_n$	9002-84-0
Polytetrahydrofuran	$(C_4H_8O)_n$	24979-97-3
Polytriazine	$(C_{24}H_{12}N_6)_n$	33411-58-4
Poly(triazolequinazoline)	$(C_{30}H_{16}N_8)_n$	31742-67-3
Poly(tridecanolactone)	$(C_{13}H_{24}O_2)_n$	unavailable
Polytrifluorochloroethylene	$(C_2ClF_3)_n$	9002-83-9
Polytrifluorovinyl chloride	$(C_2ClF_3)_n$	9002-83-9
Poly-N-(β-trimethylsilylethyl)azetidine	$(C_8H_{19}NSi)_n$	59789-07-0
Poly-N-(β-trimethylsilylethyl)azetidine, zinc chloride complex	$(C_8H_{19}Cl_2NSiZn)_n$	59789-07-0
Poly-N-(β-trimethylsilylethyl) ethylenimine	$(C_7H_{17}NSi)_n$	54691-50-8
Poly-L-tryptophane	$(C_{11}H_{10}N_2O)_n$	27813-82-7
Poly-L-tyrosine	$(C_9H_9NO_2)_n$	25619-78-7
Poly-δ-valerolactone	$(C_5H_8O_2)_n$	26354-94-9
Poly-L-valine	$(C_5H_9NO)_n$	25609-85-2
Polyvinyl alcohol	$(C_2H_4O)_n$	9002-89-5
Polyvinyl chloride	$(C_2H_3Cl)_n$	93050-82-9
Polyvinyldimethylbenzylsilane	$(C_{11}H_{16}Si)_n$	26715-68-4
Polyvinyldimethylphenylsilane	$(C_{10}H_{14}Si)_n$	26744-16-1
Polyvinylenediphenylenesilyl,germyl-α,ω-dihydride copolymer	$(C_{28}H_{24}GeSi)_n$	66160-70-1

Polyvinylenediphenylgermane	$(C_{14}H_{12}Ge)_n$	60130-27-0
Polyvinylenediphenylgermyl-α,ω-dihydride	$(C_{14}H_{12}Ge)_n$	60130-27-0
Polyvinylenediphenylsilane	$(C_{14}H_{12}Si)_n$	66160-69-8
Polyvinylenediphenylsilyl-α,ω-dihydride	$(C_{14}H_{12}Si)_n$	66160-69-8
Polyvinylidene chloride	$(C_2H_2Cl_2)_n$	9002-85-1
Polyvinyltrimethylsilane	$(C_5H_{12}Si)_n$	25036-32-2
Potassium acetate	$C_2H_3KO_2$	127-08-2
Potassium butyrate	$C_4H_7KO_2$	589-39-9
Potassium hydrogen *cis*-butenedioate	$C_4H_3O_4K$	689-82-7
Potassium hydrogen *trans*-butenedioate	$C_4H_3O_4K$	20272-14-4
Potassium hydrogen fumarate	$C_4H_3O_4K$	20272-14-4
Potassium hydrogen maleate	$C_4H_3O_4K$	689-82-7
Potassium 2-methylpropanoate	$C_4H_7KO_2$	19455-20-0
Potassium propionate	$C_3H_5KO_2$	327-62-8
Potassium sodium tartrate tetrahydrate	$C_4H_4KNaO_6\cdot4H_2O$	6381-59-5
Potassium tetraphenyl borate	$C_{24}H_{20}BK$	3244-41-5
Potassium tetraphenyl boron	$C_{24}H_{20}BK$	3244-41-5
Potassium thiocyanate	CKNS	333-20-0
Praseodymium isothiocyanate heptahydrate	$C_3N_3PrS_3\cdot7H_2O$	113614-86-1
Prehnitene	$C_{10}H_{14}$	488-23-3
Proline(L)	$C_5H_9NO_2$	147-85-3
Propaldehyde	C_3H_6O	123-38-6
Propanal	C_3H_6O	123-38-6
Propane	C_3H_8	74-98-6
1,2-Propanediamine	$C_3H_{10}N_2$	78-90-0
1,2-Propanediol	$C_3H_8O_2$	57-55-6
1-Propanethiol	C_3H_8S	107-43-1
2-Propanethiol	C_3H_8S	75-33-2
1,2,3-Propanetriol	$C_3H_8O_3$	56-81-5
1,2,3-Propanetriol-d_3	$C_3H_5D_3O_3$	7325-16-8
Propanoic acid	$C_3H_6O_2$	79-09-4
1-Propanol	C_3H_8O	71-23-8
2-Propanol	C_3H_8O	67-63-0
Propanone	C_3H_6O	67-64-1
Propanone clathrate hydrate	$C_3H_6O\cdot17H_2O$	18879-06-6
Propanoyl chloride	C_3H_5ClO	79-03-8
Propene	C_3H_6	115-07-1
Propene polysulfone	$(C_3H_6O_2S)_n$	30475-44-6
2-Propen-1-ol	C_3H_6O	107-18-6
2-Propenyl ethanoate	$C_5H_8O_2$	591-87-7
β-Propiolactone	$C_3H_4O_2$	57-57-8
Propionic acid	$C_3H_6O_2$	79-09-4
Propionitrile	C_3H_5N	107-12-0
4-Propionyl-4′-*n*-butanoyloxyazobenzene	$C_{19}H_{20}N_2O_3$	76204-68-7
Propionyl chloride	C_3H_5ClO	79-03-8
4-Propionyl-4′-*n*-decanoyloxyazobenzene	$C_{25}H_{32}N_2O_3$	76204-62-1
4-Propionyl-4′-*n*-dodecanoyloxyazobenzene	$C_{27}H_{36}N_2O_3$	76204-60-9
4-Propionyl-4′-*n*-heptadecanoyloxyazobenzene	$C_{32}H_{46}N_2O_3$	76204-55-2
4-Propionyl-4′-*n*-heptanoyloxyazobenzene	$C_{22}H_{26}N_2O_3$	76204-65-4
4-Propionyl-4′-*n*-hexadecanoyloxyazobenzene	$C_{31}H_{44}N_2O_3$	76204-56-3
4-Propionyl-4′-*n*-hexanoyloxyazobenzene	$C_{21}H_{24}N_2O_3$	76204-66-5
4-Propionyl-4′*n*-*n*-onanoyloxyazobenzene	$C_{24}H_{30}N_2O_3$	76204-63-2
4-Propionyl-4′-*n*-octadecanoyloxyazobenzene	$C_{33}H_{48}N_2O_3$	76212-79-8
4-Propionyl-4′-*n*-octanoyloxyazobenzene	$C_{23}H_{28}N_2O_3$	76204-64-3
4-Propionyl-4′-*n*-pentadecanoyloxyazobenzene	$C_{30}H_{42}N_2O_3$	76204-57-4
4-Propionyl-4′-*n*-tetradecanoyloxyazobenzene	$C_{29}H_{40}N_2O_3$	76204-58-5
4-Propionyl-4′-*n*-tridecanoyloxyazobenzene	$C_{28}H_{38}N_2O_3$	76204-59-6
4-Propionyl-4′-*n*-undecanoyloxyazobenzene	$C_{26}H_{34}N_2O_3$	76204-30-9
2-Propoxyethanol	$C_5H_{12}O_2$	2807-30-9
2-*n*-Propoxyethanol	$C_5H_{12}O_2$	2807-30-9
1-*n*-Propoxy-2-methoxyethane	$C_6H_{14}O_2$	500005-28-7
N-(*n*-Propyl)acetamide	$C_5H_{11}NO$	5331-48-6
n-Propyl acetate	$C_5H_{10}O_2$	109-60-4
n-Propyl alcohol	C_3H_8O	71-23-8
n-Propylamine	C_3H_9N	107-10-8
n-Propylammonium bromide	$C_3H_{10}BrN$	4905-83-3
n-Propylbenzene	C_9H_{12}	103-65-1
trans,trans-4′-Propylbicyclohexyl-4-carbonitrile	$C_{16}H_{27}N$	65355-35-3
4′-Propylbiphenyl-4-carbonitrile	$C_{16}H_{15}N$	58743-76-3
n-Propyl bromide	C_3H_7Br	106-94-5
n-Propyl chloride	C_3H_7Cl	540-54-5
n-Propyl cyanide	C_4H_7N	109-74-0
n-Propylcyclohexane	C_9H_{18}	1678-92-8
n-Propylcyclopentane	C_8H_{16}	2040-96-2
α-*n*-Propyldecalin	$C_{13}H_{24}$	91972-45-1
Propyldiammonium cadmium tetrachloride	$C_3H_{12}CdCl_4N_2$	60970-45-8
Propyldiammonium manganese tetrachloride	$C_3H_{12}Cl_4MnN_2$	59683-18-0
Propylene	C_3H_6	115-07-1
Propylene carbonate	$C_4H_6O_3$	108-32-7
Propylene dichloride	$C_3H_6Cl_2$	78-87-5
Propylene glycol	$C_3H_8O_2$	57-55-6
Propylene oxide	C_3H_6O	75-56-9
Propylene oxide clathrate hydrate	$C_3H_6O\cdot17H_2O$	20392-75-0
N-(*n*-Propyl)ethanamide	$C_5H_{11}NO$	5331-48-6
Propyl ethanoate	$C_5H_{10}O_2$	109-60-4
Propyl formate	$C_4H_8O_2$	110-74-7
4-Propyl-4-heptanol	$C_{10}H_{22}O$	2198-72-3
n-Propyl iodide	C_3H_7I	107-08-2
n-Propyl mercaptan	C_3H_8S	107-03-9
Propyl methanoate	$C_4H_8O_2$	110-74-7
n-Propyl methyl ketone	$C_5H_{10}O$	107-87-9
Propyl N-phenylcarbamate	$C_{10}H_{13}NO_2$	5532-90-1
n-Propyl propanoate	$C_6H_{12}O_2$	106-36-5
Propyl propionate	$C_6H_{12}O_2$	106-36-5
Propyl silicate	$C_{12}H_{28}O_4Si$	682-01-9
n-Propylurea	$C_4H_{10}N_2O$	627-06-5
Pseudocumene	C_9H_{12}	95-63-6
Pulegone	$C_{10}H_{16}O$	89-82-7
Purine	$C_5H_4N_4$	120-73-0
Pyrazine	$C_4H_4N_2$	290-37-9
Pyrazole	$C_3H_4N_2$	288-13-1
Pyrene	$C_{16}H_{10}$	129-00-0
Pyrene-picric acid	$C_{22}H_{13}N_3O_7$	1732-41-8
Pyrene-pyromellitic dianhydride charge transfer complex	$C_{26}H_{12}O_6$	6863-59-8
Pyridine	C_5H_5N	110-86-1
Pyridium hexafluorophosphate	$C_5H_6F_6NP$	16941-15-1
Pyridium iodide	C_5H_6IN	18820-83-2
Pyrocatechin	$C_6H_6O_2$	120-80-9
Pyromellitic dianhydride	$C_{10}H_2O_6$	89-32-7
Pyrotartaric acid	$C_5H_8O_4$	498-21-5
Pyrrole	C_4H_5N	109-97-7
Pyrrolidine	C_4H_9N	123-75-1
Pyrrolidine-2-carboxylic acid(L)	$C_5H_9NO_2$	147-85-3
2-Pyrrolidone	C_4H_7NO	616-45-5
α-Pyrrolidone	C_4H_7NO	616-45-5
Pyrroyl manganese tricarbonyl	$C_7H_4MnNO_3$	32761-36-7

Q

Quadricyclane	C_7H_8	278-06-8
m-Quaterphenyl	$C_{24}H_{18}$	1166-18-3
p-Quaterphenyl	$C_{24}H_{18}$	135-70-6
Quinhydrone	$C_{12}H_{10}O_4$	106-34-3
Quinoline	C_9H_7N	91-22-5
β-Quinol carbon monoxide clathrate	$C_{18}H_{18}O_6\cdot0.460CO$	unavailable
β-Quinol-methane clathrate	$C_{18.1}H_{18.6}O_6$	unavailable

Quinone	$C_6H_4O_2$	106-51-4
p-Quinquephenyl	$C_{30}H_{22}$	3073-05-0
Quinuclidine	$C_7H_{13}N$	100-76-5
R		
R227	C_3HF_7	431-89-0
RDX	$C_3H_6N_6O_6$	121-82-4
Resorcin	$C_6H_6O_2$	108-46-3
Resorcinol	$C_6H_6O_2$	108-46-3
Retene	$C_{18}H_{18}$	483-65-8
Ribitol	$C_5H_{12}O_5$	488-81-3
Ribose(D)	$C_5H_{10}O_5$	50-69-1
Rigidex 50 polymer	$(CH_2)_n$	9002-88-4
Rochelle salt	$C_4H_4KNaO_6\cdot 4H_2O$	6381-59-5
Rubber	$(C_5H_8)_n$	9003-31-0
Rubidium butyrate	$C_4H_7O_2Rb$	38869-23-7
Rubidium formate	CHO_2Rb	3495-35-0
Rubidium propionate	$C_3H_5O_2Rb$	19559-54-7
Rubidium tetraphenyl borate	$C_{24}H_{20}BRb$	5971-93-7
Rubidium tetraphenyl boron	$C_{24}H_{20}BRb$	5971-93-7
Ruthenocene	$C_{10}H_{10}Ru$	1287-13-4
S		
Sabinene	$C_{10}H_{16}$	3387-41-5
Salicylaldehyde	$C_7H_6O_2$	90-02-8
Salicylic acid	$C_7H_6O_3$	121-91-5
Salicylic acid-acetamide complex	$C_9H_{11}NO_4$	unavailable
N-Salicylidene-β-alanine	$C_{10}H_{11}NO_3$	34295-85-7
N-Salicylidene-*m*-aminobenzoic acid	$C_{14}H_{11}NO_3$	841-12-3
Samarium isothiocyanate hexahydrate	$C_3N_3S_3Sm\cdot 6H_2O$	113614-84-9
Sarcosine	$C_3H_7NO_2$	107-97-1
Scandium ethanoate	$C_6H_9O_6Sc$	3804-23-7
Sebacic acid	$C_{10}H_{18}O_4$	111-20-6
β-Selenodiglycol	$C_4H_{10}O_2Se$	27974-49-8
Selenophene	C_4H_4Se	288-05-1
Selenophene chromium tricarbonyl	$C_7H_4CrO_3Se$	12078-16-9
Semicarbazide	CH_5N_3O	57-56-7
Semicarbazide hydrochloride	CH_6ClN_3O	563-41-7
Serine(DL)	$C_3H_7NO_3$	302-84-1
Serine(L)	$C_3H_7NO_3$	56-45-1
Silicon tetramethyl	$C_4H_{12}Si$	75-76-3
Silver phenylacetylenide	C_8H_5Ag	33440-88-9
β-Sitosterol	$C_{29}H_{50}O$	83-46-5
Sodium acetate	$C_2H_3NaO_2$	127-09-3
Sodium acetate trihydrate	$C_2H_3NaO_2\cdot 3H_2O$	6131-90-4
Sodium butyrate	$C_4H_7NaO_2$	156-54-7
Sodium ethanoate	$C_2H_3NaO_2$	127-09-3
Sodium formate	$CHNaO_2$	141-53-7
Sodium methanoate	$CHNaO_2$	141-53-7
Sodium methoxide	CH_3NaO	124-41-4
Sodium *p*-nitrophenoxide dihydrate	$C_6H_4NNaO_3\cdot 2H_2O$	42083-62-5
Sodium oxalate	$C_2Na_2O_4$	62-76-0
β-Sodium palmitate	$C_{16}H_{31}NaO_2\cdot 0.01H_2O$	408-35-5
δ-Sodium palmitate	$C_{16}H_{31}NaO_2$	408-35-5
ϵ-Sodium palmitate	$C_{16}H_{31}NaO_2\cdot 0.482H_2O$	408-35-5
ω-Sodium palmitate	$C_{16}H_{31}NaO_2$	408-35-5
Sodium potassium tartrate tetrahydrate	$C_4H_4KNaO_6\cdot 4H_2O$	6381-59-5
Sodium propanoate	$C_3H_5NaO_2$	137-53-7
Sodium succinate	$C_4H_4Na_2O_4$	150-90-3
Sorbitol(D)	$C_6H_{14}O_6$	50-70-4
Sorbose(L)	$C_6H_{12}O_6$	87-79-6
Spiropentane	C_5H_8	157-40-4
Squaric acid	$C_4H_2O_4$	2892-51-5
Stearic acid	$C_{18}H_{36}O_2$	57-11-4
Stilbene	$C_{14}H_{12}$	588-59-0
trans-Stilbene	$C_{14}H_{12}$	103-30-0
Strontium dicalcium propionate	$C_{18}H_{30}Ca_2O_{12}Sr$	54993-39-4
Styphnic acid	$C_6H_3N_3O_8$	82-71-3
Styrene	C_8H_8	100-42-5
Styrene-d_8	C_8D_8	19361-62-7
Suberic acid	$C_8H_{14}O_4$	505-48-6
Succinamide	$C_4H_8N_2O_2$	110-14-5
Succinic acid	$C_4H_6O_4$	110-15-6
Succinimide	$C_4H_5NO_2$	123-56-8
Succinonitrile	$C_4H_4N_2$	110-61-2
Sucrose	$C_{12}H_{22}O_{11}$	57-50-1
T		
Tartaric acid	$C_4H_6O_6$	87-69-4
Taurine	$C_2H_7NO_3S$	107-35-7
Teflon	$(C_2F_4)_n$	9002-84-0
Teflon, annealed	$(C_2F_4)_n$	9002-84-0
Teflon, drawn	$(C_2F_4)_n$	9002-84-0
Teflon, molded	$(C_2F_4)_n$	9002-84-0
Teflon, powder	$(C_2F_4)_n$	9002-84-0
Teflon, quenched	$(C_2F_4)_n$	9002-84-0
Tellurophene chromium tricarbonyl	$C_7H_4CrO_3Te$	39015-36-6
m-Tercylcohexyl	$C_{18}H_{32}$	1706-50-9
o-Tercylcohexyl	$C_{18}H_{32}$	2456-43-1
p-Tercylcohexyl	$C_{18}H_{32}$	1795-19-3
Terephthal-*bis*-*n*-butylaniline	$C_{28}H_{32}N_2$	29743-21-3
Terephthalic acid	$C_8H_6O_4$	569-51-7
Terephthalic bisamidrazone	$C_8H_{12}N_6$	19173-40-1
Terephthalodinitrile	$C_8H_4N_2$	623-26-7
Terephthaloyl dichloride	$C_8H_4Cl_2O_2$	100-20-9
Terephthalyl chloride	$C_8H_4Cl_2O_2$	100-20-9
m-Terphenyl	$C_{18}H_{14}$	92-06-8
o-Terphenyl	$C_{18}H_{14}$	84-15-1
p-Terphenyl	$C_{18}H_{14}$	92-94-4
p-Terphenyl-d_{14}	$C_{18}D_{14}$	1718-51-0
3,3′,4,4′-Tetraaminodiphenyl ether	$C_{12}H_{14}N_4O$	2676-59-7
3,3′,4,4′-Tetraaminodiphenyl oxide	$C_{12}H_{14}N_4O$	2676-59-7
Tetraamylstannane	$C_{20}H_{44}Sn$	3765-65-9
Tetraamyl tin	$C_{20}H_{44}Sn$	3765-65-9
1,4,8,11-Tetraazacyclotetradecane	$C_{10}H_{24}N_4$	295-37-4
1,4,8,11-Tetraazacyclotetradecane copper (II) nitrate	$C_{10}H_{24}N_4\cdot Cu(NO_3)_2$	73746-94-8
1,3,5,7-Tetraazatricyclo[3.3.1.1^{3,7}]decane	$C_6H_{12}N_4$	100-97-0
1,2,4,5-Tetrabromobenzene	$C_6H_2Br_4$	636-28-2
Tetrabromomethane	CBr_4	558-13-4
1,1,2,2-Tetrabromoethane	$C_2H_2Br_4$	79-27-6
Tetrabutoxytitanium	$C_{16}H_{36}O_4Ti$	5593-70-4
Tetra-*n*-butylammonium bromide	$C_{16}H_{36}BrN$	1643-19-2
Tetrabutyl silicate	$C_{16}H_{36}O_4Si$	4766-57-8
1,2,3,4-Tetrachlorobenzene	$C_6H_2Cl_4$	634-66-2
1,2,3,5-Tetrachlorobenzene	$C_6H_2Cl_4$	634-90-2
1,2,4,5-Tetrachlorobenzene	$C_6H_2Cl_4$	95-94-3
Tetrachloro-*p*-benzoquinone	$C_6Cl_4O_2$	118-75-2
Tetrachlorobis-(butylammonium) manganese II	$C_8H_{24}Cl_4MnN_2$	58675-48-2
Tetrachlorobis-(decylammonium) manganese II	$C_{20}H_{48}Cl_4MnN_2$	53188-91-3
Tetrachlorobis-(deuteromethylammonium) manganese II	$C_2H_6Cl_4D_6MnN_2$	unavailable
Tetrachlorobis-(ethylammonium) manganese II	$C_4H_{16}Cl_4MnN_2$	12070-79-0
Tetrachlorobis-(methylammonium) cadmium II	$C_2H_{12}CdCl_4N_2$	53188-86-6
Tetrachlorobis-(methylammonium) manganese II	$C_2H_{12}Cl_4MnN_2$	12121-86-7
Tetrachlorobis-(pentylammonium) manganese II	$C_{10}H_{28}Cl_4MnN_2$	58675-49-3
Tetrachlorobis-(2-propeneammonium) cadmium II	$C_6H_{16}CdCl_4N_2$	82794-54-5

Tetrachlorobis-(*n*-propylammonium) cadmium II	$C_6H_{20}CdCl_4N_2$	53188-87-7
Tetrachlorobis-(*n*-propylammonium) manganese II	$C_6H_{20}Cl_4MnN_2$	52495-27-9
1,1,1,2-Tetrachlorodifluoroethane	$C_2Cl_4F_2$	76-11-9
1,1,2,2-Tetrachloro-1,2-difluoroethane	$C_2Cl_4F_2$	76-12-0
1,1,2,2-Tetrachloroethane	$C_2H_2Cl_4$	79-34-5
Tetrachloroethene	C_2Cl_4	127-18-4
Tetrachloroethylene	C_2Cl_4	127-18-4
Tetrachloromethane	CCl_4	56-23-5
1,1,1,3-Tetrachloropropane	$C_3H_4Cl_4$	1070-78-6
n-Tetracosane	$C_{24}H_{50}$	646-31-1
1,2,4,5-Tetracyanobenzene	$C_{10}H_2N_4$	712-74-3
1,2,4,5-Tetracyanobenzene-pyrene complex	$C_{26}H_{12}N_4$	7371-17-7
Tetracyclo[3.2.0.0.^{2,7}.0^{4,6}]heptane	C_7H_8	278-06-8
Tetracyclopropylsuccinonitrile	$C_{16}H_{20}N_2$	19219-01-3
n-Tetradecane	$C_{14}H_{30}$	629-59-4
1-Tetradecanethiol	$C_{14}H_{30}S$	2079-95-0
Tetradecanoic acid	$C_{14}H_{28}O_2$	544-63-8
1-Tetradecanol	$C_{14}H_{30}O$	112-72-1
2-Tetradecanone	$C_{14}H_{28}O$	2345-27-9
1-Tetradecene-urea adduct	$C_{2.4}H_{6.9}N_2O$	27610-35-1
n-Tetradecyl alcohol	$C_{14}H_{30}O$	112-72-1
n-Tetradecyl mercaptan	$C_{14}H_{30}S$	2079-95-0
Tetraethylammonium bromide	$C_8H_{20}BrN$	71-91-0
Tetraethylammonium iodide	$C_8H_{20}IN$	68-05-3
Tetraethylammonium tetrabromoferrate	$C_8H_{20}Br_4FeN$	21279-19-6
Tetraethylammonium tetrachloroferrate	$C_8H_{20}Cl_4FeN$	14240-75-6
Tetraethylcarbamide	$C_9H_{20}N_2O$	1187-03-7
1,1,3,3-Tetraethyl-5,5-dimethylcyclotrisiloxane	$C_{10}H_{26}O_3Si_3$	110505-51-6
1,1,3,3-Tetraethyl-5,5-diphenylcylotrisiloxane	$C_{20}H_{30}O_3Si_3$	108543-32-4
Tetraethylene glycol	$C_8H_{18}O_5$	112-60-7
Tetraethylenepentamine	$C_8H_{23}N_5$	112-57-2
Tetraethylgermane	$C_8H_{20}Ge$	597-63-7
Tetraethyl lead	$C_8H_{20}Pb$	78-00-2
Tetraethylmethane	C_9H_{20}	1067-20-5
Tetraethyl silicate	$C_8H_{20}O_4Si$	78-10-4
Tetraethylsilane	$C_8H_{20}Si$	631-36-7
Tetraethyl silicon	$C_8H_{20}Si$	631-36-7
Tetraethyl tin	$C_8H_{20}Sn$	597-64-8
Tetraethylurea	$C_9H_{20}N_2O$	1187-03-7
Tetrafluorethene	C_2F_4	116-14-3
1,2,3,4-Tetrafluorobenzene	$C_6H_2F_4$	551-62-2
1,2,3,5-Tetrafluorobenzene	$C_6H_2F_4$	2367-82-0
1,2,4,5-Tetrafluorobenzene	$C_6H_2F_4$	327-54-8
Tetrafluoroethylene	C_2F_4	116-14-3
Tetrafluoromethane	CF_4	75-73-0
Tetra-*n*-hexylammonium perchlorate	$C_{24}H_{52}ClNO_4$	4656-81-9
1,2,3,4-Tetrahydroanthracene	$C_{14}H_{14}$	2141-42-6
exo-Tetrahydrodicyclopentadiene	$C_{10}H_{16}$	2825-82-3
Tetrahydrofuran	C_4H_8O	109-99-9
Tetrahydrofuran clathrate hydrate	$C_4H_8O \cdot 17H_2O$	18879-05-5
Tetrahydrofurfuryl alcohol	$C_5H_{10}O_2$	97-99-4
Tetrahydro-1,4-isoxazine	C_4H_9NO	110-91-8
1,2,3,4-Tetrahydro-9-methylcarbazole	$C_{13}H_{15}N$	6303-88-4
1,2,3,4-Tetrahydronaphthalene	$C_{10}H_{11}$	119-64-2
1,2,3,4-Tetrahydrophenanthrene	$C_{14}H_{14}$	1013-08-7
Tetrahydrophthalic anhydride	$C_8H_8O_3$	85-43-8
Tetrahydropyran	$C_5H_{10}O$	142-68-7
Tetrahydropyran-2-methanol	$C_6H_{12}O_2$	100-72-1
4,5,9,10-Tetrahydropyrene	$C_{16}H_{14}$	781-17-9
1,4,5,6-Tetrahydropyrimidine	$C_4H_8N_2$	1606-49-1
1,2,3,4-Tetrahydroquinoline	$C_9H_{11}N$	635-46-1
5,6,7,8-Tetrahydroquinoline	$C_9H_{11}N$	10500-57-9
1,2,3,4-Tetrahydroxybutane	$C_4H_{10}O_4$	149-32-6
Tetraiodomethane	CI_4	507-25-5
Tetrakis(μ_3-methoxo-2,4-pentanedionato(methanol) nickel (II)	$C_{28}H_{56}Ni_4O_{16}$	18432-56-9
Tetrakis(methylamine)platinum dibromide	$C_4H_{20}Br_2N_4Pt$	15273-28-6
trans-Tetrakis(methylamine)platinum tetrabromide	$C_4H_{20}Br_4N_4Pt$	131415-64-0
Tetrakis(methylthia)methane	$C_5H_{12}S_4$	6156-25-3
Tetrakis(pentane-2,4-dionato)zirconium(IV)	$C_{20}H_{28}O_8Zr$	17501-44-9
Tetrakis(1,1,1-trifluoropentane-2,4-dionato)zirconium(IV)	$C_{20}H_{16}F_{12}O_8Zr$	17499-68-3
Tetra-μ_3-methoxy-tetrakis-[salicylaldehydato(methanol)nickel(II)]	$C_{36}H_{48}Ni_4O_{16}$	18432-56-0
Tetramethylammonium bromide	$C_4H_{12}BrN$	64-20-0
Tetramethylammonium chloride	$C_4H_{12}ClN$	75-57-0
Tetramethylammonium hexacyanotrimethylenecyclopropanide	$C_{16}H_{12}N_7$	89187-04-3
Tetramethylammonium hydrogen dichloride	$C_4H_{13}Cl_2N$	5906-64-0
Tetramethylammonium iodide	$C_4H_{12}IN$	75-58-9
Tetramethylammonium platinum iodide	$C_4H_{20}I_2N_4Pt$	131145-80-7
Tetramethylammonium tetrabromozincate(II)	$C_8H_{24}Br_4N_2Zn$	2041-07-3
Tetramethylammonium tetrachloroferrate(III)	$C_4H_{12}Cl_4FeN$	15649-95-5
Tetramethylammonium trichlorocadmate	$C_4H_{12}CdCl_3N$	15976-91-7
Tetramethylammonium trichloromanganate(II)	$C_4H_{12}Cl_3MnN$	18616-15-0
1,2,3,4-Tetramethylbenzene	$C_{10}H_{14}$	488-23-3
1,2,3,5-Tetramethylbenzene	$C_{10}H_{14}$	527-53-7
1,2,4,5-Tetramethylbenzene	$C_{10}H_{14}$	95-93-2
2,3,4,5-Tetramethylbenzoic acid	$C_{11}H_{14}O_2$	2529-39-7
2,3,4,6-Tetramethylbenzoic acid	$C_{11}H_{14}O_2$	2408-38-0
2,3,5,6-Tetramethylbenzoic acid	$C_{11}H_{14}O_2$	2604-45-7
2,4,5,7-Tetramethyl-4,5-*bis*(4-*tert*-butylphenyl)octane	$C_{32}H_{50}$	85668-75-3
2,2,3,3-Tetramethylbutane	C_8H_{18}	594-82-1
Tetramethylcarbamide	$C_5H_{12}N_2O$	632-22-0
1,1,10,10-Tetramethylcyclooctadecane	$C_{22}H_{44}$	23014-56-0
1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane	$C_{16}H_{22}OSi_2$	56-33-7
Tetramethyldisilacyclobutane	$C_6H_{16}Si_2$	1627-98-1
1,1,3,3-Tetramethyl-1,3-disilacyclobutane	$C_6H_{16}Si_2$	1627-98-1
Tetramethyldisiletan	$C_6H_{16}Si_2$	1627-98-1
Tetramethylethylene	C_6H_{12}	563-78-0
Tetramethylgermane	$C_4H_{12}Ge$	865-52-2
3,7,11,15-Tetramethyl-1-hexadecen-3-ol	$C_{20}H_{38}O$	60046-87-9
3,7,11,15-Tetramethyl-1-hexadecyn-3-ol	$C_{20}H_{38}O$	29171-23-8
1,3,5,7-Tetramethyl-2,4,6,8,9,10-hexathiaadamantane	$C_8H_{12}S_6$	6327-74-3
2,2,5,5-Tetramethylhex-3-ene	$C_{10}H_{20}$	22808-06-4
1,1,4,7-Tetramethylindan	$C_{13}H_{18}$	1078-04-3
1,1,4,6-Tetramethylindan	$C_{13}H_{18}$	941-60-4
Tetramethyl lead	$C_4H_{12}Pb$	75-74-1
2,2,4,4-Tetramethyl-3-oxapentane	$C_8H_{18}O$	6163-66-2
2,6,10,14-Tetramethylpentadecane	$C_{19}H_{40}$	1921-70-6
2,2,4,4-Tetramethylpentan-3-ol	$C_9H_{20}O$	14609-79-9
2,2,3,3-Tetramethylpentane	C_9H_{20}	7154-79-2
2,2,4,4-Tetramethylpentane	C_9H_{20}	1070-87-7
N,N,N′,N′-Tetramethyl-*p*-phenylene-diamine perchlorate	$C_{10}H_{16}N_2ClO_4$	38668-38-2
2,4,6,8-Tetramethyl-2,4,6,8-tetraphenyl-cyclosiloxane	$C_{28}H_{32}Si_4O_4$	77-63-6
Tetramethylsilane	$C_4H_{12}Si$	75-76-3
Tetramethyl silicate	$C_4H_{12}O_4Si$	681-84-5
Tetramethyl stannane	$C_4H_{12}Sn$	594-27-6
Tetramethylsuccinic acid	$C_8H_{14}O_4$	630-51-3
Tetramethylsuccinonitrile	$C_8H_{12}N_2$	3333-52-6
1,1,3,3-Tetramethyl-5,5,7,7-tetraphenyl-cyclotetrasiloxane	$C_{28}H_{32}O_4Si_4$	1693-47-6

1,3,5′7′-Tetramethyl-1′,3′,5,7-tetraphenylcyclotetrasiloxane	$C_{28}H_{32}O_4Si_4$	77-63-4
1,3,5,7-Tetramethyl-2,4,6,8-tetrathiaadamantane	$C_{10}H_{16}S_4$	7000-79-5
Tetramethylthiuram disulfide	$C_6H_{12}N_2S_4$	137-26-8
Tetramethylthiuram monosulfide	$C_6H_{12}N_2S_3$	97-74-5
Tetramethyl tin	$C_4H_{12}Sn$	594-27-4
Tetramethylurea	$C_5H_{12}N_2O$	632-22-4
2,4,6,N-Tetranitroethylaniline	$C_8H_7N_5O_8$	6052-13-7
2,4,6,N-Tetranitro-N-methyltoluidine	$C_8H_7N_5O_8$	43072-20-4
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine	$C_4H_8N_8O_8$	2691-41-0
1,3,5,7-Tetranitro-1,3,5,7-cyclooctahydrotetrazocine	$C_4H_8N_8O_8$	2691-41-0
1,3,5,7-Tetranitro-1,3,5,7-cyclooctahydrotetrazocine(α)	$C_4H_8N_8O_8$	2691-41-0
1,3,5,7-Tetranitro-1,3,5,7-cyclooctahydrotetrazocine(β)	$C_4H_8N_8O_8$	2691-41-0
1,3,5,7-Tetranitro-1,3,5,7-cyclooctahydrotetrazocine(δ)	$C_4H_8N_8O_8$	2691-41-0
1,3,5,7-Tetranitro-1,3,5,7-cyclooctahydrotetrazocine(γ)	$C_4H_8N_8O_8$	2691-41-0
2,5,8,11-Tetraoxadodecane	$C_8H_{18}O_4$	112-49-2
Tetrapentyltin	$C_{20}H_{44}Sn$	3765-65-9
1,1,1,2-Tetraphenylethane	$C_{26}H_{22}$	2294-94-2
1,1,2,2-Tetraphenylethane	$C_{26}H_{22}$	632-50-8
Tetraphenylethylene	$C_{26}H_{20}$	632-51-9
Tetraphenylmethane	$C_{25}H_{20}$	630-76-2
Tetraphenylsilane	$C_{24}H_{20}Si$	1048-08-4
Tetraphenylstannane	$C_{24}H_{20}Sn$	595-90-4
Tetraphenyl tin	$C_{24}H_{20}Sn$	595-90-4
Tetra-*n*-propylammonium iodide	$C_{12}H_{28}IN$	631-40-3
Tetrapropylene glycol	$C_{12}H_{26}O_5$	25657-08-3
Tetrapropyl silicate	$C_{12}H_{28}O_4Si$	682-01-9
n-Tetratriacontane	$C_{34}H_{70}$	14167-59-0
Tetrazole	CH_2N_4	288-94-8
Tetroxan	$C_4H_8O_4$	293-30-1
Tetryl	$C_7H_5N_5O_8$	479-45-8
Tetryl-*bis*(trinitrotoluene) complex	$C_{21}H_{15}N_{11}O_{20}$	unavailable
Tetryl-picric acid complex	$C_{13}H_8N_8O_{15}$	unavailable
Thallium acetate	$C_2H_3O_2Tl$	563-68-8
Thallium butyrate	$C_4H_7O_2Tl$	63424-49-7
Thallium (I) *n*-decanoate	$C_{10}H_{19}O_2Tl$	18993-51-6
Thallium *n*-dodecanoate	$C_{12}H_{23}O_2Tl$	18993-51-6
Thallium formate	CHO_2Tl	992-98-3
Thallium heptanoate	$C_7H_{13}O_2Tl$	34244-91-2
Thallium hexadecanoate	$C_{16}H_{31}O_2Tl$	33734-55-3
Thallium hexanoate	$C_6H_{11}O_2Tl$	34244-90-1
Thallium nonanoate	$C_9H_{17}O_2Tl$	34244-92-3
Thallium octadecanoate	$C_{18}H_{35}O_2Tl$	33734-56-4
Thallium octanoate	$C_8H_{15}O_2Tl$	18993-50-5
Thallium pentanoate	$C_5H_9O_2Tl$	34244-89-8
Thallium propionate	$C_3H_5O_2Tl$	63424-48-6
Thallium tetradecanoate	$C_{14}H_{27}O_2Tl$	18993-53-8
Thallium tridecanoate	$C_{13}H_{25}O_2Tl$	80006-41-3
Thallium undecanoate	$C_{11}H_{21}O_2Tl$	34244-93-4
THAM	$C_4H_{11}NO_3$	77-86-1
Thiaadamantane	$C_9H_{14}S$	281-25-4
2-Thiabutane	C_3H_8S	624-89-5
Thiacyclobutane	C_3H_6S	287-27-4
Thiacyclohexane	$C_5H_{10}S$	1613-51-0
Thiacyclopentane	C_4H_8S	110-01-0
4-Thiaheptane	$C_6H_{14}S$	111-47-7
2-Thiahexane	$C_5H_{12}S$	628-29-5
3-Thiahexane	$C_5H_{12}S$	4110-50-3
5-Thianonane	$C_8H_{18}S$	544-40-1
Thianthrene	$C_{12}H_8S_2$	92-85-3
2-Thiapentane	$C_4H_{10}S$	3877-15-4
3-Thiapentane	$C_4H_{10}S$	352-93-2
2-Thiapropane	C_2H_6S	75-18-3
Thiazole	C_3H_3NS	288-47-1
Thioacetamide	C_2H_5NS	62-55-5
Thiobenzamide	C_7H_7NS	2227-79-4
Thiocarbohydrazide	CH_6N_4S	2231-57-4
β-Thiolactic acid	$C_3H_6O_2S$	107-96-0
3-Thiolpropanoic acid	$C_3H_6O_2S$	107-96-0
Thiophene	C_4H_4S	110-02-1
Thiophene chromium tricarbonyl	$C_7H_4CrO_3S$	12078-15-8
Thiophenol	C_6H_6S	108-98-5
Thiosemicarbazide	CH_5N_3S	79-19-6
Thiourea	CH_4N_2S	62-56-6
Thiourea carbon tetrachloride inclusion compound	$C_3H_{12}N_6S_3{\cdot}CCl_4$	70938-79-3
Thiourea-cycloheptane adduct	$C_{10}H_{26}N_6S_3$	39822-97-4
Thiourea-cyclohexane adduct	$C_9H_{24}N_6S_3$	33561-77-2
Thiourea-cyclooctane adduct	$C_{11}H_{28}N_6S_3$	39822-99-6
Thiourea-2,2-dimethylbutane adduct	$C_9H_{26}N_6S_3$	39822-98-5
Thiourea-ferrocene	$C_{13}H_{22}FeN_6S_3$	54899-85-3
Thiourea nitrate	$CH_5N_3O_3S$	55011-91-1
Thiourea 1,1,2,2-tetrachloroethane clathrate	$(CH_4N_2S)_3{\cdot}C_2H_2Cl_4$	145195-87-5
Thioxanthone	$C_{13}H_8OS$	492-22-8
Thymine	$C_5H_6N_2O_2$	65-71-4
Tin tetraamyl	$C_{20}H_{44}Sn$	3765-65-9
γ-TNT	$C_7H_5N_3O_6$	118-96-7
α-Tocopherol acetate	$C_{31}H_{52}O_3$	58-95-7
Toluene	C_7H_8	108-88-3
m-Toluic acid	$C_8H_8O_2$	99-04-7
o-Toluic acid	$C_8H_8O_2$	118-90-1
p-Toluic acid	$C_8H_8O_2$	99-94-5
m-Toluidine	C_7H_9N	108-44-1
o-Toluidine	C_7H_9N	95-53-4
p-Toluidine	C_7H_9N	106-49-0
p-Toluidine-phenol complex	$C_{13}H_{15}NO$	14489-32-8
2,4-Tolylenediisocyanate	$C_9H_6N_2O_2$	584-84-9
Triacetamide nitrate	$C_6H_{16}N_4O_6$	54800-07-6
Triacetin	$C_9H_{14}O_6$	102-76-1
n-Triacontane	$C_{30}H_{62}$	638-68-6
Tri-L-alanine	$C_9H_{17}N_3O_4$	5874-90-8
Triamantane	$C_{18}H_{24}$	13349-10-5
Triaquo hexacetate chromate chloride hexahydrate	$C_{12}H_{36}ClCr_3O_{22}$	12366-60-8
s-Triazine	$C_3H_3N_3$	290-87-9
Triazine triol	$C_3H_3N_3O_3$	108-80-5
1,2,4-Triazole	$C_2H_3N_3$	288-88-0
1,2,4-Triazol-3-one	$C_2H_3N_3O$	930-33-6
Tribenzyl-*n*-hexadecylsilane	$C_{37}H_{54}Si$	unavailable
2,4,6-Tribromoaniline	$C_6H_4Br_3N$	147-82-0
Tribromomethane	$CHBr_3$	75-25-2
2,4,6-Tribromophenol	$C_6H_3Br_3O$	118-79-6
1,2,3-Tribromopropane	$C_3H_5Br_3$	96-11-7
Tri(*tert*-butyl)methane	$C_{13}H_{28}$	35660-96-9
Tri-*tert*-butylmethanol	$C_{13}H_{28}O$	41902-42-5
Tri-*n*-butylphosphate	$C_{12}H_{27}O_4P$	126-73-8
Tributyrin	$C_{15}H_{26}O_6$	60-01-5
Tricaproin	$C_{21}H_{38}O_6$	621-70-5
α,α,α-Trichloroacetaldehyde	C_2HCl_3O	75-87-6
Trichloroacetic acid	$C_2HCl_3O_2$	76-03-9
1,2,4-Trichlorobenzene	$C_6H_3Cl_3$	120-82-1
2,2,3-Trichlorobutanal	$C_4H_5Cl_3O$	76-36-8
2,2,2-Trichloroethanal	C_2HCl_3O	75-87-6
1,1,1-Trichloroethane	$C_2H_3Cl_3$	71-55-6
1,1,2-Trichloroethane	$C_2H_3Cl_3$	79-00-5
Trichloroethene	C_2HCl_3	79-01-6
Trichloroethylene	C_2HCl_3	79-01-6
Tri-(2-chloroethyl)phosphate	$C_6H_{12}Cl_3O_4P$	115-96-8
Trifluorochloroethene	C_2ClF_3	359-29-5
Trifluorochloroethylene	C_2ClF_3	359-29-5
Trichloromethane	$CHCl_3$	67-66-3
Trichloromethylsilane	CH_3Cl_3Si	75-79-6

Trichlorophenylstannane	$C_6H_5Cl_3Sn$	1124-19-2
1,2,3-Trichloropropane	$C_3H_5Cl_3$	98-18-4
o-Trichlorosilylbiphenyl	$C_{12}H_9Cl_3Si$	18030-62-1
p-Trichlorosilylbiphenyl	$C_{12}H_9Cl_3Si$	18030-61-0
β-Trichlorosilylpropionitrile	$C_3H_4Cl_3NSi$	1071-22-3
α,α,α-Trichlorotoluene	$C_7H_5Cl_3$	98-07-7
1,3,5-Trichloro-2,4,6-trichlorobenzene	$C_6Cl_3F_3$	319-88-0
1,1,1-Trichlorotrifluoroethane	$C_2Cl_3F_3$	354-58-5
1,1,2-Trichloro-1,2,2-trifluoroethane	$C_2Cl_3F_3$	76-13-1
1,1,1-Trichloro-3,3,3-trifluoropropane	$C_3H_2Cl_3F_3$	7125-83-9
1,3,5-Trichloro-2,4,6-trimethylbenzene	$C_9H_9Cl_3$	5324-68-5
1,2,3-Trichloro-4,5,6-trimethylbenzene	$C_9H_9Cl_3$	19219-81-9
n-Tricosane	$C_{23}H_{48}$	638-67-5
Tricresyl phosphate	$C_{21}H_{21}O_4P$	78-30-8
Tricyclo[5.2.1.0^{2,6}]decane	$C_{10}H_{16}$	6004-38-2
Tricyclo[3.3.1.1^{3,7}]decane	$C_{10}H_{16}$	281-23-2
Tricyclo[3.3.2.0^{2,8}]deca-2,7,9-triene	$C_{10}H_{10}$	1005-51-2
Tricyclo[6.2.1.1^{3,6}]dodecane	$C_{12}H_{20}$	281-84-5
Tricyclo[2.2.1.0^{2,6}]heptane	C_7H_{10}	279-19-6
1,1,3-Tricyclohexylpropane	$C_{21}H_{38}$	55682-89-8
Tricyclopentadienyl yttrium	$C_{15}H_{15}Y$	1294-07-1
n-Tridecane	$C_{13}H_{28}$	629-50-5
Tridecanedioic acid	$C_{13}H_{24}O_4$	638-53-9
Tridecanoic acid	$C_{13}H_{26}O_2$	638-53-9
Tridecanoin	$C_{33}H_{62}O_6$	621-71-6
1-Tridecanol	$C_{13}H_{28}O$	112-70-9
Tridecanolactone	$C_{13}H_{24}O_2$	1725-04-8
n-Tridecyl alcohol	$C_{13}H_{28}O$	112-70-9
Tridecyl methyl ketone	$C_{15}H_{30}O$	2345-28-0
Triethanolamine	$C_6H_{15}NO_3$	102-71-6
Triethanolamine borate	$C_6H_{12}BNO_3$	283-56-7
Triethylaluminum	$C_6H_{15}Al$	97-93-8
Triethylamine	$C_6H_{15}N$	121-44-8
Triethylamineborane	$C_6H_{18}BN$	1722-26-5
Triethylantimony	$C_6H_{15}Sb$	617-85-6
Triethylarsine	$C_6H_{15}As$	617-75-4
Triethylbismuth	$C_6H_{15}Bi$	617-77-6
Triethylboron	$C_6H_{15}B$	97-94-9
Triethylenediamine	$C_6H_{12}N_2$	280-57-9
Triethylene glycol	$C_6H_{14}O_4$	112-27-6
Triethylenetetramine	$C_6H_{18}N_4$	112-24-3
Triethylgallium	$C_6H_{15}Ga$	1115-99-7
Triethylindium	$C_6H_{15}In$	923-34-2
Triethylstibine	$C_6H_{15}Sb$	617-85-6
Trifluoroacetonitrile	C_2F_3N	353-85-5
Trifluoroacetyl fluoride	C_2F_4O	354-34-7
1,1,1-Trifluoro-3-chloropropane	$C_3H_4ClF_3$	460-35-5
1,1,1-Trifluoro-3,3-dichloropropane	$C_3H_3Cl_2F_3$	460-69-5
1,1,1-Trifluoroethane	$C_2H_3F_3$	420-46-2
Trifluoromethane	CHF_3	75-46-7
Trifluoromethanethiol	CHF_3S	1493-15-8
α (Trifluoromethoxy) α,α difluoromethyl acetate	$C_4H_3F_5O_3$	2195-84-8
3-Trifluoromethylbenzoic acid	$C_7H_5F_3O_2$	454-92-2
Trifluoromethyl cyanide	C_2F_3N	353-85-5
Trifluoromethyl (2-hydroxy-1-propenyl) ketone	$C_5H_5F_3O_2$	65847-85-0
3-Trifluoromethyl nitrobenzene	$C_7H_4F_3NO_2$	98-46-4
2-[3-(Trifluoromethyl)-phenyl]amino-3-pyridinecarboxylic acid	$C_{13}H_9F_3N_2O_2$	4394-00-7
2-[3-(Trifluoromethyl)-phenyl]amino-3 -pyridinecarboxylic acid. β-morpholino ethyl ester	$C_{19}H_{20}F_3N_3O_3$	65847-85-0
α,α,α-Trifluorotoluene	$C_7H_5F_3$	98-08-8
m-Trifluorotoluic acid	$C_7H_5F_3O_2$	454-92-2
α,α,α-Trifluoro-*m*-toluic acid	$C_7H_5F_3O_2$	454-92-2
Triglycine	$C_6H_{11}N_3O_4$	139-13-9
Triglycine fluoroberyllate	$C_6H_{17}BeF_4N_3O_6$	2396-72-7
Triglycine fluoroberyllate, deuterated	$C_6D_{17}BeF_4N_3O_6$	unavailable
Triglycine sulfate	$C_6H_{17}N_3O_{10}S$	513-29-1
Triglycine sulfate, deuterated	$C_6D_{17}N_3O_{10}S$	17237-73-9
Triglycine sulfate-triglycine selenate	$C_6H_{17}N_3O_{10}S\cdot C_6H_{17}N_3O_{10}Se$	unavailable
Triglyme	$C_8H_{18}O_4$	112-49-2
1,1,1-Trihydroxymethylpropane	$C_6H_{10}O_3$	77-99-6
1,2,3-Trihydroxypropane	$C_3H_8O_3$	56-81-5
1,2,3-Trihydroxypropane-d_3	$C_3H_5D_3O_3$	7325-16-8
Triiodomethane	CHI_3	75-47-8
Triiron dodecacarbonyl	$C_{12}Fe_3O_{12}$	17685-52-8
Trilaurin	$C_{39}H_{74}O_6$	538-24-9
Trimargarin	$C_{54}H_{104}O_6$	2438-40-6
Trimellitic anhydride	$C_9H_7O_5$	552-30-7
Trimethylaluminum	C_3H_9Al	75-24-
Trimethylamine	C_3H_9N	75-50-3
Trimethylamineborane	$C_3H_{12}BN$	75-22-9
Trimethylamine-triborane	$C_3H_{16}B_3N$	57808-48-7
Trimethylammonium trichlorocadmate	$C_3H_{10}CdCl_3N$	68778-49--
N,N,2-Trimethylalanine methyl ester	$C_7H_{15}NO_2$	140653-59--
2,N,N-Trimethylaniline	$C_9H_{13}N$	609-72-2
Trimethylarsine	C_3H_9As	593-88--
1,2,3-Trimethylbenzene	C_9H_{12}	526-73-8
1,2,4-Trimethylbenzene	C_9H_{12}	95-63-6
1,3,5-Trimethylbenzene	C_9H_{12}	108-67-8
2,4,6-Trimethylbenzonitrile	$C_{10}H_{11}N$	2571-52-0
2,4,6-Trimethylbenzonitrile N-oxide	$C_{10}H_{11}NO$	2902-57-0
Trimethyl borane	C_3H_9B	593-90-8
Trimethyl borate	$C_3H_9BO_3$	121-43-7
2,2,3-Trimethylbutane	C_7H_{16}	464-06-2
Trimethyl cyanurate	$C_6H_9N_3O_3$	877-89--
2,5,6-Trimethyl-2-cyclohexen-1-one	$C_9H_{14}O$	20030-30-2
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	$C_{13}H_{20}O$	79-77-6
3,7,11-Trimethyl-1-dodecyne-3-ol	$C_{15}H_{28}O$	1604-35-9
Trimethylene oxide	C_3H_6O	503-30-0
Trimethylgallium	C_3H_9Ga	1445-79-0
Trimethylhydrazine	$C_3H_{10}N_2$	1741-01-1
Trimethylhydroquinone	$C_9H_{12}O_2$	700-13-0
Trimethylindium	C_3H_9In	3385-78-2
Trimethylolethane	$C_5H_{12}O_3$	77-85-0
Trimethylolethane tetrahydrate	$C_5H_{12}O_3\cdot 4H_2O$	142381-76-8
6,10,14-Trimethyl-3,5-pentadecadien-2-one	$C_{18}H_{32}O$	1604-32-0
6,10,14-Trimethyl-2-pentadecanone	$C_{18}H_{36}O$	502-69-2
2,2,4-Trimethylpentane	C_8H_{18}	540-84-1
2,3,3-Trimethylpentane	C_8H_{18}	560-21--
2,3,4-Trimethylpentane	C_8H_{18}	565-75-3
2,4,4-Trimethyl-1-pentene	C_8H_{16}	107-39-1
2,4,4-Trimethyl-2-pentene	C_8H_{16}	107-40--
2,3,6-Trimethylphenol	$C_9H_{12}O$	2416-94-6
2,4,6-Trimethylphenol	$C_9H_{12}O$	527-60-6
2,4,6-Trimethylphenyl isocyanide	$C_{10}H_{11}N$	57116-96-8
2,3,6-Trimethylpyridine	$C_8H_{11}N$	1462-84-0
cis-(2,4,6-Trimethyl-2,4,6-triphenyl)cyclotrisiloxane	$C_{21}H_{24}O_3Si_3$	3424-57-5
trans-Tri-2,4,6-methylphenylcyclotrisiloxane	$C_{21}H_{24}O_3Si_3$	6138-53-0
2,2,N-Trimethylpropanamide	$C_6H_{13}NO$	6830-83-7
2,4,6-Trimethylpyridine	$C_8H_{11}N$	108-75-8
N-(β-Trimethylsilylethyl)azetidine, zinc chloride complex	$C_8H_{19}Cl_2NSiZn$	42525-64--
N-(β-Trimethylsilylethyl)ethylenimine	$C_7H_{17}NSi$	18387-12-7
N-(β-Trimethylsilylethyl)trimethylenimine	$C_8H_{19}NSi$	42525-64--
Trimethylsulfonylmethane	$C_4H_{10}O_6S_3$	67294-81-9
2,4,6-Trimethyl-1,3,5-trioxane	$C_6H_{12}O_3$	123-63-7
cis-1,3,5-Trimethyl-1,3,5-triphenylcyclotrisiloxane	$C_{21}H_{24}O_3Si_3$	3424-57-5
trans-1,3,5-Trimethyl-1,3,5-triphenylcyclotrisiloxane	$C_{21}H_{24}O_3Si_3$	6138-53-0
1,3,6-Trimethyluracil	$C_7H_{10}N_2O_2$	13509-52-9

1,1,3-Trimethylurea	$C_4H_{10}N_2O$	632-14-4
Trimyristin	$C_{45}H_{86}O_6$	555-45-3
1,3,5-Tri-2-naphthylbenzene	$C_{36}H_{24}$	7059-70-3
1,3,5-Trinitrobenzene	$C_6H_3N_3O_6$	99-35-4
2,4,6-Trinitro-N-(methylnitro)-*m*-toluidene	$C_8H_7N_5O_8$	43072-20-4
2,4,6-Trinitrophenol	$C_6H_3N_3O_7$	29663-11-4
2,4,6-Trinitrophenylethyl nitramine	$C_8H_7N_5O_8$	6052-13-7
2,4,6-Trinitrophenylmethyl nitramine	$C_7H_5N_5O_8$	479-45-8
2,4,6-Trinitroresorcinol	$C_6H_3N_3O_8$	82-71-3
1,3,5-Trinitroso-1,3,5-triazacyclohexane	$C_3H_6N_6O_3$	1116-76-3
2,4,5-Trinitrotoluene	$C_7H_5N_3O_6$	610-25-3
2,4,6-Trinitrotoluene	$C_7H_5N_3O_6$	118-96-7
1,3,5-Trinitro-1,3,5-triazacyclohexane	$C_3H_6N_6O_6$	121-82-4
Trioctanoin	$C_{27}H_{50}O_6$	538-23-8
Tri-*n*-octylamine	$C_{24}H_{51}N$	1116-76-3
1,3,5-Trioxane	$C_3H_6O_3$	110-88-3
2,5,8-Trioxanonane	$C_6H_{14}O_3$	111-96-6
3,6,9-Trioxaundecane	$C_8H_{18}O_3$	112-36-7
Tripalmitin	$C_{51}H_{98}O_6$	555-44-2
Triphenylamine	$C_{18}H_{15}N$	603-34-9
Triphenylarsine	$C_{18}H_{15}As$	603-32-7
1,3,5-Triphenylbenzene	$C_{24}H_{18}$	612-71-5
Triphenylbismuthine	$C_{18}H_{15}Bi$	603-33-8
Triphenylcarbinol	$C_{19}H_{16}O$	76-84-6
Triphenylchloromethane	$C_{19}H_{15}Cl$	76-83-5
Triphenylchlorosilane	$C_{18}H_{15}ClSi$	76-86-8
Triphenylene	$C_{18}H_{12}$	217-59-4
Triphenylene picric acid	$C_{24}H_{15}N_3O_7$	72454-49-0
1,1,1-Triphenylethane	$C_{20}H_{18}$	5271-39-6
1,1,2-Triphenylethane	$C_{20}H_{18}$	1520-42-9
Triphenylethylene	$C_{20}H_{16}$	58-72-0
Triphenylmethane	$C_{19}H_{16}$	519-73-3
Triphenyl phenylethynyl tin	$C_{26}H_{20}Sn$	1247-08-1
Triphenylphosphate	$C_{18}H_{15}O_4P$	115-86-6
Triphenylphosphine	$C_{18}H_{15}P$	603-35-0
Triphenylphosphine oxide	$C_{18}H_{15}OP$	791-28-6
2,4,6-Triphenylpyridine	$C_{23}H_{17}N$	580-35-8
Triphenylstibene	$C_{18}H_{15}Sb$	603-36-1
Triphenyl-s-triazine	$C_{21}H_{15}N_3$	493-77-6
Triphenyl-1,3,5-triazine	$C_{21}H_{15}N_3$	493-77-6
Triphenyl vinyl tin	$C_{20}H_{18}Sn$	2117-48-8
Tripropionin	$C_{12}H_{20}O_6$	139-45-7
Tripropylaluminum	$C_9H_{21}Al$	102-67-0
Tripropylene glycol	$C_9H_{20}O_4$	1638-16-0
Triptycene	$C_{20}H_{14}$	477-75-8
TRIS	$C_4H_{11}NO_3$	77-86-1
Tris(di-*n*-butyldithiocarbamato)antimony (III)	$C_{27}H_{54}N_3S_6Sb$	14907-93-8
Tris(di-*n*-butyldithiocarbamato)arsenic (III)	$C_{27}H_{54}AsN_3S_6$	48233-55-2
Tris(di-*n*-butyldithiocarbamato)bismuth (III)	$C_{27}H_{54}BiN_3S_6$	34410-99-6
Tris(di-*n*-butyldithiocarbamato)phosphorus (III)	$C_{27}H_{54}N_3PS_6$	69267-83-0
Tris-(cyclopentadienylcobalt)disulfide	$C_{15}H_{15}Co_3S_2$	11105-79-6
Tris(hydroxymethyl)aminomethane	$C_4H_{11}NO_3$	77-86-1
Tris(methylammonium) nonachlorodibismuthate	$C_3H_{18}Bi_2Cl_9N_3$	72318-16-2
Tris(3-methylpentane-2,4-dionato)iron(III)	$C_{18}H_{27}FeO_6$	13978-46-6
Tris(2-picolylamine)iron chloride ethanolate	$C_{20}H_{30}Cl_2FeN_6O$	18433-69-7
Tris(sarcosine) calcium chloride	$C_9H_{21}CaCl_2N_3O_6$	10051-96-4
Tristearin	$C_{57}H_{110}O_6$	555-43-1
Trithiocarbonic acid	CH_2S_3	594-08-1
n-Tritriacontane	$C_{33}H_{68}$	630-05-7
anti, trans-Truxane	$C_{18}H_{16}$	25456-55-7
syn, trans-Truxane	$C_{18}H_{16}$	23358-17-0
Tryptophane(L)	$C_{11}H_{12}N_2O_2$	73-22-3
Tyrosine(L)	$C_9H_{11}NO_3$	60-18-4

U

n-Unatriacontane	$C_{31}H_{64}$	630-04-6
n-Undecane	$C_{11}H_{24}$	1120-21-4
Undecanedioic acid	$C_{11}H_{20}O_4$	1852-04-6
n-Undecane-urea adduct	$C_{2.2}H_{6.6}N_2O$	1191-63-5
Undecanoic acid	$C_{11}H_{22}O_2$	112-37-8
1-Undecanol	$C_{11}H_{24}O$	112-42-5
Undecanolactone	$C_{11}H_{20}O_2$	710-04-3
6-Undecanone	$C_{11}H_{22}O$	927-49-1
1-Undecene	$C_{11}H_{22}$	821-95-4
n-Undecyl alcohol	$C_{11}H_{24}O$	112-42-5
Undecylcyanobiphenyl	$C_{24}H_{31}N$	65860-74-4
n-Untriacontane	$C_{31}H_{64}$	630-04-6
Uracil	$C_4H_4N_2O_2$	66-22-8
Uranium pentaethylate	$C_{10}H_{25}O_5U$	unavailable
Urea	CH_4N_2O	57-13-6
Urea-1-decene adduct	$C_{2.3}H_{6.7}N_2O$	24494-58-4
Urea-1-dodecene adduct	$C_{2.2}H_{6.5}N_2O$	38588-33-9
Urea-1-eicosene adduct	$C_{2.4}H_{6.8}N_2O$	24494-31-7
Urea-1-hexadecene adduct	$C_{2.3}H_{6.7}N_2O$	24494-57-3
Urea nitrate	$CH_5N_3O_4$	17687-37-5
Urea-1-octadecene adduct	$C_{2.4}H_{6.8}N_2O$	38588-35-1
Urea-phenol complex	$C_{13}H_{16}N_2O_3$	5168-44-5
Urea-1-tetradecene adduct	$C_{2.4}H_{6.9}N_2O$	27610-35-1
Urea-trioxane inclusion compound	$C_{10}H_{22}N_2O_{10}$	20351-17-1
Urea-*n*-undecane adduct	$C_{2.2}H_{6.6}N_2O$	1191-63-5
Urethane	$C_3H_7NO_2$	51-79-6
Uric acid	$C_5H_4N_4O_3$	69-93-2

V

Vinylidene chloride	$C_2H_2Cl_2$	75-35-4
Vinyl bromide	C_2H_3Br	593-60-2
Vinyl chloride	C_2H_3Cl	75-01-4
Vinyl cyanide	C_3H_3N	107-13-1
Vinyl acetate	$C_4H_6O_2$	108-05-4
Valeraldehyde	$C_5H_{10}O$	110-62-3
Valeral	$C_5H_{10}O$	110-62-3
δ-Valerolactone	$C_5H_8O_2$	542-28-9
Valeryl chloride	C_5H_9ClO	638-29-9
Valeronitrile	C_5H_9N	110-59-8
n-Valeric acid	$C_5H_{10}O_2$	109-52-4
Valine(D)	$C_5H_{11}NO_2$	640-68-6
Valine(L)	$C_5H_{11}NO_2$	72-18-4
Valine(DL)	$C_5H_{11}NO_2$	516-06-3
Vanadocene	$C_{10}H_{10}V$	1277-47-0
Vinyltrimethylsilane	$C_5H_{12}Si$	754-05-2
Vinyl isobutyl ether	$C_6H_{12}O$	109-53-5
Vinyl *n*-butyl ether	$C_6H_{12}O$	111-34-2
Vinyldimethylphenylsilane	$C_{10}H_{14}Si$	1125-26-4
Vinyldimethylbenzylsilane	$C_{11}H_{16}Si$	18001-46-2

W

WNC 18 polymer	$(CH_2)_n$	9002-88-4
Wurster's Blue perchlorate	$C_{10}H_{16}N_2ClO_4$	38668-38-1

X

Xanthine	$C_5H_4N_4O_2$	57-41-0
Xanthone	$C_{13}H_8O_2$	90-47-1
m-Xylene	C_8H_{10}	108-38-3
o-Xylene	C_8H_{10}	95-47-6
p-Xylene	C_8H_{10}	106-42-3
Xylitol	$C_5H_{12}O_5$	87-99-0
α-Xylose(D)	$C_5H_{10}O_5$	58-86-6

Y		
Ytterbium isothiocyanate hexahydrate	$C_3N_3S_3Yb \cdot 6H_2O$	91862-08-7
Yttrium ethylsulfate	$C_6H_{15}O_{12}S_3Y \cdot 9H_2O$	13040-17-0
Yttrium isothiocyanate hexahydrate	$C_3N_3S_3Y \cdot 6H_2O$	91862-09-8
Z		
Zinc acetate	$C_4H_6O_4Zn$	557-34-6
Zinc acetate dihydrate	$C_4H_6O_4Zn \cdot 2H_2O$	5970-45-6
Zinc acetylacetonate	$C_{10}H_{14}O_4Zn$	14024-63-6
Zinc(II) *n*-decanoate	$C_{20}H_{38}O_4Zn$	13040-17-0
Zinc(II) *n*-dodecanoate	$C_{24}H_{46}O_4Zn$	2452-01-
Zinc(II) *n*-hexadecanoate	$C_{32}H_{62}O_4Zn$	4991-47-
Zinc(II) *n*-hexanoate	$C_{12}H_{22}O_4Zn$	20779-08-
Zinc(II) *n*-octadecanoate	$C_{36}H_{70}O_4Zn$	557-05-
Zinc(II) *n*-octanoate	$C_{16}H_{30}O_4Zn$	557-09-
Zinc(II) *n*-tetradecanoate	$C_{28}H_{54}O_4Zn$	16260-27-
Zirconium acetylacetonate	$C_{20}H_{28}O_8Zr$	17501-44-
Zirconium α,α,α-trifluoroacetylacetonate	$C_{20}H_{16}F_{12}O_8Zr$	17499-68-

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