# Heat Capacities and Entropies of Organic Compounds in the Condensed Phase Volume II

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# Heat Capacities and Entropies of Organic Compounds in the Condensed Phase Volume II

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This compilation of data on the heat capacities, entropies, and phase transitions of organic compounds in the condensed phase supplements the document published earlier on this subject, namely, "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). It provides data on approximately 1300 organic compounds. About half of the articles examined contain data published prior to 1982. A total of 565 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 from the articles examined and evaluated.

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

## Contents



## 1. Introduction

This compilation provides heat capacity and entropy data on approximately 1300 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. A total of 565 articles have been examined, evaluated, and referenced.

This compilation is a supplement to an earlier document published in 1984, namely, "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). Since 1984, two 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 (1985).

The latter two 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 organic oxygen compounds. The discus-

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sions on specific compounds provided by Wilhoit, Chao, and Hall were helpful in the assignment of a rating to our evaluation of those data.

## 2. Scope of the Search

References containing data on the heat capacities and entropies of organic compounds in the condensed phase were obtained through a search of the files of the Chemical Thermodynamics Data Center of the National Institute of Standards and Technology. Additional references were located through the Bulletin of Chemical Thermodynamics and through Chemical Abstracts. 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.

Our previous publication [1], covered the literature from 1881 to the beginning of 1982. About half of the 565 papers referenced in this publication contain measurements performed for that same period of time with the remaining half covering the period from 1982 to most of 1989.

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), temperature scale, 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 converted to the International System of Units (SI Units). Except for very precise data, corrections involving energy units for most measurements since about 1930 are often within the uncertainty of the data. Older data are of lower precision so that corrections are not needed. In general, transition temperatures are those reported by the investigator. The effort to convert each investigator's temperature scale to the 1968 International Practical Temperature Scale (IPTS-68) was not warranted. Hence, the reported values may have a systematic error of up to 0.1 K. Fortunately, modern high-precision measurements are usually based on IPTS-68.

## 3. Arrangement of the Data

The table of heat capacities, entropies, and phase transitions given in this paper contains data entries for a variety of organic compounds. The entries here, as in the 1984 J. Phys. Chem. Ref. Data publication [1], are arranged in the order of the empirical formulae of the compounds; isomers are further separated by their Wiswesser Line Notation [2]. The latter notation system has been used to represent the structure of the organic compound. Under a given organic substance, the data from the pertinent papers are included. The data from each paper form a separate entry, complete with identification of the reference source. When there are several reference entries for a compound, they are arranged chronologically by year.

For each entry the data given are: molecular (empirical) formula for the compound, physical state, reference code, compound name(s), followed by the values for the heat capacity, entropy, and, where available, phase transition data. The entry of information is completed by the molecular weight, Wiswesser Line Notation for the compound, and a graduated indication of the quality of the data. The formula given is the empirical formula 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 their chemical symbols. One or more names are given for each compound. No attempt has been made to conform to a rigorously systematic nomenclature. Common names and systematic names are used; alternate names have been given freely. All names used appear in the Compound Name-Formula Index in Sec. 8, which should assist the reader who is aware of the compound name but not its empirical formula.

The bibliography is listed in Sec. 9. The reference code is of the form XXAAA/BBBN where XX are the last two digits of the year of publication of the paper, AAA is the first three letters of the last name of the first author and BBB is the first three letters of the last name of the second author (if present). Authors after the first two are disregarded. $N$ is a digit from 2 to 9 used to indicate a second, third, ...paper with the same year and author codes. Thus, 60BRO/SMI2 refers to a paper 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 $\Delta S$ 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 1987 IUPAC Table of International Atomic Weights [3]. Two 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 fomulae. 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 [4]). 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
$CCl_4$
$CHCl_3$
$CH_4$
$CO_2$
$C_2Cl_3O_2$
$C_2H_2Cl_2$
$C_2H_3Cl$
$C_2H_4$
$C_2H_4O_2$
$C_2H_6$
$C_2H_6O$

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 infinitesmal 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:

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

Actual heat capacity measurements, or $C_{sat}$, for liquids and solids are normally made with the sample in equilibrium with its own vapor 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 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 infinitesmal change in entropy:

$$dS = dQ/T \ .$$

Entropy and heat capacity are related by the following expressions:

$(\partial S/\partial T)_v = C_v/T$, at constant volume,
$(\partial S/\partial T)_p = C_p/T$, at constant pressure,
$(\partial S/\partial T) = C_{sat}/T$, 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,

$$S_T^\circ = S_0^\circ(\text{zero point}) + \int_0^{T_1} (C_p/T)dT \,(\text{extrapolation}) +$$
$$\int_{T_1}^{T_2} (C_p/T)dT + \Delta H_{T_2}/T_2 \,(\text{phase change}) +$$
$$\int_{T_2}^{T_3} (C_p/T)dT + \Delta H_{T_3}/T_3 \,(\text{phase change}) +$$
$$\int_{T_3}^{T} (C_p/T)dT$$

For additional discussions on the concept of entropy, the reader should consult references [5] and [6].

*Phase Transitions*. A process by which a substance undergoes a change of physical state, i.e., solid-solid, solid-liquid, solid-gas, or liquid-gas, is known as a phase transition or phase change. The phase change is accompanied by a transfer of energy (commonly referred to as latent heat) and a change in volume while both temperature and pressure remain constant. For a phase change which is carried out reversibly (i.e., under equilibrium conditions) at a constant temperature and pressure, the total Gibbs energy remains unchanged. If there is an enthalpy (or heat) change, then it follows that there will also be an entropy change for the process, because:

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

These equations are applicable only for the temperature and pressure at which the phases are in equilibrium.

For phase changes — solid-solid, solid-liquid, solid-gas, liquid-gas — encountered in the accompanying tables in Sec. 7, $\Delta H$ refers to the isothermal enthalpy change at the transition temperature. Corrections can be applied to the experimental data for premelting effects to isothermal conditions. The pressure, unless specified, is the vapor pressure of the substance at the transition temperature; the correction to a standard state pressure is usually negligible at ordinary pressures for a solid-solid transition and for fusion. The entropy change is taken as $\Delta H/T$ at the equilibrium pressure.

Some investigators have reported the measurement of anomalous phase changes in which the volume and entropy are continuous, but the heat capacity is discontinuous. During such phase changes no latent heat is present and the shape of the curve of the heat capacity plotted as a function of temperature often resembles the Greek letter lambda at the transition point. Such a transition is called a "lambda transition". In order to differentiate these anomalous transitions from ordinary phase changes, it has become customary to identify normal phase changes as phase changes of the first order and atypical phase changes as those of the second order. The discontinuity which occurs in a first order phase transition is a commonly observed phenomenon; however, the discontinuity associated with a second order phase transition has been more difficult to identify and/or interpret. Sometimes the discontinuous nature of the heat capacity is questioned in a second order transition because experimental measurements show a peak or a hump at the transition temperature rather than an unambiguous discontinuity.

A phase change which is accompanied by changes in the entropy and 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,

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

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,

$$C_p/T = (\partial S/\partial T)_P = -(\partial^2 G/\partial T^2)_P$$

$$KV = -(\partial V/\partial P)_T = -(\partial^2 G/\partial P^2)_T$$

$$\beta V = (\partial V/\partial T)_P = (\partial^2 G/\partial T \partial P)_{T,P},$$

where $K$ is the isothermal compressibility and $\beta$ is the volume expansivity. The relationship between these quantities and the pressure and temperature is given below by Ehrenfest's eq. [7].

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

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

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 references [8, 9, and 10].

## 5. Acknowledgements

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

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: $C_p = 0.538657 + 9.11129\times10^{-6}T - 90.2725T^{-1} - 43449.3T^{-2} + 1.59309\times10^{7}T^{3} - 1.43688\times10^{9}T^{-4}$ 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$^{-1}$·K$^{-1}$.
**Entropy** 298.15 K, $S = 5.51$ J·mol$^{-1}$·K$^{-1}$
$S^{\circ}_T = 0.4585$ J·g$^{-1}$·K$^{-1}$.
**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) 81ISA/WAN
Graphite; Carbon, graphite
**Heat Capacity** 300 K, $C_p = 10.05$ J·mol$^{-1}$·K$^{-1}$
Temperature range 80 to 300 K.
$C_p = 8.729\times10^{-4}T + 6.27\times10^{-6}T^{2} + 6.309\times10^{-9}T^{3}$ 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.

$CBr_4$ (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

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

$CCl_4$ (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) 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, $\Delta H = 4631$ J·mol$^{-1}$
$\Delta S = 20.52$ J·mol$^{-1}$·K$^{-1}$
(c,II/c,Ib)
c,I/liq 250.53 K, $\Delta H = 2562$ J·mol$^{-1}$
$\Delta S = 10.226$ J·mol$^{-1}$·K$^{-1}$
(c,Ib/liq). Data also given for (c,Ia/liq):
246.00 K, $\Delta H = 1830$ J·mol$^{-1}$.
$\Delta S = 7.44$ 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

**$CF_3Br$** (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

**$CF_4$** (liq) 69ENO/SHI
Carbon tetrafluoride; Tetrafluoromethane; Freon 14
**Heat Capacity**
Temperature range 4 to 100 K.
**Phase Changes**
c,II/c,I 76.09 K, $\Delta H = 1462.3$ J·mol$^{-1}$
$\Delta S = 19.20$ J·mol$^{-1}$·K$^{-1}$
c,I/liq 89.529 K, $\Delta H = 705.4$ J·mol$^{-1}$
$\Delta S = 7.87$ J·mol$^{-1}$·K$^{-1}$
**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) 84GOL/KOL
Tribromomethane; Bromoform
**Phase Changes**
c/liq 281.84 K, $\Delta H = 11046$ J·mol$^{-1}$
$\Delta S = 39.2$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 252.7309
**Wiswesser Line Notation** EYEE
**Evaluation** A

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

**$CHNaO_2$** (c) 83FRA/PLA
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 in 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, $\Delta H = 1214$ J·mol$^{-1}$
$\Delta S = 2.47$ J·mol$^{-1}$·K$^{-1}$
c,I/liq 530.46 K, $\Delta H = 17710$ J·mol$^{-1}$
$\Delta S = 33.39$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 68.0075
**Wiswesser Line Notation** VHO .NA
**Evaluation** A

**$CHO_2Tl$** (c) 76MEI/SEY
Thallium formate
**Phase Changes**
c,I/liq 374 K, $\Delta H = 10878$ J·mol$^{-1}$
$\Delta S = 28.9$ J·mol$^{-1}$·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·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 10 to 320 K. Interpolated data.
**Entropy** 300 K, $S = 25.52$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 14.0268
**Wiswesser Line Notation** /*1*/
**Evaluation** A
Branched, high pressure polyethylene.

**$(CH_2)_n$** (c) 62WUN
Polyethylene
**Heat Capacity** 300 K, $C_p = 24.53$ J·mol$^{-1}$·K$^{-1}$
Temperature range 1 to 420 K.
Extrapolated value to 100% crystalline phase.
**Entropy** 300 K, $S = 24.04$ J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 415 K, $\Delta H = 3879$ J·mol$^{-1}$
$\Delta S = 9.35$ J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 1 to 420 K.
Extrapolated value to 100% amorphous phase.
**Entropy** 300 K, $S = 31.96$ J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 415 K, $\Delta H = 3879$ J·mol$^{-1}$
$\Delta S = 9.35$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 14.0268
**Wiswesser Line Notation** /*1*/
**Evaluation** A

**$(CH_2)_n$** (c) 78STE
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

**$CH_2Cl_2$** (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

**$CH_2N_2$** (c) 83DEW/DEK
Cyanamid
**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, $\Delta H$ = 7272 J·mol$^{-1}$
$\Delta S$ = 22.82 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 42.0402
**Wiswesser Line Notation** ZCN
**Evaluation** B($C_p$), A(Phase changes).

**$CH_3Cl_3Si$** (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 + 0.04132$T$ + 100930$T^{-2}$
(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, $\Delta H$ = 8945 J·mol$^{-1}$
$\Delta S$ = 45.31 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 149.4792
**Wiswesser Line Notation** G-SI-GG1
**Evaluation** A
Debye temperature = 98.84 K.

**$CH_3NO$** (liq) 76SKO/SUU
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) 83DEW/DEK
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, $\Delta H$ = 8667 J·mol$^{-1}$
$\Delta S$ = 31.448 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 45.0408
**Wiswesser Line Notation** ZVH
**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, $\Delta H$ = 93.55 J·mol$^{-1}$
$\Delta S$ = 4.557 J·mol$^{-1}$·K$^{-1}$
Lambda transition.
c,I/liq 90.67 K, $\Delta H$ = 939.2 J·mol$^{-1}$
$\Delta S$ = 10.36 J·mol$^{-1}$·K$^{-1}$
liq/g 99.54 K, $\Delta H$ = 8519 J·mol$^{-1}$
$\Delta S$ = 85.58 J·mol$^{-1}$·K$^{-1}$
$p$ = 32.81 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) 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, $\Delta H$ = 13610 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 13900 J·mol$^{-1}$
$\Delta S$ = 34.25 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 60.0554
**Wiswesser Line Notation** ZVZ
**Evaluation** A

**$CH_4N_2O$** (c) 87DEL/FER
Urea
**Phase Changes**
c/liq 406.5 K, $\Delta H$ = 14790 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 14500 J·mol$^{-1}$
$\Delta S$ = 35.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 60.0554
**Wiswesser Line Notation** ZVZ
**Evaluation** B

**$CH_4N_2S$** (c) 67WES/CHA
Thiourea
**Heat Capacity** 298.15 K, $C_p$ = 96.90 J·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 298.15 K
**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, $\Delta S$ = 0.17 J·mol$^{-1}$·K$^{-1}$; 171.2 K, $\Delta S$ = 0.04 J·mol$^{-1}$·K$^{-1}$; 200 K, $\Delta S$ = 0.71 J·mol$^{-1}$·K$^{-1}$. A slight hump in the heat capacity appears between 210 and 260K.

**$CH_4N_2S$** (c) 82TOR/SAB
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 from 67WES/CHA.
**Phase Changes**
c/g 298.15 K, $\Delta H$ = 112000 J·mol$^{-1}$
$\Delta S$ = 375.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 76.1160
**Wiswesser Line Notation** ZYZUS
**Evaluation** B

**$CH_4O$** (liq) 82VIL/CAS
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/SOM
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) 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) 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) 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

**$CH_4O$** (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, $\Delta H$ = 1540 J·mol$^{-1}$
$\Delta S$ = 14.95 J·mol$^{-1}$·K$^{-1}$
Glass transition.
c/liq 175.22 K
**Molecular Weight** 32.0420
**Wiswesser Line Notation** Q1
**Evaluation** A

**$CH_4N_2S·HNO_3$** (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, $\Delta H$ = 34.0 J·mol$^{-1}$
$\Delta S$ = 0.130 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 139.1288
**Wiswesser Line Notation** ZYZUS &WNQ
**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

**$CH_5N_3S$** (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, $\Delta H$ = 125800 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 70.0 J·mol$^{-1}$
$\Delta S$ = 0.250 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 91.1306
**Wiswesser Line Notation** ZYMZUS
**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 $\alpha'$ to metastable $\delta$.
**Molecular Weight** 158.9696
**Wiswesser Line Notation** Z1 &IH
**Evaluation** A
Data given for $\beta'$ phase from 10 to 220 K.
$\beta'$ to $\alpha'$ phase transition at 220 K,
$\Delta H$ = 2970 J·mol$^{-1}$, $\Delta S$ = 13.5 J·mol$^{-1}$·K$^{-1}$.

**$CH_6N_4S$** (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, $\Delta H$ = 152100 J·mol$^{-1}$
$\Delta S$ = 510.1 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 106.1452
**Wiswesser Line Notation** ZMYMZUS
**Evaluation** B

**$C_2Br_2F_4$** (liq) 88VES/ZAB
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$^{-1}$) = 131.53 + 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/SCH
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 experimental 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) 84GOL/KOL
Chlorotrifluoroethene; Chlorotrifluoroethylene;
Trichlorofluoroethene; Trichlorofluoroethylene
**Phase Changes**
c/liq 118.3 K, $\Delta H$ = 5282 J·mol$^{-1}$
$\Delta S$ = 44.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 116.4702
**Wiswesser Line Notation** GYFUYFF
**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, $\Delta H$ = 2326 J·mol$^{-1}$
$\Delta S$ = 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) 87OTT/WOO
1,1,1-Trichlorotrifluoroethane
**Phase Changes**
c,II/c,I 148 K
Solid-plastic crystal.
c,I/liq 287.52 K, $\Delta H$ = 4110 J·mol$^{-1}$
$\Delta S$ = 14 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 187.3762
**Wiswesser Line Notation** GXGGXFFF
**Evaluation** A

**$C_2Cl_3F_3$** (liq) 88SVO/VES
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 + 0.200 ($T$/K) (298 to 318 K).
**Molecular Weight** 187.3762
**Wiswesser Line Notation** GXGGXFFF
**Evaluation** A

**$C_2Cl_4$** (liq) 86NOV/RAB
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, $\Delta H$ = 820 J·mol$^{-1}$
$\Delta S$ = 5.26 J·mol$^{-1}$·K$^{-1}$
c/liq 250.81 K, $\Delta H$ = 10880 J·mol$^{-1}$
$\Delta S$ = 43.38 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 165.8340
**Wiswesser Line Notation** GYGUYGG
**Evaluation** A

**$C_2Cl_4F_2$** (c) 84GOL/KOL
1,1,1,2-Tetrachlorodifluoroethane
**Phase Changes**
c/liq 314.2 K, $\Delta H$ = 3990 J·mol$^{-1}$
$\Delta S$ = 12.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 203.8308
**Wiswesser Line Notation** GXGGXGFF
**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, $\Delta H$ = 2565 J·mol$^{-1}$
$\Delta S$ = 8.08 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 345 K, $\Delta H$ = 8222 J·mol$^{-1}$
$\Delta S$ = 23.8 J·mol$^{-1}$·K$^{-1}$
c,I/liq 458 K, $\Delta H$ = 9749 J·mol$^{-1}$
$\Delta S$ = 23.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 236.7400
**Wiswesser Line Notation** GXGGXGGG
**Evaluation** B($C_p$), A(Phase changes)

**$C_2D_{12}C_{16}N_2Sn$** (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, $\Delta H$ = 2810 J·mol$^{-1}$
$\Delta S$ = 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

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

**$C_2F_4O$** (liq) 71HOD
Trifluoroacetyl fluoride
**Heat Capacity**
Temperature range 14 to 214 K.
**Phase Changes**
c/liq 113.69 K, $\Delta H$ = 4869 J·mol$^{-1}$
$\Delta S$ = 42.83 J·mol$^{-1}$·K$^{-1}$
liq/g 214.10 K, $\Delta H$ = 19267 J·mol$^{-1}$
$\Delta S$ = 89.99 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 116.0150
**Wiswesser Line Notation** FXFFVF
**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) 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

**$C_2HBrClF_3$** (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 318K).
**Molecular Weight** 197.3821
**Wiswesser Line Notation** GYEXFFF
**Evaluation** A

**$C_2HCl_3$** (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

**$C_2HCl_3O_2$** (c) 1895PIC
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

**$(C_2H_2Cl_2)_n$** (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

**$C_2H_2Cl_2O_2$** (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, $\Delta H$ = 7644 J·mol$^{-1}$
$\Delta S$ = 26.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 128.9426
**Wiswesser Line Notation** QVYGG
**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, $\Delta H$ = 544 J·mol$^{-1}$
$\Delta S$ = 2.62 J·mol$^{-1}$·K$^{-1}$
c,I/liq 230.8 K, $\Delta H$ = 9172 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 356 J·mol$^{-1}$
$\Delta S$ = 1.74 J·mol$^{-1}$·K$^{-1}$
c,II/liq 230.3 K, $\Delta H$ = 9521 J·mol$^{-1}$
$\Delta S$ = 41.51 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 167.8498
**Wiswesser Line Notation** GYGYGG
**Evaluation** A
Data for (c,II).

**$C_2H_2CuO_4{\cdot}4D_2O$** (c) 76MAT/KUM
Copper (II) formate tetradeuterate
**Heat Capacity** 300.16 K, $C_p$ = 329.69 J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S$ = 3.814 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 233.7054
**Wiswesser Line Notation** OVH 2 .CU &QH4 &14/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·mol$^{-1}$·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·mol$^{-1}$
$\Delta S$ = 3.546 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 225.6422
**Wiswesser Line Notation** OVH 2 .CU &QH4
**Evaluation** B

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

**$(C_2H_3Cl)_n$** (c) 55ALF/DOL
Polyvinyl chloride
**Heat Capacity** 298 K, $C_p$ = 59.47 J·mol$^{-1}$·K$^{-1}$
Temperature range 253 to 393 K.
$C_p$ calculated from equation. $C_p$(cal·g$^{-1}$·K$^{-1}$) = 0.2092 + $7.29\times10^{-4}T$, where $T<60$ °C for L-38 PVC.
$C_p$(cal·g$^{-1}$·K$^{-1}$) = 0.2048 + $8.46\times10^{-4}T$, where $T<60$ °C for annealed PVC.
**Molecular Weight** 62.4984
**Wiswesser Line Notation** /*YG1*/
**Evaluation** A
$T$(glass) = 78.5 °C.

**$(C_2H_3Cl)_n$** (gls) 67LEB/RAB
Polyvinyl chloride
**Heat Capacity** 298.15 K, $C_p$ = 59.96 J·mol$^{-1}$·K$^{-1}$
Temperature range 58 to 300 K.
Value per monomer unit.
**Entropy** 298.15 K, $S$ = 65.10 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 62.4984
**Wiswesser Line Notation** /*YG1*/
**Evaluation** B

**$C_2H_3ClO_2$** (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, $\Delta H$ = 16296 J·mol$^{-1}$
$\Delta S$ = 48.74 J·mol$^{-1}$·K$^{-1}$
$\alpha$-Isomer.
c/liq 329.16 K, $\Delta H$ = 13933 J·mol$^{-1}$
$\Delta S$ = 42.33 J·mol$^{-1}$·K$^{-1}$
$\beta$-Isomer.
**Molecular Weight** 94.4975
**Wiswesser Line Notation** QV1G
**Evaluation** D

**$C_2H_3Cl_3$** (liq) 82MAR
1,1,1-Trichloroethane; Methylchloroform
**Phase Changes**
c,II/c,I 224.5 K, $\Delta H$ = 7470 J·mol$^{-1}$
$\Delta S$ = 33.3 J·mol$^{-1}$·K$^{-1}$
c,I/liq 240.9 K, $\Delta H$ = 1550 J·mol$^{-1}$
$\Delta S$ = 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

**$C_2H_3LiO_2{\cdot}2H_2O$** (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, $\Delta H$ = 24250 J·mol$^{-1}$
$\Delta S$ = 74.7 J·mol$^{-1}$·K$^{-1}$
Transition of dihydrate to anhydrous salt and aqueous solution.
**Molecular Weight** 102.0159
**Wiswesser Line Notation** OV1 .LI &QH 2
**Evaluation** B

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

**$(C_2H_3NO)_n$** (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.
$C_p = 37.744 + 0.218T - 2.333\times10^{-6}T^2$.
**Molecular Weight** 57.0518
**Wiswesser Line Notation** /*MV1*/
**Evaluation** B
Same data as in 81FIN/KUM. $\beta$-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.
$C_p = 57.598 + 0.05T + 2.357\times10^{-4}T^2$.
**Molecular Weight** 57.0518
**Wiswesser Line Notation** /*MV1*/
**Evaluation** B
Same data as in 81FIN/KUM. $3_1$ helical structure.

**$C_2H_3N_3$** (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

**$C_2H_3NaO_2$** (c) 83FRA/PLA
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, $\Delta S$ = 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) 84MEI/GRO
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, $\Delta H$ = 37860 J·mol$^{-1}$
$\Delta S$ = 114.2 J·mol$^{-1}$·K$^{-1}$
Transition of trihydrate to anhydrous salt and aqueous solution.
**Molecular Weight** 136.0799
**Wiswesser Line Notation** OV1 .N*A* &QH 3
**Evaluation** B

**$C_2H_3O_2Tl$** (c) 76MEI/SEY
Thallium acetate
**Phase Changes**
c,I/liq 404 K, $\Delta H$ = 17573 J·mol$^{-1}$
$\Delta S$ = 43.5 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 15 to 170 K.
**Phase Changes**
c/liq 103.95 K, $\Delta H$ = 3351 J·mol$^{-1}$
$\Delta S$ = 32.23 J·mol$^{-1}$·K$^{-1}$
liq/g 169.40 K, $\Delta H$ = 13544 J·mol$^{-1}$
$\Delta S$ = 79.95 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 16 to 169 K.
**Entropy** 170 K, $S$ = 117.8 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 103.97 K, $\Delta H$ = 3351 J·mol$^{-1}$
$\Delta S$ = 32.23 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 28.0536
**Wiswesser Line Notation** 1U1
**Evaluation** A
A reevaluation of the original measured data from: 37EGA/KEM.

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

**$C_2H_4F_2$** (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

**$C_2H_4N_2O_2$** (c) 83LEB/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 x 10$^{-4}$ $T^3$ − 0.0923 $T^2$ + 31.3779 $T$ − 3457.8187 J·mol$^{-1}$·K$^{-1}$ (298 to 350 K).
**Molecular Weight** 88.0658
**Wiswesser Line Notation** VHMMVH
**Evaluation** B

**$C_2H_4O$** (liq) 88LEB/VAS
Ethanal
**Heat Capacity** 298.15 K, $C_p$ = 89.05 J·mol$^{-1}$·K$^{-1}$
Temperature range 13 to 300 K.
**Entropy** 298.15 K, $S$ = 117.3 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 149.78 K, $\Delta H$ = 2310 J·mol$^{-1}$
$\Delta S$ = 15.43 J·mol$^{-1}$·K$^{-1}$
liq/liq 242.9 K, $\Delta H$ = 1716 J·mol$^{-1}$
$\Delta S$ = 7.35 J·mol$^{-1}$·K$^{-1}$
Lambda type transition.
**Molecular Weight** 44.0530
**Wiswesser Line Notation** VH1
**Evaluation** A

**$(C_2H_4O)_n$** (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

**$(C_2H_4O)_n$** (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

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

**$C_2H_4O_2$** (liq) 1895PIC
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, $\Delta H$ = 11126 J·mol$^{-1}$
$\Delta S$ = 38.36 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 60.0524
**Wiswesser Line Notation** QV1
**Evaluation** D

**$C_2H_4O_2$** (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) 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

**$C_2H_5NO$** (liq) 76SKO/SUU
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

**$C_2H_5NO$** (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, $\Delta H$ = 15590 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 15606 J·mol$^{-1}$
$\Delta S$ = 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) 86EMO/NAU
Acetamide; Ethanamide
**Phase Changes**
c/liq 342.15 K, $\Delta H$ = 12522 to 12877 J·mol$^{-1}$
$\Delta S$ = 36.6 to 37.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 59.0676
**Wiswesser Line Notation** ZV1
**Evaluation** A
Unstable form.

**$C_2H_5NO_2$** (c) 76BER/BOU
Methyl carbamate
**Phase Changes**
c/liq 328.6 K, $\Delta H$ = 16700 J·mol$^{-1}$
$\Delta S$ = 51.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 75.0672
**Wiswesser Line Notation** ZVO1
**Evaluation** A

**$C_2H_5NO_4$·0.5$H_2O$** (c) 89FUK/MAT
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 $\Delta H$ = 0.37 $J$ mol$^{-1}$
$\Delta$S = 3.01 J·mol$^{-1}$·K$^{-1}$
Order − disorder transition
**Molecular Weight** 116.0734
**Wiswesser Line Notation** ZH QVVQ &QH 0.5
**Evalation** A

**$C_2D_5NO_4$·0.5$D_2O$** (c) 89FUK/MAT
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 $\Delta H$ =0.56 J mol$^{-1}$
$\Delta S$ =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 &2/4/7/10/11/H-2
**Evaluation** A

**$C_2H_5NS$** (c) 82SAB/TOR
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, $\Delta H$ = 82800 J·mol$^{-1}$
$\Delta S$ = 277.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 75.1282
**Wiswesser Line Notation** ZY1&US
**Evaluation** B

**$C_2H_6$** (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, $\Delta H$ = 2282 J·mol$^{-1}$
$\Delta S$ = 25.48 J·mol$^{-1}$·K$^{-1}$
c/liq 90.341 K, $\Delta H$ = 583 J·mol$^{-1}$
$\Delta S$ = 6.46 J·mol$^{-1}$·K$^{-1}$
Triple point.
**Molecular Weight** 30.0694
**Wiswesser Line Notation** 2H
**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 + 0.06453$T$ + 283310$T^{-2}$
(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, $\Delta H$ = 8828 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 2.6 J·mol$^{-1}$
$\Delta S$ = 0.007 J·mol$^{-1}$·K$^{-1}$
c,I/liq 389 K, $\Delta H$ = 14.6 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 15750 J·mol$^{-1}$
$\Delta S$ = 42.1 J·mol$^{-1}$·K$^{-1}$
**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, $\Delta H$ = 1090 J·mol$^{-1}$
$\Delta S$ = 4.18 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 122.0804
**Wiswesser Line Notation** QVVQ &ZZ
**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, $\Delta H$ = 4973 J·mol$^{-1}$
$\Delta S$ = 31.3 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 46.0688
**Wiswesser Line Notation** Q2
**Evaluation** B

**$C_2H_6O$** (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) 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) 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/OLS
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/SOM
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) 86TAN/TOY
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

**$(C_2H_6OSi)_n$** (liq) 78LEB/MUK
Poly(dimethylsiloxane)
**Heat Capacity** 298.15 K, $C_p$ = 117.8 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, $\Delta H$ = 4540 J·mol$^{-1}$
$\Delta S$ = 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

**$C_2H_6O_2$** (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) 82ZAR
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

**$C_2H_6Zn$** (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, $\Delta H$ = 1061 J·mol$^{-1}$
$\Delta S$ = 5.05 J·mol$^{-1}$·K$^{-1}$
c,I/liq 230.13 K, $\Delta H$ = 6830 J·mol$^{-1}$
$\Delta S$ = 29.67 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 95.4494
**Wiswesser Line Notation** 1-ZN-1
**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, $\Delta H$ = 13638 J·mol$^{-1}$
$\Delta S$ = 51.60 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 60.0986
**Wiswesser Line Notation** 1MM1
**Evaluation** A

**$C_2H_8N_2$** (liq) 88BOB/KAM
1,2-Diaminoethane; 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

**$C_2H_{12}B_{10}$** (liq) 81GOR/ZAL

*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, | $\Delta H$ = 41 J·mol$^{-1}$ |
| | | $\Delta S$ = 0.73 J·mol$^{-1}$·K$^{-1}$ |
| c,II/c,I | 165 K, | $\Delta H$ = 1903 J·mol$^{-1}$ |
| | | $\Delta S$ = 9.50 J·mol$^{-1}$·K$^{-1}$ |
| c,I/liq | 280.1 K, | $\Delta H$ = 4326 J·mol$^{-1}$ |
| | | $\Delta S$ = 14.8 J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 144.2168

**Wiswesser Line Notation**

**Evaluation** A

**$C_2H_{12}Br_6N_2Te$** (c) 86ONO/MAT

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, | $\Delta H$ = 1677 J mol$^{-1}$ |
| | | $\Delta S$ = 13.0 J·mol$^{-1}$·K$^{-1}$ |
| c,III/c,II | 163.9 K, | $\Delta H$ = 885 J·mol$^{-1}$·K−1 |
| | | $\Delta$S = 5.4 J·mol$^{-1}$·K$^{-1}$ |
| c,II/c,I | 288.9 K, | $\Delta H$ = 4594 J·mol$^{-1}$ |
| | | $\Delta S$ = 15.9 J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 671.1542

**Wiswesser Line Notation** ZH&1 2 -TE- E6

**Evaluation** A

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

Tetrachlorobis-(methylammonium) manganese II

**Phase Changes**

| | | |
|---|---|---|
| c,III/c,II | 257 K, | $\Delta H$ = 4.8 J·mol$^{-1}$ |
| | | $\Delta S$ = 0.017 J·mol$^{-1}$·K$^{-1}$ |
| c,II/c,I | 393 K, | $\Delta H$ = 3.6 J·mol$^{-1}$ |
| | | $\Delta S$ = 0.007 J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 260.8802

**Wiswesser Line Notation** ZH&1 2 -MN- G4

**Evaluation** A

**$C_2H_{12}Cl_6Te$** (c) 88ONO/MAT

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, | $\Delta H$ = 470 J·mol$^{-1}$ |
| | | $\Delta S$ = 6.4 J·mol$^{-1}$·K$^{-1}$ |
| c,V/c,IV | 136.8 K, | $\Delta H$ = 1810 J·mol$^{-1}$ |
| | | $\Delta S$ = 14.9 J·mol$^{-1}$·K$^{-1}$ |

Lambda type transition.

| | | |
|---|---|---|
| c,IV/c,III | 155 K, | $\Delta H$ = 390 J·mol$^{-1}$ |
| | | $\Delta S$ = 2.5 J·mol$^{-1}$·K$^{-1}$ |
| c,III/c,II | 226.0 K, | $\Delta H$ = 330 J·mol$^{-1}$ |
| | | $\Delta S$ = 1.7 J·mol$^{-1}$·K$^{-1}$ |
| c,II/c,I | 439 K, | $\Delta H$ = 4400 J·mol$^{-1}$ |
| | | $\Delta S$ = 9.8 J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 376.4348

**Wiswesser Line Notation** ZH&1 2 -TE- G4

**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 mol$^{-1}$K$^{-1}$

**Phase Changes**

| | | |
|---|---|---|
| c,III/c,II | 66.1 K, | $\Delta H$ = 403 J·mol$^{-1}$·K$^{-1}$ |
| | | $\Delta S$ = 6.1 *J* mol-1K$^{-1}$ |
| c,II/c,I | 115.6 K, | $\Delta H$ = 2555 J·mol$^{-1}$ |
| | | $\Delta$S = 22.1 J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 718.1547

**Wiswesser Line Notation** ZH&1 2 -TE- I6

**Evaluation** A

**$C_3H_2N_2$** (c) 87WAS/OLE

Malononitrile

**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

**$C_3H_3Cl_3$** (liq) 84GOL/KOL

1,1,2-Trichloroethane

**Phase Changes**

| | | |
|---|---|---|
| c/liq | 237.9 K, | $\Delta H$ = 10880 J·mol$^{-1}$ |
| | | $\Delta S$ = 45.7 J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 145.4157

**Wiswesser Line Notation** GYG1G

**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).

**$C_3H_4Cl_3Si$** (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, | $\Delta H$ = 21242 J·mol$^{-1}$ |
| | | $\Delta S$ = 69.0 J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 174.5091

**Wiswesser Line Notation** NC2-SI-GGG

**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, $\Delta H$ = 12821 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 12800 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 13800 J·mol$^{-1}$
$\Delta S$ = 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

**$C_3H_4N_2O$** (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, $\Delta H$ = 1200 J·mol$^{-1}$
$\Delta S$ = 3.46 J·mol$^{-1}$·K$^{-1}$
c,I/liq 387.3 K, $\Delta H$ = 21700 J·mol$^{-1}$
$\Delta S$ = 56.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 84.0774
**Wiswesser Line Notation** ZV1CN
**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, $\Delta H$ = 9509.7 J·mol$^{-1}$
$\Delta S$ = 33.3 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 72.0634
**Wiswesser Line Notation** QV1U1
**Evaluation** A

**$C_3H_4O_2$** (liq) 83LEB/YEV
$\beta$-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, $\Delta H$ = 9410 J·mol$^{-1}$
$\Delta S$ = 39.23 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 72.0634
**Wiswesser Line Notation** T4OVTJ
**Evaluation** A

**$C_3H_5KO_2$** (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, $\Delta H$ = 515 J·mol$^{-1}$
$\Delta S$ = 2.02 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 352.5 K
c,I/liq 638.3 K
**Molecular Weight** 112.1696
**Wiswesser Line Notation** OV2 .KA
**Evaluation** A

**$C_3H_5LiO_2$** (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

**$C_3H_5NO_4$** (liq) 81LEB/RYA
Methyl ester of nitroacetic acid;
Methyl nitroacetate
**Heat Capacity** $C_p$ = 205.8 J·mol$^{-1}$·K$^{-1}$
Temperature range 298 to 343 K. Data given over temperature range.
**Molecular Weight** 119.0768
**Wiswesser Line Notation** WN1VO1
**Evaluation** B

**$C_3H_5NaO_2$** (c) 83FRA/WES
Sodium propanoate
**Heat Capacity** 298.15 K, $C_p$ = 134.4 J·mol$^{-1}$·K$^{-1}$
Temperature range 9 to 580 K.
**Entropy** 298.15 K, $S$ = 152.1 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,III/c,II 467.00 K, $\Delta H$ = 3209 J·mol$^{-1}$
$\Delta S$ = 6.87 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 491.00 K, $\Delta H$ = 4357 J·mol$^{-1}$
$\Delta S$ = 8.87 J·mol$^{-1}$·K$^{-1}$
c,I/liq 561.91 K, $\Delta H$ = 13280.0 J·mol$^{-1}$
$\Delta S$ = 23.63 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 96.0611
**Wiswesser Line Notation** OV2 .NA
**Evaluation** A

**$C_3H_5O_2Tl$** (c) 76MEI/SEY
Thallium propionate
**Phase Changes**
c,II/c,I 365 K, $\Delta H$ = 377 J·mol$^{-1}$
$\Delta S$ = 1.05 J·mol$^{-1}$·K$^{-1}$
c,I/liq 468 K, $\Delta H$ = 9205 J·mol$^{-1}$
$\Delta S$ = 20.1 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 320 to 480 K.
**Phase Changes**
c,II/c,I 364.8 K, $\Delta H$ = 316 J·mol$^{-1}$
$\Delta S$ = 0.83 J·mol$^{-1}$·K$^{-1}$
c,I/liq 468.0 K, $\Delta H$ = 10476 J·mol$^{-1}$
$\Delta S$ = 22.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 277.4413
**Wiswesser Line Notation** OV2 .TL
**Evaluation** A

**$C_3H_6$** (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, $\Delta H$ = 3002 J·mol$^{-1}$
$\Delta S$ = 34.18 J·mol$^{-1}$·K$^{-1}$
liq/g 225.35 K, $\Delta H$ = 18418 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 3003 J·mol$^{-1}$
$\Delta S$ = 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.

**$(C_3H_6)_n$** (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, $\Delta H$ = 600 J·mol$^{-1}$ (38% crystallinity).

**$C_3H_6Cl_2Si$** (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

**$C_3H_6N_2O_4$** (c) 78GOD/RAC
2,2-Dinitropropane
**Heat Capacity** 300 K, $C_p$ = 205 J·mol$^{-1}$·K$^{-1}$
Temperature range 100 to 347 K.
$C_p$ estimated from graph.
**Phase Changes**
c,III/c,II 259.67 K, $\Delta H$ = 1870 J·mol$^{-1}$
$\Delta S$ = 7.20 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 267.7 K, $\Delta H$ = 11276 J·mol$^{-1}$
$\Delta S$ = 42.13 J·mol$^{-1}$·K$^{-1}$
c,I/liq 324.5 K, $\Delta H$ = 2636 J·mol$^{-1}$
$\Delta S$ = 8.12 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 134.0914
**Wiswesser Line Notation** WNX1&1&NW
**Evaluation** D($C_p$), B(Phase changes)

**$C_3H_6O$** (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

**$C_3H_6O$·17$H_2O$** (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, $\Delta H$ = 92700 J·mol$^{-1}$
$\Delta S$ = 345.1 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 364.3382
**Wiswesser Line Notation** T3OTJ B1 &QH 17
**Evaluation** A

**$C_3H_6O$** (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, $\Delta H$ = 8590 J·mol$^{-1}$
**Molecular Weight** 58.0798
**Wiswesser Line Notation** VH2
**Evaluation** A

**$C_3H_6O_2$** (liq) 69CLE/MEL
1,3-Dioxolan
**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, $\Delta H$ = 2677 J·mol$^{-1}$
$\Delta S$ = 18.8 J·mol$^{-1}$·K$^{-1}$
c,I/liq 175.93 K, $\Delta H$ = 6567 J·mol$^{-1}$
$\Delta S$ = 37.3 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 74.0792
**Wiswesser Line Notation** T5O COTJ
**Evaluation** B

**$C_3H_6O_2$·17$H_2O$** (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, $\Delta H$ = 99100 J·mol$^{-1}$
$\Delta S$ = 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) 82BIR/SIK
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.
$C_p = 129.7 - 0.1263\ T + 0.0007486\ T^2$ J·mol$^{-1}$·K$^{-1}$.
**Molecular Weight** 74.0792
**Wiswesser Line Notation** QV2
**Evaluation** C

**$(C_3H_6O_2)_n$** (c) 69CLE/MEL
Poly-1,3-dioxolan
**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, $\Delta H$ = 16698 J·mol$^{-1}$
$\Delta S$ = 5.14 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 74.0792
**Wiswesser Line Notation** /*1O1O1*/
**Evaluation** B

**$C_3H_6O_3$** (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

**$C_3H_6O_3$** (liq) 83SAN/CIO
Methylene glycol acetate
**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−1K−1) = 0.033053$T$ − 7.401
**Molecular Weight** 87.0549
**Wiswesser Line Notation** Q1OV1
**Evaluation** D

**$C_3H_7NO$** (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** 61.0834
**Wiswesser Line Notation** VHN1&1
**Evaluation** B

**$C_3H_7NO_2$** (c) 83SKO/SAB
3-Aminopropanoic acid
**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) 76BER/BOU
Ethyl carbamate; Urethane
**Phase Changes**
c/liq 321.7 K, $\Delta H$ = 20900 J·mol$^{-1}$
$\Delta S$ = 64.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 75.0871
**Wiswesser Line Notation** ZVO2
**Evaluation** A

**$C_3H_7NO_2$** (c) 83DEW/DEK
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, $\Delta H$ = 16794 J·mol$^{-1}$
$\Delta S$ = 52.25 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 89.0938
**Wiswesser Line Notation** ZVO2
**Evaluation** B($C_p$), A(Phase changes).

**$C_3H_7NO_3$** (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, $\Delta H$ = 10010 J·mol$^{-1}$
$\Delta S$ = 52.43 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 105.0932
**Wiswesser Line Notation** WNOY1&1
**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$^{-1}$·K$^{-1}$.
**Molecular Weight** 44.0962
**Wiswesser Line Notation** 3H
**Evaluation** A
Sample purity, 99.95 mol%.

**$C_3H_8N_2O$** (c) 87DEL/FER
1,3-Dimethylurea
**Phase Changes**
c/liq 379.5 K, $\Delta H$ = 13620 J·mol$^{-1}$
$\Delta S$ = 35.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 88.1090
**Wiswesser Line Notation** 1MVM1
**Evaluation** A

**$C_3H_8N_2O$** (c) 87DEL/FER
1,1-Dimethylurea
**Phase Changes**
c/liq 454.0 K, $\Delta H$ = 29610 J·mol$^{-1}$
$\Delta S$ = 65.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 88.1090
**Wiswesser Line Notation** ZVN1&1
**Evaluation** A

**$C_3H_8N_2O$** (c) 87DEL/FER
Ethylurea; Monoethylurea
**Phase Changes**
c/liq 367.8 K, $\Delta H$ = 13940 J·mol$^{-1}$
$\Delta S$ = 37.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 88.1090
**Wiswesser Line Notation** ZVM2
**Evaluation** A

**$C_3H_8O$** (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** A
Data from 76FOR/BEN.

**$C_3H_8O$** (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) 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) 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

**$C_3H_8O_2$** (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) 44YOS
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
**Phase Changes**
c/liq 292 K, $\Delta H$ = 18303 J·mol$^{-1}$
$\Delta S$ = 62.7 J·mol$^{-1}$·K$^{-1}$
**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

**$C_3H_9Al$** 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$^{-1}$
c/liq 288.43 K, $\Delta H$ = 8790.6 J·mol$^{-1}$
$\Delta S$ = 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
Trimethyl arsine
**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, $\Delta H$ = 8962 J·mol$^{-1}$
$\Delta S$ = 48.03 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 120.0257
**Wiswesser Line Notation** 1-AS-1&1
**Evaluation** A

**$C_3H_9ClSi$** (liq) 71SAM/KOS
Chlorotrimethylsilane
**Heat Capacity** 298.15 K, $C_p$ = 187.5 J·mol$^{-1}$·K$^{-1}$
Temperature range 12.38 to 303.05 K.
$C_p$(liq) = 18.19046 + 0.077664$T$ + 309052$T^{-2}$ cal·mol$^{-1}$·K$^{-1}$.
Value is calculated from equation.
Deposited in VINITI, No 2501–71, 18 January 1971.
**Entropy** 298.15 K, S = 275.1 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 185.1 K, $\Delta H$ = 695 J·mol$^{-1}$
$\Delta S$ = 3.75 J·mol$^{-1}$·K$^{-1}$
c,I/liq 217.97 K, $\Delta H$ = 9682 J·mol$^{-1}$
$\Delta S$ = 44.39 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 108.6426
**Wiswesser Line Notation** G-SI-1&1&1
**Evaluation** B
$T_{Debye}$ = 115.8 K.

**$C_3H_9Ga$** (liq) 88LEB/SMI
Trimethylgallium
**Heat Capacity** 298.15 K, $C_p$ = 188.0 J·mol$^{-1}$·K$^{-1}$
Temperature range 0 to 330 K.
**Entropy** 298.15 K, S = 252.1 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 244.5 K, $\Delta H$ = 333 J·mol$^{-1}$
$\Delta S$ = 1.36 J·mol$^{-1}$·K$^{-1}$
c,I/liq 257.81 K, $\Delta H$ = 10602 J·mol$^{-1}$
$\Delta S$ = 41.1 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 114.8241
**Wiswesser Line Notation** 1-GA-1&1
**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, $\Delta H$ = 710 J·mol$^{-1}$
$\Delta S$ = 2.4 J·mol$^{-1}$·K$^{-1}$
DSC study yields $\Delta H$ = 725 J·mol$^{-1}$·K$^{-1}$ at 305 K.
c,II/c,I 336 K, $\Delta H$ = 640 J·mol$^{-1}$
$\Delta S$ = 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.

**$C_4Br_2Cl_2F_6$** (liq) 88SVO/VES
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) 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

**$C_4H_2O_3$** (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, $\Delta H$ = 13550 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 13600 J·mol$^{-1}$
$\Delta S$ = 41.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 98.0580
**Wiswesser Line Notation** T5VOVJ
**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, $\Delta H$ = 300 J·mol$^{-1}$
$\Delta S$ = 0.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 114.0574
**Wiswesser Line Notation** L4VVJ CQ DQ
**Evaluation** B

**$C_4H_3Cl_3OS$** (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 $\Delta H$ = 20370 J·mol$^{-1}$
$\Delta S$ = 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-1U12U1
**Evaluation** A

**$C_4H_3F_5O_3$** (liq) 84GOL/KOL
α-(Trifluoromethoxy)-α,α-difluoromethyl acetate
**Phase Changes**
c/liq 167.4 K, $\Delta H$ = 8510 J·mol$^{-1}$
$\Delta S$ = 50.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 194.0579
**Wiswesser Line Notation** FXFFOXFFVO1
**Evaluation** A

**$C_4H_4KNaO_6{\cdot}4H_2O$** (c) 38HIC/HOO
Sodium potassium tartrate tetrahydrate;
Rochelle salt
**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, $\Delta H$ = 42752 J·mol$^{-1}$
$\Delta S$ = 130.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 282.2209
**Wiswesser Line Notation** OVYQYQVO .K .NA &QH4
**Evaluation** B

**$C_4H_4N_2$** (c) 87RAI/SIN
Succinonitrile; 1,4-Butanedinitrile
**Phase Changes**
c/liq 334 K, $\Delta H$ = 3704 J·mol$^{-1}$
$\Delta S$ = 11.1 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 80.0890
**Wiswesser Line Notation** NC2CN
**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)

**$C_4H_4O_4$** (c,II) 77LEB/EVS
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, $\Delta H$ = 1840 J·mol$^{-1}$
$\Delta S$ = 5.90 J·mol$^{-1}$·K$^{-1}$
c,I/liq 356.2 K, $\Delta H$ = 14800 J·mol$^{-1}$
$\Delta S$ = 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, $C_p$ = 133.3 J·mol$^{-1}$·K$^{-1}$
Temperature range 8 to 400 K.
**Entropy** 298.15 K, S = 157.2 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 312.1 K, $\Delta H$ = 1810 J·mol$^{-1}$
$\Delta S$ = 5.80 J·mol$^{-1}$·K$^{-1}$
c,I/liq 356.2 K, $\Delta H$ = 14800 J·mol$^{-1}$
$\Delta S$ = 41.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 116.0732
**Wiswesser Line Notation** T6OV DOVTJ
**Evaluation** A
See also 77EVS/BEL.

**$C_4H_4O_4$** (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, $\Delta H$ = 1810 J·mol$^{-1}$
$\Delta S$ = 5.80 J·mol$^{-1}$·K$^{-1}$
c,I/liq 356.2 K, $\Delta H$ = 14800 J·mol$^{-1}$
$\Delta S$ = 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 $S_T°$ = 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, $\Delta H$ = 1840.0 J·mol$^{-1}$
$\Delta S$ = 5.90 J·mol$^{-1}$·K$^{-1}$
c,I/liq 356.2 K, $\Delta H$ = 14800 J·mol$^{-1}$
$\Delta S$ = 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** T6OV VOTJ
**Evaluation** A

**$C_4H_4O_4$** (c) 82LEB/KUL2
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, $\Delta H$ = 13400 J·mol$^{-1}$
$\Delta S$ = 32.29 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 116.0732
**Wiswesser Line Notation** T6OV VOTJ
**Evaluation** A

**$(C_4H_4O_4)_n$** (c) 77LEB/EVS
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, $\Delta H$ = 23500 J·mol$^{-1}$
$\Delta S$ = 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/YEV
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, $\Delta H$ = 23500 J·mol$^{-1}$
$\Delta S$ = 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/KUL2
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

**$C_4H_4S$** (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

**$C_4H_5NO$** (liq) 79DZH/KAR
$\beta$-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
$\alpha$-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$^{-1}$·K$^{-1}$.
**Molecular Weight** 83.0896
**Wiswesser Line Notation** VHY1&CN
**Evaluation** C

**$(C_4H_6)_n$** (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 284 K
**Molecular Weight** 54.0914
**Wiswesser Line Notation** /*2U2*/ -C
**Evaluation** A

**$(C_4H_6)_n$** (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 $\Delta H$ = 7980 J·mol$^{-1}$
$\Delta S$ = 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

**$C_4H_6N_2O_2$** (c) 82LEB/KUL
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

**$C_4H_6O \cdot 17H_2O$** (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, $\Delta H$ = 92900 J·mol$^{-1}$
$\Delta S$ = 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 $H_2O$.

**$C_4H_6O$** (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) 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, $\Delta H$ = 9729 J·mol$^{-1}$
$\Delta S$ = 49.26 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 86.0902
**Wiswesser Line Notation** 1U1VO1
**Evaluation** A

**$C_4H_6O_2$** (liq) 83LEB/YEV
$\tau$-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, $\Delta H$ = 9570 J·mol$^{-1}$
$\Delta S$ = 41.56 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 86.0902
**Wiswesser Line Notation** T5OVTJ
**Evaluation** A

**$C_4H_6O_2$** (liq) 84VAS/PET
Methacrylic acid; $\alpha$-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; $\alpha$-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; $\alpha$-Methyl acrylic acid
**Phase Changes**
c/liq 287.5 K, $\Delta H$ = 8062.5 J·mol$^{-1}$
$\Delta S$ = 28.04 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 86.0902
**Wiswesser Line Notation** QVY1&U1
**Evaluation** A

**$(C_4H_6O_2)_n$** (c) 67PAV/RAB
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·°C (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) 76VAS/KOR
Propylene carbonate
**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, $\Delta H$ = 9617 J·mol$^{-1}$
$\Delta S$ = 42.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 102.0896
**Wiswesser Line Notation** T5OVOTJ D1
**Evaluation** A

**$C_4H_6O_3$** (liq) 84VAS/PET
Propylene carbonate
**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, $\Delta H$ = 9620 J·mol$^{-1}$
$\Delta S$ = 42.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 102.0896
**Wiswesser Line Notation** T5OVOTJ D1
**Evaluation** A

**$C_4H_6O_4Mg$** (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.

**$C_4H_6O_4Mg·4H_2O$** (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, $\Delta H$ = 35800 J·mol$^{-1}$
$\Delta S$ = 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

**$C_4H_6O_4Zn$** (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

**$C_4H_7KO_2$** (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, $\Delta H$ = 409 J·mol$^{-1}$
$\Delta S$ = 3.33 J·mol$^{-1}$·K$^{-1}$
c,VI/c,VB 142.3 K, $\Delta H$ = 269 J·mol$^{-1}$
$\Delta S$ = 1.88 J·mol$^{-1}$·K$^{-1}$
Bifurcated transitions.
c,VB/c,V*A* 250 K
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
c,I/liq 626.1 K
Solid-liquid crystal.
**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) 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

**$C_4H_7NO$** (liq) 62KOL/PAU
α-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, $\Delta H$ = 13920 J·mol$^{-1}$
$\Delta S$ = 46.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 85.1033
**Wiswesser Line Notation** T5MVTJ
**Evaluation** B

**$C_4H_7O_2Tl$** (c) 76MEI/SEY
Thallium butyrate
**Phase Changes**
c,I/liq 459 K, $\Delta H$ = 6694 J·mol$^{-1}$
$\Delta S$ = 14.2 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 320 to 480 K.
**Phase Changes**
c,I/liq 456.7 K, $\Delta H$ = 7691 J·mol$^{-1}$
$\Delta S$ = 16.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 291.4681
**Wiswesser Line Notation** OV3 .TL
**Evaluation** A

**$C_4H_8$** (liq) 71RAB/LEB
2-Methylpropene; Isobutene
**Heat Capacity** 266.26 K, $C_p$ = 121.3 J·mol$^{-1}$·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) 83CHA/HAL
*cis*-2-Butene
**Heat Capacity** 298.15 K, $C_p$ = 127 J·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 367 K.
**Entropy** 298.15 K, $S$ = 220 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 134.26 K, $\Delta H$ = 7309 J·mol$^{-1}$
$\Delta S$ = 54.4 J·mol$^{-1}$·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) 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, $\Delta H$ = 9757 J·mol$^{-1}$
$\Delta S$ = 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.

**$C_4H_8$** (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, $\Delta H$ = 3848 J·mol$^{-1}$
$\Delta S$ = 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: 46AST/FIN, 49SCH/SAG, 36TOD/PAR.

**$(C_4H_8)_n$** (c) 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

**$C_4H_8Cl_2$** (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

**$C_4H_8N_8O_8$** (c,$\alpha$) 70LIC
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine($\alpha$); Octogen($\alpha$); HMX
**Heat Capacity** 298 K, $C_p$ = 307 J·mol$^{-1}$·K$^{-1}$
Temperature range 203 to 523 K. $\alpha$-Phase.
$C_p$ = 0.0991 + 5×10$^{-4}$$T$ cal·K$^{-1}$·g$^{-1}$ (−70 to 250 °C).
**Phase Changes**
c,II/c,I 193–201 K, $\Delta H$ = 7398 J·mol$^{-1}$
$\alpha$-$\delta$ Transition.
Data also given for the following transitions:
$\beta$-$\delta$; $T$ = 167 to 183 °C; $\Delta H$ = 9801 J·mol$^{-1}$.
$\tau$-$\delta$; $T$ = 175 to 182 °C; $\Delta H$ = 2788 J·mol$^{-1}$.
**Molecular Weight** 296.1560
**Wiswesser Line Notation** T8N CN EN GNTJ ANW CNW ENW GNW
**Evaluation** B
Data also given for the following polymorphic forms:
$\beta$-HMX; $C_p$(298 K) = 301 J·mol$^{-1}$·K$^{-1}$;
$C_p$ = 0.0935 + 5×10$^{-4}$$T$ cal·K$^{-1}$·g$^{-1}$ (−70 to 250 °C);
$\tau$-HMX; $C_p$(298 K) = 328 J·mol$^{-1}$·K$^{-1}$;
$C_p$ = 0.1159 + 5×10$^{-4}$$T$ cal·K$^{-1}$·g$^{-1}$ (−70 to 250 °C);
$\delta$-HMX; $C_p$(298 K) = 387 J·mol$^{-1}$·K$^{-1}$;
$C_p$ = 0.1642 + 5×10$^{-4}$$T$ cal·K$^{-1}$·g$^{-1}$ (-70 to 250 °C).

**$C_4H_8N_8O_8$** (c,$\beta$) 83KOS/SHO
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine($\beta$); Octogen($\beta$); HMX
**Heat Capacity** 315 K, $C_p$ = 321.0 J·mol$^{-1}$·K$^{-1}$
Temperature range 294 to 486 K. $\beta$-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,$\beta$) 84KOS/SHO
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine($\beta$); Octogen($\beta$); 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,beta/c,delta)
**Molecular Weight** 296.1560
**Wiswesser Line Notation** T8N CN EN GNTJ ANW CNW ENW GNW
**Evaluation** C

**$C_4H_8O$** (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) 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) 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) 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, $\Delta H$ = 8540 J·mol$^{-1}$
$\Delta S$ = 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) 79LEB/LIT
Tetrahydrofuran; Oxolane
**Heat Capacity** 298.15 *K*
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 $\Delta H = 8540$ *J* mol$^{-1}$
$\Delta S = 51.83$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 72.1066
**Wiswesser Line Notation** T5OTU
**Evaluation** A

**$C_4H_8O \cdot 17H_2O$** (liq) 85HAN
Tetrahydrofuran clathrate hydrate
**Heat Capacity**
Temperature range 95 to 260 K.
**Phase Changes**
c/liq 277.3 K, $\Delta H = 99100$ J·mol$^{-1}$
$\Delta S = 357.4$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 378.3650
**Wiswesser Line Notation** T5OTJ &QH 17
**Evaluation** A
Actual formula: $C_4H_8O \cdot 17H_2O$.

**$C_4H_8O \cdot 17H_2O$** (c) 82LEA/MUR
Tetrahydrofuran clathrate hydrate
**Heat Capacity**
Temperature range 120 to 260 K.
Data given graphically.
**Phase Changes**
c/liq 277.4 K, $\Delta H = 98000$ J·mol$^{-1}$
$\Delta S = 353.2$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 378.3650
**Wiswesser Line Notation** T5OTJ &QH 17
**Evaluation** A
Actual formula: $C_4H_8O \cdot 16.9H_2O$

**$C_4H_8O \cdot 17H_2O$** (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, $\Delta H = 96980$ J·mol$^{-1}$
$\Delta S = 349.6$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 378.3650
**Wiswesser Line Notation** T5OTJ &QH 17
**Evaluation** A
Actual formula: $C_4H_8O \cdot 16.64H_2O$.

**$(C_4H_8O)_n$** (c) 77LEB/LIT
Polytetrahydrofuran
**Phase Changes**
c,II/c,I 186 K
Glass point.
c/liq 316 K, $\Delta H = 11000$ J·mol$^{-1}$
$\Delta S = 34.8$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 72.1066
**Wiswesser Line Notation** /*O4*/
**Evaluation** A

**$(C_4H_8O)_n$** (c) 77LEB/LIT2
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, $\Delta H = 11000$ J·mol$^{-1}$
$\Delta S = 34.8$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 72.1066
**Wiswesser Line Notation** /*O4*/
**Evaluation** A
$T$(glass) = 186 K.

**$C_4H_8O_2$** (liq) 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** 20V1
**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) 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) 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** 30VH
**Evaluation** B

**$C_4H_8O_2$** (liq) 82BIR/SIK
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 − 0.08156 $T$ + 0.0008541 $T^2$ J·mol$^{-1}$·K$^{-1}$.
**Molecular Weight** 88.1060
**Wiswesser Line Notation** QVY1&1
**Evaluation** C

**$C_4H_8O_2$·17$H_2O$** (liq) 85HAN
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, $\Delta H$ = 89900 J·mol$^{-1}$
$\Delta S$ = 333.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 394.3644
**Wiswesser Line Notation** T6O COTJ &QH 17
**Evaluation** A
Actual formula: $C_4H_8O_2$·17$H_2O$.

**$C_4H_8O_2$** (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) 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) 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

**$C_4H_8O_3$** (liq) 83SAN/CIO
Ethylene glycol acetate
**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$^{-1}$) = 0.042568$T$ - 10.686
**Molecular Weight** 101.0817
**Wiswesser Line Notation** Q2OV1
**Evaluation** D

**$C_4H_8S_2$** (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, $\Delta H$ = 800 J·mol$^{-1}$
$\Delta S$ = 2.5 J·mol$^{-1}$·K$^{-1}$
c,I/liq 327.2 K, $\Delta H$ = 14400 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 21600 J·mol$^{-1}$
$\Delta S$ = 56.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 120.2272
**Wiswesser Line Notation** T6S DSTJ
**Evaluation** B

**$C_4H_9Cl$** (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

**$C_4H_9NO$** (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/JIM
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, $\Delta H$ = 86000 J·mol$^{-1}$
$\Delta S$ = 288.4 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 87.1212
**Wiswesser Line Notation** ZVY1&1
**Evaluation** A

**$C_4H_9NO_2$** (c) 83SKO/SAB
4-Aminobutanoic acid; $\tau$-Aminobutyric 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) 84GRU/BOU
$\alpha$-Aminobutyric acid (L); 2-Aminobutanoic acid (L)
**Phase Changes**
c,II/c,I 356 K, $\Delta H$ = 530 J·mol$^{-1}$
$\Delta S$ = 1.49 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 103.1206
**Wiswesser Line Notation** ZY2&QV -L
**Evaluation** B

**$C_4H_{10}Hg$** (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, $\Delta H$ = 10500 J·mol$^{-1}$
$\Delta S$ = 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 DMTU
**Evaluation** D

**$C_4H_{10}N_2O$** (c) 87DEL/FER
1,1,3-Trimethylurea
**Phase Changes**
c/liq 344.4 K, $\Delta H$ = 14300 J·mol$^{-1}$
$\Delta S$ = 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/FER
Isopropylurea; Monoisopropylurea
**Phase Changes**
c,II/c,I 375.5 K, $\Delta H$ = 2310 J·mol$^{-1}$
c/liq 427.4 K, $\Delta H$ = 17400 J·mol$^{-1}$
$\Delta S$ = 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/FER
Propylurea; Monopropylurea
**Phase Changes**
c/liq 381.0 K, $\Delta H$ = 14630 J·mol$^{-1}$
$\Delta S$ = 38.4 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 102.1358
**Wiswesser Line Notation** ZVM3
**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) 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/SOM
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) 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$^{-1}$
**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) 76SKO/SUU
*tert*-Butyl alchohol; 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) 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) 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

**$(C_4H_{10}OSi)_n$** (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, $\Delta H$ = 2070 J·mol$^{-1}$
$\Delta S$ = 10.2 J·mol$^{-1}$·K$^{-1}$
Degree of crystallinity = 72%.
c/liq 295 K, $\Delta H$ = 2876 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 2070 J·mol$^{-1}$
$\Delta S$ = 10.2 J·mol$^{-1}$·K$^{-1}$
Degree of crystallinity = 72%.
c,I/liq 295 K, $\Delta H$ = 2860 J·mol$^{-1}$
$\Delta S$ = 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

**$C_4H_{10}O_2$** (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, $\Delta H$ = 18700 J·mol$^{-1}$
$\Delta S$ = 63.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 90.1218
**Wiswesser Line Notation** Q4Q
**Evaluation** A

**$C_4H_{10}O_2Se$** (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, $\Delta H$ = 110 J·mol$^{-1}$
$\Delta S$ = 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) 82ZAR
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

**$C_4H_{10}O_3$** (c) 89ZHA/YAN
1,1,1-Trihydroxymethylpropane
**Heat Capacity** 301.29 K 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** 106.1212
**Wiswesser Line Notation** QXQQY1&1
**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.
$C_p = 155.76 + 2.780\times10^{-2}T + 8.100\times10^{-5}T^2$.
**Molecular Weight** 90.1830
**Wiswesser Line Notation** SH4
**Evaluation** B

**$C_4H_{10}Zn$** (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, $\Delta H$ = 18050 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 275.4 J·mol$^{-1}$
$\Delta S$ = 2.12 J·mol$^{-1}$·K$^{-1}$
c,I/liq 236.98 K, $\Delta H$ = 16634 J·mol$^{-1}$
$\Delta S$ = 70.19 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 123.5030
**Wiswesser Line Notation** 2-ZN-2
**Evaluation** A

**$C_4H_{11}NO$** (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**

**Molecular Weight** 89.1370

**Wiswesser Line Notation** Z301

**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

**$C_4H_{11}N_3O_7$** (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.

$C_p = -0.0108 + 0.231\times10^{-2}T - 0.631\times10^{-5}T^2 + 0.830\times10^{-8}T^3$ cal·g$^{-1}$·K$^{-1}$ (80 to 300 K).

$C_p$ value calculated from equation.

**Phase Changes**

c,II/c,I 206.5 K, $\Delta H$ = 1072 J·mol$^{-1}$; $\Delta S$ = 5.19 J·mol$^{-1}$·K$^{-1}$

**Molecular Weight** 213.1468

**Wiswesser Line Notation** Z1VQ 2 &WNQ

**Evaluation** C

**$C_4H_{12}Cl_3MnN$** (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

**$C_4H_{12}Cl_4FeN$** (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, $\Delta H$ = 498.9 J·mol$^{-1}$; $\Delta S$ = 1.98 J·mol$^{-1}$·K$^{-1}$

c,V/c,$IV$ 291.4 K, $\Delta H$ = 2524 J·mol$^{-1}$; $\Delta S$ = 10.7 J·mol$^{-1}$·K$^{-1}$

c,IV/c,III 307.4 K, $\Delta H$ = 734.3 J·mol$^{-1}$; $\Delta S$ = 2.38 J·mol$^{-1}$·K$^{-1}$

c,III/c,II 347.0 K, $\Delta H$ = 713.1 J·mol$^{-1}$; $\Delta S$ = 2.05 J·mol$^{-1}$·K$^{-1}$

c,II/c,I 381.0 K, $\Delta H$ = 5319.6 J·mol$^{-1}$; $\Delta S$ = 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, $\Delta H$ = 7447.1 J·mol$^{-1}$; $\Delta S$ = 40.39 J·mol$^{-1}$·K$^{-1}$

liq/g 285 K, $\Delta H$ = 28125 J·mol$^{-1}$; $\Delta S$ = 98.7 J·mol$^{-1}$·K$^{-1}$; P = 1 atm

**Molecular Weight** 132.7288

**Wiswesser Line Notation** 1-GE-1&1&1

**Evaluation** A

**$C_4H_{12}O_4Si$** (liq) 08KAH/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, $\Delta H$ = 30900 J·mol$^{-1}$; $\Delta S$ = 78.4 J·mol$^{-1}$·K$^{-1}$

**Molecular Weight** 152.2219

**Wiswesser Line Notation** 1O-SI-O1&O1&O1

**Evaluation** D

**$C_4H_{12}Pb$** (liq) 54STA/WAR

Tetramethyl lead

**Phase Changes**

c/liq 242.92 K, $\Delta H$ = 10799 J·mol$^{-1}$; $\Delta S$ = 44.43 J·mol$^{-1}$·K$^{-1}$

**Molecular Weight** 267.3388

**Wiswesser Line Notation** 1-PB-1&1&1

**Evaluation** B

**$C_4H_{12}Sn$** (liq) 54STA/WAR

Tetramethyl tin; Tetramethyl stannane

**Phase Changes**

c/liq 218.18 K, $\Delta H$ = 9439 J·mol$^{-1}$; $\Delta S$ = 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, $\Delta H$ = 9234 J·mol$^{-1}$; $\Delta S$ = 42.35 J·mol$^{-1}$·K$^{-1}$

**Molecular Weight** 178.8488

**Wiswesser Line Notation** 1-SN-1&1&1

**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, $\Delta H = 43.6$ J·mol$^{-1}$
$\Delta S = 0.20$ J·mol$^{-1}$·K$^{-1}$
c,II/c,I 424 K, $\Delta H = 4.1$ J·mol$^{-1}$
$\Delta S = 0.009$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 288.9338
**Wiswesser Line Notation** 2ZH2 .MN G4
**Evaluation** A

**$C_5F_{12}$** (liq) 83CAM/DIA
*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) 84GOL/KOL
Perfluoromethyldiethylamine
**Phase Changes**
c/liq 150.1 K, $\Delta H = 4600$ J·mol$^{-1}$
$\Delta S = 30.6$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 321.0409
**Wiswesser Line Notation** FXFFXFFNXFFF&XFFXFFF
**Evaluation** A

**$C_5H_3F_7O_2$** (liq) 84GOL/KOL
Methyl perfluorobutanoate
**Phase Changes**
c/liq 191.4 K, $\Delta H = 11770$ J·mol$^{-1}$
$\Delta S = 61.5$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 228.0663
**Wiswesser Line Notation** XFFFXFFXFFVO1
**Evaluation** A

**$C_5H_5F_3O_2$** (liq) 84GOL/KOL
Trifluoromethyl (2-hydroxy-1-propenyl) ketone
**Phase Changes**
c/liq 232.4 K, $\Delta H = 8450$ J·mol$^{-1}$
$\Delta S = 36.4$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 154.0885
**Wiswesser Line Notation** QY1&U1VXFFF
**Evaluation** A

**$C_5H_6$** (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, $\Delta H = 8010$ J·mol$^{-1}$
$\Delta S = 45.4$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 66.1024
**Wiswesser Line Notation** L5 AHJ
**Evaluation** A

**$C_5H_6N_2O_2$** (c) 1889EYK
Thymine
**Phase Changes**
c/liq 321.3 K, $\Delta H = 17510$ J·mol$^{-1}$
**Molecular Weight** 126.1146
**Wiswesser Line Notation** T6MVMVJ E1
**Evaluation** C

**$C_5H_7N$** (liq) 86STE/CHI
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/TOD
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, $\Delta H = 7824.8$ J·mol$^{-1}$
$\Delta S = 36.07$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 81.1170
**Wiswesser Line Notation** T5NJ A1
**Evaluation** A

**$C_5H_7N$** (liq) 88MES/TOD
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, $\Delta H = 7824.77$ J·mol$^{-1}$
**Molecular Weight** 81.1170
**Wiswesser Line Notation** T5NJ A1
**Evaluation** A

**$C_5H_7NO_2$** (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$^{-1}$
**Phase Changes**
c,II/c,I 162.5 K
Glass transition.
Transition temperature estimated from graph.
c,I/liq 246.8 K, $\Delta H = 11780$ J·mol$^{-1}$
$\Delta S = 47.73$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 113.1158
**Wiswesser Line Notation** NC1VO2
**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, $\Delta H = 5756$ J·mol$^{-1}$
$\Delta S = 41.6$ 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, $\Delta H$ = 5755 J·mol$^{-1}$
$\Delta S$ = 41.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 68.1182
**Wiswesser Line Notation** L4YTJ AU1
**Evaluation** A

**$C_5H_8$** (liq) 78LEB/TSV2
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, $\Delta H$ = 5755 J·mol$^{-1}$
$\Delta S$ = 41.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 68.1182
**Wiswesser Line Notation** L4YTJ AU1
**Evaluation** A

**$(C_5H_8)_n$** (liq) 76LEB/RAB
Polypentenamer
**Heat Capacity**
Temperature range 14 to 322 K.
**Phase Changes**
c/liq 293 K, $\Delta H$ = 8075 J·mol$^{-1}$
$\Delta S$ = 27.56 J·mol$^{-1}$·K$^{-1}$
100% crystallinity.
**Molecular Weight** 68.1182
**Wiswesser Line Notation** /*YU4*/
**Evaluation** A
$T$(glass) = 173 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, $\Delta H$ = 8080 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 5200 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 8900 J·mol$^{-1}$
$\Delta S$ = 28.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 68.1182
**Wiswesser Line Notation** /*YU4* -T/
**Evaluation** B
$T$(glass) = 175 K.

**$C_5H_8O_2$** (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, $\Delta H$ = 14435 J·mol$^{-1}$
$\Delta S$ = 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,I/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, $\Delta H$ = 13451 J·mol$^{-1}$
$\Delta S$ = 59.65 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 100.1170
**Wiswesser Line Notation** 1UY1&VO1
**Evaluation** A

**$C_5H_8O_2$** (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, $\Delta H$ = 14497 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 457 J·mol$^{-1}$
$\Delta S$ = 3.88 J·mol$^{-1}$·K$^{-1}$
c,III/c,II 122–155 K, $\Delta H$ = 310 J·mol$^{-1}$
$\Delta S$ = 2.2 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 180–225 K, $\Delta H$ = 205 J·mol$^{-1}$
$\Delta S$ = 0.90 J·mol$^{-1}$·K$^{-1}$
c,I/liq 262.82 K, $\Delta H$ = 10530 J·mol$^{-1}$
$\Delta S$ = 39.46 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 100.1170
**Wiswesser Line Notation** T6OVTJ
**Evaluation** A

**$(C_5H_8O_2)_n$** (c) 67PAV/RAB
Poly(methyl methacrylate)
**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)
**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

**$C_5H_9LiO_2$** (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, $\Delta H$ = 665 J·mol$^{-1}$
$\Delta S$ = 3.24 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 319.06 K, $\Delta H$ = 2745 J·mol$^{-1}$
$\Delta S$ = 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

**$C_5H_9NO$** (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, $S$ = 164.9 J·mol$^{-1}$
**Phase Changes**
c/liq 342.305 K, $\Delta H$ = 16096 J·mol$^{-1}$
$\Delta S$ = 33.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 99.1299
**Wiswesser Line Notation** T6MVTU
**Evaluation** B

**$C_5H_9NO_4$** (c) 75SAK/SEK
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.

**$C_5H_9O_2Tl$** (c) 76MEI/SEY
Thallium pentanoate
**Phase Changes**
c,II/c,I 354.6 K, $\Delta H$ = 2259 J·mol$^{-1}$
$\Delta S$ = 6.28 J·mol$^{-1}$·K$^{-1}$
c,I/liq 455 K, $\Delta H$ = 5439 J·mol$^{-1}$
$\Delta S$ = 12.1 J·mol$^{-1}$·K$^{-1}$
Solid-mesophase.
liq/liq 487 K, $\Delta H$ = 3054 J·mol$^{-1}$
$\Delta S$ = 6.28 J·mol$^{-1}$·K$^{-1}$
Mesophase-isotropic.
**Molecular Weight** 305.4949
**Wiswesser Line Notation** OV4 .TL
**Evaluation** B

**$C_5H_9O_2Tl$** (c) 84FER/LOP
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, $\Delta H$ = 2104 J·mol$^{-1}$
$\Delta S$ = 5.99 J·mol$^{-1}$·K$^{-1}$
c,I/liq 455.0 K, $\Delta H$ = 5704 J·mol$^{-1}$
$\Delta S$ = 12.5 J·mol$^{-1}$·K$^{-1}$
Solid to mesophase.
**Molecular Weight** 305.4949
**Wiswesser Line Notation** OV4 .TL
**Evaluation** A
Mesophase to isotropic liquid phase change data also given:
488.0 K; $\Delta H$ = 3051 J·mol$^{-1}$;
$\Delta S$ = 6.24 J·mol$^{-1}$·K$^{-1}$.

**$C_5H_{10}$** (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, $\Delta H$ = 5359 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 7579 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 7911 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 7112 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 8352 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 5807 J·mol$^{-1}$
$\Delta S$ = 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.

**$C_5H_{10}O$** (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) 70HAR/HEA
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) 70HAR/HEA
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) 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; Diethylketone
**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) 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) 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
Valeral; *n*-Pentanal; Valeraldehyde
**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, $\Delta H$ = 499 J·mol$^{-1}$
$\Delta S$ = 3.34 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 183.9 K, $\Delta H$ = 4809 J·mol$^{-1}$
$\Delta S$ = 26.22 J·mol$^{-1}$·K$^{-1}$
c,I/liq 272.1 K, $\Delta H$ = 2520 J·mol$^{-1}$
$\Delta S$ = 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) 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) 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** 30V1
**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

**$C_5H_{10}O_3$** (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$^{-1}$) = 0.024460$T$ - 4.667
**Molecular Weight** 118.1322
**Wiswesser Line Notation** 1V0201
**Evaluation** D

**$C_5H_{10}O_5$** (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

**$C_5H_{11}N$** (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) 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, $\Delta H$ = 14847.9 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 14853.69 J·mol$^{-1}$
$\Delta S$ = 56.67 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 85.1486
**Wiswesser Line Notation** T6MTJ
**Evaluation** A

**$C_5H_{11}NO$** (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, $\Delta H$ = 86600 J·mol$^{-1}$
$\Delta S$ = 290.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 101.1480
**Wiswesser Line Notation** ZVX1&1&1
**Evaluation** A

**$C_5H_{11}NO_2$** (c) 84GRU/BOU
Norvaline (L); α-Aminovaleric acid (L)
**Phase Changes**
c,II/c,I 273 K, $\Delta H$ = 40 J·mol$^{-1}$
$\Delta S$ = 0.16 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 117.1474
**Wiswesser Line Notation** QVYZ3 -L
**Evaluation** B

**$C_5H_{11}NO_2$** (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

**$C_5H_{11}NO_2S$** (c) 84GRU/BOU
Methionine (L)
**Phase Changes**
c,III/c,II 307 K, $\Delta H$ = 1980 J·mol$^{-1}$
$\Delta S$ = 6.45 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 393 K, $\Delta H$ = 150 J·mol$^{-1}$
$\Delta S$ = 0.38 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 149.2074
**Wiswesser Line Notation** QVYZ2S1 -L
**Evaluation** B

**$C_5H_{11}NO_2S$** (c) 84GRU/BOU
Methionine (DL)
**Phase Changes**
c,III/c,II 326 K, $\Delta H$ = 820 J·mol$^{-1}$
$\Delta S$ = 2.51 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 380 K
**Molecular Weight** 149.2074
**Wiswesser Line Notation** QVYZ2S1
**Evaluation** B

**$C_5H_{12}N_2O$** (c) 87DEL/FER
1,3-Diethylurea
**Phase Changes**
c,II/c,I 339.4 K, $\Delta H$ = 1870 J·mol$^{-1}$
$\Delta S$ = 55.1 J·mol$^{-1}$·K$^{-1}$
c/liq 383.4 K, $\Delta H$ = 12460 J·mol$^{-1}$
$\Delta S$ = 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, | $\Delta H$ = 7020 J·mol$^{-1}$ |
| c,II/c,I | 344.9 K, | $\Delta H$ = 880 J·mol$^{-1}$ |
| c/liq | 369.3 K, | $\Delta H$ = 14550 J·mol$^{-1}$ |
| | | $\Delta S$ = 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, | $\Delta H$ = 33130 J·mol$^{-1}$ |
| | | $\Delta S$ = 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 140–310 K.
**Phase Changes**

| | | |
|---|---|---|
| c,II/c,I | 195–225 K, | $\Delta H$ = 2000 J·mol$^{-1}$ |
| | | $\Delta S$ = 9.61 J·mol$^{-1}$·K$^{-1}$ |
| | Reversible transition. | |
| c,I/liq | 384.43 K, | $\Delta H$ = 16100 J·mol$^{-1}$ |
| | | $\Delta S$ = 41.9 J·mol$^{-1}$·K$^{-1}$ |
| c/g | 326 K, | $\Delta H$ = 96800 J·mol$^{-1}$ |
| | | $\Delta S$ = 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

**$C_5H_{12}O$** (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) 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) 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
Methyl *n*-butyl ether; 2-Oxahexane
**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) 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) 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) 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

**$C_5H_{12}O$** (liq) 83DAP/DEL
2-Methyl-2-butanol; *tert*-Pentanol;
*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) 88PIE/SOM
2-Methyl-2-butanol; *tert*-Pentanol;
*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

**$C_5H_{12}O_2$** (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

**$C_5H_{12}O_4$** (c) 50HOS/NAG
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane; Pentaerythritol
**Phase Changes**
c,II/c,I 457 K, $\Delta H$ = 35146 J·mol$^{-1}$
$\Delta S$ = 76.9 J·mol$^{-1}$·K$^{-1}$
c,I/liq 529 K, $\Delta H$ = 5439 J·mol$^{-1}$
$\Delta S$ = 10.28 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 136.1474
**Wiswesser Line Notation** Q1X1Q1Q1Q
**Evaluation** B

**$C_5H_{12}O_4$** (c) 89ZHA/YAN
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane; Pentaerythritol
**Heat Capacity** 298.98 *K* 188.40 J·mol$^{-1}$·K$^{-1}$
Temperature range 277 to 510 K
**Phase Changes**
c,II/c,I 461.60 K $\Delta H$ = 41380 *J* mol$^{-1}$
$\Delta$S = 89.64 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 136.1474
**Wiswesser Line Notation** Q1X1Q1Q1Q
**Evaluation** A

**$C_5H_{12}Si$** (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, $\Delta H$ = 7657 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 7660 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 6761 J·mol$^{-1}$
$\Delta S$ = 43.51 J·mol$^{-1}$·K$^{-1}$
liq/g 355.91 K, $\Delta H$ = 32141 J·mol$^{-1}$
$\Delta S$ = 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) 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/

**$C_5H_{13}N$** (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

**$C_5H_{13}NO$** (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

**$C_5H_{14}N_2$** (liq) 84LEB/GUT
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
$\Delta H$ vaporization = 44100 J·mol$^{-1}$, temperature range = 290 to 317 K.

**$C_5H_{14}N_2O$** (liq) 88KOZ/KRA
Tetramethylurea
**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 240K);
$C_p$(liq) = 153.30 + 0.2748 J·mol$^{-1}$·K$^{-1}$ (320 to 425K).
**Phase Changes**
c/liq 272.2 K, $\Delta H$ = 13400 J·mol$^{-1}$
$\Delta S$ = 49.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 118.1784
**Wiswesser Line Notation** 1M1&VM1&1
**Evaluation** A

**$C_5H_{15}N_3$** (liq) 81LEB/RYA
Dimethylaminopropylenediamine
**Heat Capacity** 295.96 K, $C_p$ = 249.0 J·mol$^{-1}$·K$^{-1}$
Temperature range 296 to 359 K.
**Molecular Weight** 117.1936
**Wiswesser Line Notation** Z1Y1ZN1&1
**Evaluation** B

**$C_5H_{16}Cl_4Mn$** (c) 88CHH/ABE
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, $\Delta H$ = 2240 J·mol$^{-1}$
$\Delta S$ = 8.3 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 272.9314
**Wiswesser Line Notation** Z5Z &GH 2 .MN G2

**$C_6Br_2Cl_3F_9$** (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

**$C_6D_{17}BeF_4N_3O_6$** (c) 79LOI/OSB
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 $\Delta H$ = 1153 J·mol$^{-1}$
No temperature given.
**Molecular Weight** 327.9862
**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/KOS
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/KOS2
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, $\Delta H$ = 813 J·mol$^{-1}$
$\Delta S$ = 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/GON
Triglycine sulfate, deuterated
**Heat Capacity** 300 K, $C_p$ = 390 J·mol$^{-1}$·K$^{-1}$
Temperature range 100 to 400 K.
Data given graphically; $C_p$ estimated from graph.
**Phase Changes**
c,II/c,I 331.75 K, $\Delta H$ = 571 J·mol$^{-1}$
$\Delta S$ = 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.

**$C_6F_6$** (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 CD 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

**$C_6F_{14}$** (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. **70**, 1274 (1974).

**$C_6F_{15}N$** (liq) 84GOL/KOL
Perfluorotriethylamine
**Phase Changes**
c/liq 156.1 K, $\Delta H$ = 4650 J·mol$^{-1}$
$\Delta S$ = 29.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 371.0487
**Wiswesser Line Notation** FXFFXFF 3N
**Evaluation** A

**$C_6H_2Cl_4$** (c) 82MAR
1,2,4,5-Tetrachlorobenzene
**Phase Changes**
c,II/c,I 187.5 K, $\Delta H$ = 34 J·mol$^{-1}$
$\Delta S$ = 0.18 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 215.8938
**Wiswesser Line Notation** GR BG DG EG
**Evaluation** C

**$C_6H_3Br_3O$** (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) 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/YEJ
2-Chloro-1-(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,70to330K) = 146.438 + 57.0749X− 1.31699×$^2$ + 16.2918×$^3$ − 11.3899×$^4$− 26.7611X$^5$ + 5.59976X$^6$ + 21.3037X$^7$ (J·mol$^{-1}$·K$^{-1}$).
**Phase Changes**
c/liq 337.242 K, $\Delta H$ = 20298.8 J·mol$^{-1}$
$\Delta S$ = 60.190 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 230.9084
**Wiswesser Line Notation** T6NJ BXGGG FG
**Evaluation** B

**$C_6H_3N_3O_7$** (c) 79FAR/SHA
Picric acid; 2,4,6-Trinitrophenol
**Phase Changes**
c/liq 394.1 K, $\Delta H$ = 17100 J·mol$^{-1}$
$\Delta S$ = 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/SHA
Styphnic acid; 2,4,6-Trinitroresorcinol
**Phase Changes**
c/liq 454.9 K, $\Delta H$ = 33500 J·mol$^{-1}$
$\Delta S$ = 73.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 245.1050
**Wiswesser Line Notation** WNR BQ CNW DQ ENW
**Evaluation** B

**$C_6H_4BrCl$** (liq) 18NAR
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, $\Delta H$ = 12368 J·mol$^{-1}$
$\Delta S$ = 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 + 0.0002348 t cal·g$^{-1}$·K$^{-1}$.
$C_p$ value calculated from equation.
**Phase Changes**
c/liq 251.95 K, $\Delta H$ = 12288 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 18760 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 14441 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 12192 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 19614 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 13587 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 14225 J·mol$^{-1}$
$\Delta S$ = 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
**Heat Capacity**
Temperature range 194 to 353 K.
**Phase Changes**
c/liq 360.05 K, $\Delta H$ = 20530 J·mol$^{-1}$
$\Delta S$ = 57.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 235.9056
**Wiswesser Line Notation** ER 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
1,2-Chloronitrobenzene
**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) 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, $\Delta H$ = 18030 J·mol$^{-1}$
$\Delta S$ = 69.9 J·mol$^{-1}$·K$^{-1}$
liq/g 518 K, $\Delta H$ = 36900 J·mol$^{-1}$
$\Delta S$ = 71.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 157.5561
**Wiswesser Line Notation** WNR DG
**Evaluation** C

**$C_6H_4Cl_2$** (liq) 18NAR
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 + 0.0003024 t cal·g$^{-1}$·K$^{-1}$.
$C_p$ value calculated from equation.
**Phase Changes**
c/liq 255.65 K, $\Delta H$ = 12922 J·mol$^{-1}$
$\Delta S$ = 50.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 147.0036
**Wiswesser Line Notation** GR BG
**Evaluation** D

**$C_6H_4Cl_2$** (liq) 18NAR
1,3-Dichlorobenzene; *m*-Dichlorobenzene
**Heat Capacity** 298.15 K, $C_p$ = 170.9 J·mol$^{-1}$·K$^{-1}$
Temperature range 197 to 377 K.
$C_p$ = 0.27022 + 0.0003024 t cal·g$^{-1}$·K$^{-1}$.
$C_p$ value calculated from equation.
**Phase Changes**
c/liq 248.75 K, $\Delta H$ = 12590 J·mol$^{-1}$
$\Delta S$ = 50.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 147.0036
**Wiswesser Line Notation** GR CG
**Evaluation** D

**$C_6H_4Cl_2$** (c) 18NAR
1,4-Dichlorobenzene; *p*-Dichlorobenzene
**Heat Capacity** 298 K, $C_p$ = 147.6 J·mol$^{-1}$·K$^{-1}$
Temperature range 194 to 372 K.
Average specific heat over the temperature range 2.6 to 51.6 °C is 0.2400 cal·g$^{-1}$·K$^{-1}$.
**Phase Changes**
c/liq 326.05 K, $\Delta H$ = 18144 J·mol$^{-1}$
$\Delta S$ = 55.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 147.0036
**Wiswesser Line Notation** GR DG
**Evaluation** D

**$C_6H_4Cl_2$** (c) 72BOO/HAU
1,4-Dichlorobenzene; *p*-Dichlorobenzene
**Phase Changes**
c/liq 326.15 K, $\Delta H$ = 18050 J·mol$^{-1}$
$\Delta S$ = 55.3 J·mol$^{-1}$·K$^{-1}$
**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·mol$^{-1}$ |
| | | $\Delta S = 4.62$ J·mol$^{-1}$·K$^{-1}$ |
| c,II/c,I | 304.35 K, | $\Delta H = 214.5$ J·mol$^{-1}$ |
| | | $\Delta S = 0.705$ J·mol$^{-1}$·K$^{-1}$ |
| c,I/liq | 326.14 K, | $\Delta H = 18187$ J·mol$^{-1}$ |
| | | $\Delta S = 55.76$ J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 147.0036
**Wiswesser Line Notation** GR DG
**Evaluation** A
See also 76DWO/FIG.

**$C_6H_4Cl_2$** (c) 88MAR/MON2
1,4-Dichlorobenzene; *p*-Dichlorobenzene
**Heat Capacity** 180 K, $C_p = 98$ J·mol$^{-1}$·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

**$C_6H_4Cl_2O$** (c) 82POE/FAN
2,3-Dichlorophenol
**Phase Changes**

| | | |
|---|---|---|
| c/liq | 330.0 K, | $\Delta H = 21363$ J·mol$^{-1}$ |
| | | $\Delta S = 64.74$ J·mol$^{-1}$·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·mol$^{-1}$ |
| | | $\Delta S = 88.0$ J·mol$^{-1}$·K$^{-1}$ |
| liq/g | 491 K, | $\Delta H = 36780$ J·mol$^{-1}$ |
| | | $\Delta S = 74.9$ J·mol$^{-1}$·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·mol$^{-1}$ |
| | | $\Delta S = 63.18$ J·mol$^{-1}$·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·mol$^{-1}$ |
| | | $\Delta S = 67.78$ J·mol$^{-1}$·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·mol$^{-1}$ |
| | | $\Delta S = 65.12$ J·mol$^{-1}$·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·mol$^{-1}$ |
| | | $\Delta S = 61.37$ J·mol$^{-1}$·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·mol$^{-1}$ |
| | | $\Delta S = 60.14$ J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 114.0944
**Wiswesser Line Notation** FR BF
**Evaluation** B

**$C_6H_4F_2$** (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) 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

**$C_6H_4I_2$** (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.
$C_p = 0.1357 + 0.0000776t$.
$C_p$ value calculated from equation.
**Phase Changes**

| | | |
|---|---|---|
| c/liq | 296.55 K, | $\Delta H = 14079$ J·mol$^{-1}$ |
| | | $\Delta S = 47.5$ J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 329.9066
**Wiswesser Line Notation** IR BI
**Evaluation** D

**$C_6H_4I_2$** (c) 18NAR
1,3-Diiodobenzene
**Heat Capacity**
Temperature range 196 to 306 K.
**Phase Changes**
c/liq 307.35 K, $\Delta H = 15943$ J·mol$^{-1}$
$\Delta S = 51.9$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 329.9066
**Wiswesser Line Notation** IR CI
**Evaluation** D

**$C_6H_4I_2$** (c) 18NAR
1,4-Diiodobenzene
**Heat Capacity**
Temperature range 198 to 400 K.
**Phase Changes**
c/liq 402.15 K, $\Delta H = 22375$ J·mol$^{-1}$
$\Delta S = 55.6$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 329.9066
**Wiswesser Line Notation** IR DI
**Evaluation** D

**$C_6H_4N_2O_4$** (c) 72BOO/HAU
1,2-Dinitrobenzene
**Phase Changes**
c/liq 390.05 K, $\Delta H = 22750$ J·mol$^{-1}$
$\Delta S = 58.3$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 168.1086
**Wiswesser Line Notation** WNR BNW
**Evaluation** C

**$C_6H_4N_2O_4$** (c) 72BOO/HAU
1,3-Dinitrobenzene
**Phase Changes**
c/liq 363.23 K, $\Delta H = 17350$ J·mol$^{-1}$
$\Delta S = 47.8$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 168.1086
**Wiswesser Line Notation** WNR CNW
**Evaluation** C

**$C_6H_4N_2O_4$** (c) 72BOO/HAU
1,4-Dinitrobenzene
**Phase Changes**
c/liq 446.65 K, $\Delta H = 28100$ J·mol$^{-1}$
$\Delta S = 62.9$ 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, $\Delta H = 26239$ J·mol$^{-1}$
$\Delta S = 62.92$ 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, $\Delta H = 25376$ J·mol$^{-1}$
$\Delta S = 62.35$ 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, $\Delta H = 19577$ J·mol$^{-1}$
$\Delta S = 58.26$ 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, $\Delta H = 24174$ J·mol$^{-1}$
$\Delta S = 62.30$ 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, $\Delta H = 23730$ J·mol$^{-1}$
$\Delta S = 62.28$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 184.1080
**Wiswesser Line Notation** WNR CQ DNW
**Evaluation** A

**$C_6H_5Br$** (liq) 86RED
Bromobenzene
**Heat Capacity** 303.15 K, $C_p = 155.9$ J·mol$^{-1}$·K$^{-1}$
Temperature range 303.15, 313.15 K.
**Molecular Weight** 157.0095
**Wiswesser Line Notation** ER
**Evaluation** B

**$C_6H_5BrO$** (c) 1889EYK
4-Bromophenol
**Phase Changes**
c/liq 336 K, $\Delta H = 16573$ J·mol$^{-1}$
$\Delta S = 49.3$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 173.0091
**Wiswesser Line Notation** QR DE
**Evaluation** C

**$C_6H_5Cl$** (liq) 86RED
Chlorobenzene
**Heat Capacity** 303.15 K, $C_p = 150.6$ J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 112.5585
**Wiswesser Line Notation** GR
**Evaluation** A

**$C_6H_5ClO$** (liq) 82POE/FAN
2-Chlorophenol
**Phase Changes**
c/liq 283.0 K, $\Delta H = 12523$ J·mol$^{-1}$
$\Delta S = 44.25$ J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S = 48.74$ J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S = 44.51$ J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Deposited in VINITI, No 540–69, 11 March 1969.
**Molecular Weight** 256.0545
**Wiswesser Line Notation** G-GE-GGR
**Evaluation** A

**$C_6H_5Cl_3Sn$** (c) 69NUR/KOS
Phenyltrichlorostannane
**Entropy** 298.15 K, $S = 347.5$ J·mol$^{-1}$·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) 84ROU/GRO
Fluorobenzene
**Heat Capacity** 298.15 K, $C_p = 146.29$ J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 96.1039
**Wiswesser Line Notation** FR
**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, $\Delta H = 17446$ J·mol$^{-1}$
$\Delta S = 54.86$ 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, $\Delta H = 21300$ J·mol$^{-1}$
$\Delta S = 57.6$ 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, $\Delta H = 19196$ J·mol$^{-1}$
$\Delta S = 51.88$ 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, $\Delta H = 24271$ J·mol$^{-1}$
$\Delta S = 62.7$ 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, $\Delta H = 19300$ J·mol$^{-1}$
$\Delta S = 52.3$ 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, $\Delta H = 18254$ J·mol$^{-1}$
$\Delta S = 47.17$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 139.1104
**Wiswesser Line Notation** WNR DQ
**Evaluation** A

**$C_6H_5NO_3$** (c) 86SIN/KUM
4-Nitrophenol
**Phase Changes**
c/liq 385.15 K, $\Delta H = 30118$ J·mol$^{-1}$
$\Delta S = 78.2$ 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/MRA
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, $\Delta H$ = 996.6 J·mol$^{-1}$
$\Delta S$ = 8.42 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 78.1134
**Wiswesser Line Notation** 2UU2UU2
**Evaluation** A

$C_6H_6$ (liq) 65FIN/GRU
Benzene
**Heat Capacity** 300 K, $C_p$ = 135.30 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 78.1134
**Wiswesser Line Notation** R
**Evaluation** B

$C_6H_6$ (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) 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/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) 79SMI
Benzene
**Phase Changes**
c/liq 279.1 K, $\Delta H$ = 9300 J·mol$^{-1}$
$\Delta S$ = 33.3 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 78.1134
**Wiswesser Line Notation** R
**Evaluation** C

$C_6H_6$ (liq) 82GOR/SIM2
Benzene
**Heat Capacity**
Temperature range 280 to 680 K.
Data at atmospheric pressure given by the equation:
$C_p = 1.5194 - 1.299\times10^{-3}T + 6.927\times10^{-6}T^2$ kJ·kg$^{-1}$·K$^{-1}$.
**Molecular Weight** 78.1134
**Wiswesser Line Notation** R
**Evaluation** A

$C_6H_6$ (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.
$C_p = 1.3943 - 5.857\times10^{-4}T + 5.89\times10^{-6}T^2$ 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) 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) 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

$C_6H_6N_2O_2$ (c) 72BOO/HAU
3-Nitroaniline
**Phase Changes**
c/liq 384.95 K, $\Delta H$ = 23600 J·mol$^{-1}$
$\Delta S$ = 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) 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
**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
**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

**$C_6H_6O_2$** (c) 03MAG
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) 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) 82VII/GAM
1,3-Dihydroxybenzene; Resorcin; Resorcinol
**Phase Changes**
c/liq 381 K, $\Delta H$ = 20500 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 1370 J·mol$^{-1}$
$\Delta S$ = 3.71 J·mol$^{-1}$·K$^{-1}$
$\alpha$-$\beta$ phase transition.
c,I/liq 382.7 K, $\Delta H$ = 20890 J·mol$^{-1}$
$\Delta S$ = 54.59 J·mol$^{-1}$·K$^{-1}$
Fusion of $\beta$-resorcinol.
**Molecular Weight** 110.1122
**Wiswesser Line Notation** QR CQ
**Evaluation** A

**$C_6H_6O_2$** (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

**$C_6H_7N$** (liq) 01KAH
2-Methylpyridine; $\alpha$-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) 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, $\Delta H$ = 0.083 J·mol$^{-1}$
c,I/liq 276.817 K, $\Delta H$ = 12577 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 0.00 J·mol$^{-1}$
c,I/liq 276.818 K, $\Delta H$ = 12582.28 J·mol$^{-1}$
$\Delta S$ = 45.45 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 93.1280
**Wiswesser Line Notation** T6NJ D1
**Evaluation** A

**$C_6H_7N$** (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

**$C_6H_7N$·HBr** (c) 78KOJ
Aniline hydrobromide
**Heat Capacity**
Temperature range 200 to 320 K.
Data given graphically.
**Phase Changes**
c,II/c,I 230–300 K, $\Delta H$ = 1142 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 15570 J·mol$^{-1}$
$\Delta S$ = 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

**$C_6H_8N_2O_2$** (c) 84ZIE/ZIE
1,3-Dimethyluracil
**Phase Changes**
c/liq 392.5 K, $\Delta H$ = 23100 J·mol$^{-1}$
$\Delta S$ = 58.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 140.1414
**Wiswesser Line Notation** T6NVNVJ A1 C1
**Evaluation** B

**$(C_6H_8N_2O_9)_n$** (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%.

**$C_6H_8O_2$** (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, $\Delta H$ = 11325 J·mol$^{-1}$
**Molecular Weight** 112.1280
**Wiswesser Line Notation** L6V DVTJ
**Evaluation** B($C_p$), A(Phase changes).

**$C_6H_8O_4$** (c) 82LEB/KUL
Lactide(DL)
**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

**$C_6H_8O_7$** (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)

**$C_6H_9ClO_2$** (liq) 85KAR/ABD2
Chloroethyl methacrylate
**Phase Changes**
c/liq 235.1 K, $\Delta H$ = 17001 J·mol$^{-1}$
$\Delta S$ = 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** 5UU1-CU-
**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** 5UU1-CU-
**Evaluation** A

**$C_6H_9N$** (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, $\Delta H$ = 9296.0 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 9298.42 J·mol$^{-1}$
$\Delta S$ = 33.10 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 95.1438
**Wiswesser Line Notation** T5MJ B1 E1
**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

**$(C_6H_{10})_n$** (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

**$C_6H_{10}N_2O$** (liq) 80BYS
2,3-Diazabicyclo[2.2.2]oct-2-ene N-oxide
**Phase Changes**
c,III/c,II 359.2 K, $\Delta H$ = 5020 J·mol$^{-1}$
$\Delta S$ = 14.0 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 399.3 K, $\Delta H$ = 8050 J·mol$^{-1}$
$\Delta S$ = 20.2 J·mol$^{-1}$·K$^{-1}$
c,I/liq 437.9 K, $\Delta H$ = 3840 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 8659.6 J·mol$^{-1}$
$\Delta S$ = 39.22 J·mol$^{-1}$·K$^{-1}$
c,I/liq 245.21 K, $\Delta H$ = 1327.6 J·mol$^{-1}$
$\Delta S$ = 5.414 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 98.1444
**Wiswesser Line Notation** L6VTJ
**Evaluation** A

**$C_6H_{10}O$** (liq) 80NAK/SUG
Cyclohexene oxide
**Heat Capacity** 300 K, $C_p$ = 166.12 J·mol$^{-1}$·K$^{-1}$
Temperature range 13 to 300 K.
Unsmoothed experimental datum 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, $\Delta H$ = 9535.1 J·mol$^{-1}$
$\Delta S$ = 49.39 J·mol$^{-1}$·K$^{-1}$
c,I/liq 238.14 K, $\Delta H$ = 1064.5 J·mol$^{-1}$
$\Delta S$ = 4.470 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 98.1444
**Wiswesser Line Notation** T36 BOTJ
**Evaluation** A

**$C_6H_{10}O_2$** (liq) 82VIL/CAS
3,6-Dioxaoctane
**Heat Capacity** 298.15 K, $C_p$ = 261.08 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 114.1438
**Wiswesser Line Notation** 20202
**Evaluation** B

**$C_6H_{10}O_2$** (liq) 78LEB/YEV2
$\epsilon$-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, $\Delta H$ = 13820 J·mol$^{-1}$
$\Delta S$ = 50.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 114.1438
**Wiswesser Line Notation** T7OVTJ
**Evaluation** A

**$C_6H_{10}O_2$** (liq) 83LEB/YEV
$\epsilon$-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, $\Delta H$ = 13820 J·mol$^{-1}$
$\Delta S$ = 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/YEV2
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, $\Delta H$ = 16400 J·mol$^{-1}$
$\Delta S$ = 48.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 114.1438
**Wiswesser Line Notation** /*OV5*/
**Evaluation** A
$T$(glass) = 209 K.

**$C_6H_{10}O_4$** (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$^{-1}$) = 0.044175$T$ - 11.049
**Molecular Weight** 146.1426
**Wiswesser Line Notation** 1VO2OV1
**Evaluation** D

**$C_6H_{10}O_4$** (liq) 86NIL/WAD
Ethyleneglycoldiacetate
**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

**$C_6H_{10}O_4$** (c) 84VAS/PET
1,4-Butanedioic 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

**$C_6H_8O_7{\cdot}H_2O$** (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, $\Delta H$ = 14980 J·mol$^{-1}$
$\Delta S$ = 48.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 210.1402
**Wiswesser Line Notation** QV1XQVQ1VQ &QH
**Evaluation** B

**$C_6H_{11}LiO_2$** (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) 62KOL/PAU
ϵ-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, $\Delta H$ = 16096 J·mol$^{-1}$
$\Delta S$ = 47.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight 113.1567**
**Wiswesser Line Notation** T7MVTJ
**Evaluation** B

**$(C_6H_{11}NO)_n$** (c) 62KOL/PAU
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** /*MV4*/
**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

**$C_6H_{11}O_2Tl$** (c) 76MEI/SEY
Thallium hexanoate
**Phase Changes**
c,III/c,II 395 K, $\Delta H$ = 179 J·mol$^{-1}$
$\Delta S$ = 0.46 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 412 K, $\Delta H$ = 1841 J·mol$^{-1}$
$\Delta S$ = 1.84 J·mol$^{-1}$·K$^{-1}$
c,I/liq 418 K, $\Delta H$ = 4477 J·mol$^{-1}$
$\Delta S$ = 10.9 J·mol$^{-1}$·K$^{-1}$
Solid-mesophase.
liq/liq 500 K, $\Delta H$ = 3035 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 208 J·mol$^{-1}$
$\Delta S$ = 0.50 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 415.0 K, $\Delta H$ = 657 J·mol$^{-1}$
$\Delta S$ = 1.58 J·mol$^{-1}$·K$^{-1}$
c,I/liq 425.0 K, $\Delta H$ = 4598 J·mol$^{-1}$
$\Delta S$ = 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:
499.8 K; $\Delta H$ = 3941 J·mol$^{-1}$;
$\Delta S$ = 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, $\Delta H$ = 1734 J·mol$^{-1}$
$\Delta S$ = 8.62 J·mol$^{-1}$·K$^{-1}$
c,IV/c,III 280.3 K, $\Delta H$ = 2511 J·mol$^{-1}$
$\Delta S$ = 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) 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) 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) 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) 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) 86JIM/ROM
Cyclohexane
**Heat Capacity** 298.15 K, $C_p$ = 157.06 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

**$(C_6H_{12})_n$** (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, $\Delta H$ = 4774 J·mol$^{-1}$
$\Delta S$ = 10.3 J·mol$^{-1}$·K$^{-1}$
c,I/liq 511.86 K, $\Delta H$ = 24100 J·mol$^{-1}$
$\Delta S$ = 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

**$C_6H_{12}BrFeN_2S_4$** 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 $\Delta H$ = 5.77 J·mol$^{-1}$
$\Delta$S = 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

**$C_6H_{12}FeIN_2S_4$** (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.

**$C_6H_{12}O$** (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) 89VES/BAR
4-Methyl-2-pentanone; Isobutyl methyl ketone
**Heat Capacity** 298.15 K $C_p$ = 211.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 100.1602
**Wiswesser Line Notation** 1Y1&1V1
**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) 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

**$C_6H_{12}O_2$** (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** 3OV2
**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** 3OV2
**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** 4OV1
**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** 4OV1
**Evaluation** B

**$C_6H_{12}O_3$** (liq) 83SAN/CIO
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$^{-1}$) = 0.009426$T$ + 0.036
**Molecular Weight** 132.1590
**Wiswewesser Line Notation** 1VO2O2
**Evaluation** D

**$C_6H_{12}O_6$** (c) 82LIA/CHE
meso-Inositol
**Heat Capacity** 298.15 K, $C_p$ = 218.31 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 180.1572
**Wiswesser Line Notation** L6TJ AQ BQ CQ DQ EQ FQ
**Evaluation** B

**$C_6H_{12}O_6$** (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/KUS
Fructose(D)
**Heat Capacity** 303 K, $C_p$ = 232 J·mol$^{-1}$·K$^{-1}$
Temperature range 300 to 315 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) 81KAW/KUS
Mannose(D)
**Heat Capacity** 303 K, $C_p$ = 216 J·mol$^{-1}$·K$^{-1}$
Temperature range 300 to 315 K.
**Molecular Weight** 180.1572
**Wiswesser Line Notation** T6OTJ BQ CQ DQ EQ F1Q -A&E -B&CDF
**Evaluation** B

**$C_6H_{12}O_6$** (c) 81KAW/KUS
Galactose(D)
**Heat Capacity** 303 K, $C_p$ = 217 J·mol$^{-1}$·K$^{-1}$
Temperature range 300 to 315 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) 03MAG
α-Glucose(D)
**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) 81KAW/KUS
α-Glucose(D)
**Heat Capacity** 303 K, $C_p$ = 224 J·mol$^{-1}$·K$^{-1}$
Temperature range 300 to 315 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)
**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

**$C_6H_{13}N$** (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, $\Delta H$ = 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, $\Delta H$ = 18583.87 J·mol$^{-1}$
**Molecular Weight** 99.1754
**Wiswesser Line Notation** T6MTJ B1
**Evaluation** A

**$C_6H_{13}NO$** (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

**$C_6H_{13}NO_2$** (c) 84GRU/BOU
Leucine (L); 2-Amino-4-methylpentanoic acid (L)
**Phase Changes**
c,II/c,I 352 K, $\Delta H$ = 200 J·mol$^{-1}$
$\Delta S$ = 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) 84GRU/BOU
Norleucine (L); α-Aminocaproic acid (L)
**Phase Changes**
c,II/c,I 389 K, $\Delta H$ = 110 J·mol$^{-1}$
$\Delta S$ = 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/BOU
Norleucine (DL); α-Aminocaproic acid (DL)
**Phase Changes**
c,II/c,I 390 K, $\Delta H$ = 4410 J·mol$^{-1}$
$\Delta S$ = 11.31 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 131.1742
**Wiswesser Line Notation** QVYZ4
**Evaluation** B

**$C_6H_{13}NO_2$** (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

**$C_6H_{14}O_6$** (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) 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
**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

**$C_6H_{14}S$** (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.
$C_p = 221.21 + 3.060\times10^{-2}T + 8.343\times10^{-5}T^2$.
**Molecular Weight** 118.2366
**Wiswesser Line Notation** SH6
**Evaluation** B

**$C_6H_{15}Al$** (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, $\Delta H$ = 10600 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 10600 J·mol$^{-1}$
$\Delta S$ = 47.11 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 114.1660
**Wiswesser Line Notation** 2-AL-2&2
**Evaluation** A

**$C_6H_{15}B$** (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, $\Delta H$ = 11522 J·mol$^{-1}$
$\Delta S$ = 63.94 J·mol$^{-1}$·K$^{-1}$
liq/g 321.81 K
**Molecular Weight** 97.9945
**Wiswesser Line Notation** 2B2&2
**Evaluation** B

**$C_6H_{15}N$** (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

**$C_6H_{15}N_3$** (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

**$C_6H_{16}Si_2$** (c) 75GUS/KAR
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, $\Delta H$ = 10259 J·mol$^{-1}$
$\Delta S$ = 38.58 J·mol$^{-1}$·K$^{-1}$
liq/g 390.93 K, $\Delta H$ = 39480 J·mol$^{-1}$
$\Delta S$ = 91.34 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 144.3634
**Wiswesser Line Notation** T4-SI-TJ A1 A1 $C_1$ 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, $\Delta H$ = 1254 J·mol$^{-1}$
$\Delta S$ = 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) 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) 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

**$C_6H_{17}N_3O_{10}S$·$C_6H_{17}N_3O_{10}Se$** (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
$TGS_{0.10}$– $TGSe_{0.90}$

**$C_6H_{18}N_4$** (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

**$C_6H_{18}N_3OP$** (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

**$C_6H_{18}Si_2$** (liq) 59SUG/SEK
Hexamethyldisilane
**Heat Capacity** 295.67 K, $C_p$ = 255.9 J·mol$^{-1}$·K$^{-1}$
Temperature range 206 to 296 K.
Unsmoothed experimental datum.
**Phase Changes**
c,II/c,I 221.8 K, $\Delta H$ = 9749 J·mol$^{-1}$
$\Delta S$ = 43.93 J·mol$^{-1}$·K$^{-1}$
c,I/liq 287.72 K, $\Delta H$ = 3017 J·mol$^{-1}$
$\Delta S$ = 10.50 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 146.3792
**Wiswesser Line Notation** 1-SI-1&1-SI-1&1&1
**Evaluation** C

**$C_6H_{20}Cl_4MnN_2$** (c) 75BOC/ARR
Tetrachlorobis-(propylammonium) manganese II
**Phase Changes**
c,IV/c,III 323 K, $\Delta H$ = 67.2 J·mol$^{-1}$
$\Delta S$ = 0.22 J·mol$^{-1}$·K$^{-1}$
c,III/c,II 383 K, $\Delta H$ = 14.4 J·mol$^{-1}$
$\Delta S$ = 0.036 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 445 K, $\Delta H$ = 5.3 J·mol$^{-1}$
$\Delta S$ = 0.12 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 316.9874
**Wiswesser Line Notation** 3ZH 2 .MN G4
**Evaluation** A

**$C_6H_{21}N_3Si_3$** (liq) 81MEK/KAR
Hexamethyltrisilazane
**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, $\Delta H$ = 15171 J·mol$^{-1}$
$\Delta S$ = 61.38 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 219.5085
**Wiswesser Line Notation** T6-SI-M-SI-M-SI-MTJ A1 A1 $C_1$ $C_1$ 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.
$C_p = 3.2177\times10^{1} - (1.9668\times10^{-1})T + (4.0732\times10^{-4})T^2 - (2.7686\times10^{-7})T^3$ 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

**$C_7F_{16}$ (liq)** 51OLI/GRI

Perfluoroheptane; Hexadeca-fluoroheptane

**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, | $\Delta H = 6670.6$ J·mol$^{-1}$ |
| | | $\Delta S = 36.97$ J·mol$^{-1}$·K$^{-1}$ |
| c,I/liq | 221.86 K, | $\Delta H = 6947.2$ J mol$^{-1}$ |
| | | $\Delta S = 31.31$ J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 388.0514

**Wiswesser Line Notation** FXFFXFFXFFXFFXFFXF FXFFF

**Evaluation** A

**$C_7F_{16}$ (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

**$C_7H_4CrO_3S$ (c)** 78POM/CHH

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.
$C_p = 71.02 - 4.41\times10^{-1}\,T + 4.61\times10^{-3}T^2 - 5.96\times10^{-6}T^3$ 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, | $\Delta H = 1650$ J·mol$^{-1}$ |
| | | $\Delta S = 8.95$ J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 220.1628

**Wiswesser Line Notation** T5SØJ Ø-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.
$Sp = 116.8 + 2.69\times10^{-1}T + 1.48\times10^{-3}T^2 - 2.08\times10^{-6}T^3$ J·mol$^{-1}$·K$^{-1}$ (125 to 337K).
$C_p$ value calculated from equation.

**Molecular Weight** 267.0628

**Wiswesser Line Notation** T5-SE-ØJ Ø-CR-- CO 3

**Evaluation** C ($C_p$), A (Phase changes)

**$C_7H_4CrO_3Te$ (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.
$C_p = 96.85 + 1.67\times10^{-1}T + 2.44\times10^{-3}T^2 - 3.19\times10^{-6}T^3$ J·mol$^{-1}$·K$^{-1}$ (124 to 326 K).
$C_p$ value calculated from equation.

**Molecular Weight** 315.7028

**Wiswesser Line Notation** T5-TE-ØJ Ø-CR-- CO 3

**Evaluation** C ($C_p$), A (Phase changes)

**$C_7H_4F_3NO_2$ (liq)** 81LEB/RYA

3-Trifluoromethyl nitrobenzene

**Heat Capacity** $C_p = 224.0$ J·mol$^{-1}$·K$^{-1}$
Temperature range 298 to 373 K.
Heat capacity is an average value.
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.
$C_p = 172.3 - 1.16T + 7.86\times10^{-3}T^2 - 1.09\times10^{-5}T^3$ 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, | $\Delta H = 702$ J·mol$^{-1}$ |
| | | $\Delta S = 3.55$ J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 205.0515

**Wiswesser Line Notation** T5NØJ Ø-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, | $\Delta H = 1910$ J·mol$^{-1}$ |
| | | $\Delta S = 6.3$ J·mol$^{-1}$·K$^{-1}$ |
| c,I/liq | 315.5 K, | $\Delta H = 13010$ J·mol$^{-1}$ |
| | | $\Delta S = 41$ J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 205.0515

**Wiswesser Line Notation** T5NØJ Ø-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

**$C_7H_5Cl_3$** (liq) 87GOA/BOE
Benzotrichloride; α,α,α-Trichlorotoluene
**Phase Changes**
c,I/liq 235.99 K, $\Delta H$ = 13950 J·mol$^{-1}$
$\Delta S$ = 59.11 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 108.1396
**Wiswesser Line Notation** GXGGR
**Evaluation** A

**$C_7H_5F_3O_2$** (liq) 62GOO/LAC
3-Trifluoromethylbenzoic acid; *m*-Trifluorotoluic acid
**Heat Capacity** 298.15 K, $C_p$ = 223.6 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 178.1105
**Wiswesser Line Notation** QV1R CXGGG
**Evaluation** B

**$C_7H_5N$** (liq) 83BYK/LEB
Benzonitrile
**Heat Capacity** 298.15 K, $C_p$ = 165.2 J·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 330 K.
**Entropy** 298.15 K, $S$ = 209.1 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 260.33 K, $\Delta H$ = 10980 J·mol$^{-1}$
$\Delta S$ = 42.16 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 103.1232
**Wiswesser Line Notation** NCR
**Evaluation** A

**$C_7H_5N$** (liq) 84BYK/KIP
Benzonitrile
**Heat Capacity** 298.15 K, $C_p$ = 165.2 J·mol$^{-1}$·K$^{-1}$
Temperature range 14 to 330 K.
**Phase Changes**
c,I/liq 260.33 K, $\Delta H$ = 10980 J·mol$^{-1}$
$\Delta S$ = 42.16 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 103.1232
**Wiswesser Line Notation** NCR
**Evaluation** A

**$C_7H_5N$** (liq) 84LEB/BYK2
Benzonitrile
**Heat Capacity** 298.15 K, $C_p$ = 165.2 J·mol$^{-1}$·K$^{-1}$
Temperature range 25 to 330 K.
**Entropy** 298.15 K, $S$ = 209.1 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 260.332 K, $\Delta H$ = 10980 J·mol$^{-1}$
$\Delta S$ = 42.16 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 103.1232
**Wiswesser Line Notation** NCR
**Evaluation** A

**$C_7H_5N$** (liq) 85LEB/BYK
Benzonitrile
**Heat Capacity** 298.15 K, $C_p$ = 165.2 J·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 330 K.
**Entropy** 298.15 K, $S$ = 209.1 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 260.33 K, $\Delta H$ = 10980 J·mol$^{-1}$
$\Delta S$ = 42.16 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 103.1232
**Wiswesser Line Notation** NCR
**Evaluation** A

**$C_7H_6NO_2$** (c) 72BOO/HAU
4-Nitrobenzoic acid
**Phase Changes**
c/liq 512.35 K, $\Delta H$ = 36900 J·mol$^{-1}$
$\Delta S$ = 72.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 167.1208
**Wiswesser Line Notation** WNR DVQ
**Evaluation** C

**$C_7H_6N_2$** (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

**$C_7H_6O_2$** (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) 75TAT/MAT
Benzoic acid
**Heat Capacity** 299.62 K, $C_p$ = 147.07 J·mol$^{-1}$·K$^{-1}$
Temperature range 12 to 304 K
**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·mol$^{-1}$·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·mol$^{-1}$
$\Delta S = 261.0$ J·mol$^{-1}$·K$^{-1}$
c/g 298.15 K, $\Delta H = 89230$ J·mol$^{-1}$.
$\Delta S = 299.3$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 122.1232
**Wiswesser Line Notation** QVR
**Evaluation** A

**$C_7H_6O_3$** (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.
Heat capacity is an average value.
**Molecular Weight** 138.1226
**Wiswesser Line Notation** VHR CQ DQ
**Evaluation** B

**$C_7H_7F$** (liq) 62GOO/LAC
4-Fluorotoluene
**Heat Capacity** 298.15 K, $C_p = 172.3$ J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 110.1307
**Wiswesser Line Notation** FR D1
**Evaluation** B

**$C_7H_7NO_3$** (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, $\Delta H = 97200$ J·mol$^{-1}$
$\Delta S = 326.0$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 137.1990
**Wiswesser Line Notation** ZYR&US
**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.
$C_p = 187.43814 - 0.73026493T + 0.0029613602T^2 - 2.8661704\times10^{-6}T^3$ 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) 76FOR/BEN2
Toluene
**Heat Capacity** 298.15 K, $C_p = 157.026$ J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 92.1402
**Wiswesser Line Notation** 1R
**Evaluation** A
Data from 76FOR/BEN.

**$C_7H_8$** (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) 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) 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) 78STE
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

**$C_7H_8N_2O$** (c) 87FER/DEL
Phenylurea; Monophenylurea
**Phase Changes**
c/liq 420.6 K, $\Delta H = 23680$ J·mol$^{-1}$
$\Delta S = 56.3$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 136.1530
**Wiswesser Line Notation** ZVMR
**Evaluation** A

**$C_7H_8O$** (liq) 1889EYK
Anisole; Methyl phenyl ether; Methoxybenzene
**Phase Changes**
c/liq 293.2 K, $\Delta H$ = 17029 J·mol$^{-1}$
$\Delta S$ = 58.1 J·mol$^{-1}$·K$^{-1}$
**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,I/liq 268.73 K, $\Delta H$ = 12890 J·mol$^{-1}$
$\Delta S$ = 48.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 108.1396
**Wiswesser Line Notation** 1OR
**Evaluation** A

**$C_7H_8O$** (c) 82POE/FAN
2-Methylphenol; *o*-Hydroxytoluene; *o*-Cresol
**Phase Changes**
c/liq 303.0 K, $\Delta H$ = 13938 J·mol$^{-1}$
$\Delta S$ = 46.00 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 108.1396
**Wiswesser Line Notation** QR B1
**Evaluation** A

**$C_7H_8O$** (liq) 82POE/FAN
3-Methylphenol; *m*-Hydroxytoluene; *m*-Cresol
**Phase Changes**
c/liq 285.0 K, $\Delta H$ = 9413 J·mol$^{-1}$
$\Delta S$ = 33.03 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 108.1396
**Wiswesser Line Notation** QR C1
**Evaluation** A

**$C_7H_8O$** (c) 1889EYK
4-Methylphenol; *p*-Hydroxytoluene; *p*-Cresol
**Phase Changes**
c/liq 309 K, $\Delta H$ = 12247 J·mol$^{-1}$
$\Delta S$ = 39.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 108.1396
**Wiswesser Line Notation** QR D1
**Evaluation** C

**$C_7H_8O$** (c) 82POE/FAN
4-Methylphenol; *p*-Hydroxytoluene; *p*-Cresol
**Phase Changes**
c/liq 309.0 K, $\Delta H$ = 11887 J·mol$^{-1}$
$\Delta S$ = 38.47 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 108.1396
**Wiswesser Line Notation** QR D1
**Evaluation** A

**$C_7H_9N$** (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) 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 $C_1$ D1
**Evaluation** B
Specific heat anomaly with peak at 293.5 K,
$\Delta H$ = 65.6 J·mol$^{-1}$,
$\Delta S$ = 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

**$C_7H_9N$** (c) 1889EYK
4-Methylaniline; *p*-Toluidine
**Phase Changes**
c/liq 315.6 K, $\Delta H$ = 17280 J·mol$^{-1}$
**Molecular Weight** 107.1548
**Wiswesser Line Notation** ZR D1
**Evaluation** C

**$C_7H_8O_2 \cdot H_2O$** (c) 82VII/GAM
Orcinol monohydrate; 3,5-Dihydroxytoluene monohydrate
**Phase Changes**
c/liq 328.0 K, $\Delta H$ = 26360 J·mol$^{-1}$
$\Delta S$ = 80.4 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 142.1542
**Wiswesser Line Notation** QR CQ E1 &QH
**Evaluation** B

**$C_7H_9NO$** (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

**$C_6H_7N \cdot CH_2O$** (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.

**$C_7H_{10}$** (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

**$C_7H_{10}$** (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

**$C_7H_{10}N_2O$** (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, $\Delta H$ = 15800 J·mol$^{-1}$
$\Delta S$ = 42.4 J·mol$^{-1}$·K$^{-1}$
c,I/liq 411.4 K, $\Delta H$ = 2600 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 21200 J·mol$^{-1}$
$\Delta S$ = 55.1 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 154.1682
**Wiswesser Line Notation** T6NVNVJ A1 C1 F1
**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) 88LEB/KUL
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) 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, $\Delta H$ = 7070 J·mol$^{-1}$; $\Delta S$ = 45.8 J·mol$^{-1}$·K$^{-1}$

c,II/c,I 208.26 K $\Delta H$ = 730 J·mol$^{-1}$; $\Delta S$ = 3.5 J·mol$^{-1}$·K$^{-1}$

c,I/liq 217.75 K $\Delta H$ = 820 J·mol$^{-1}$; $\Delta S$ = 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, $\Delta H$ = 7800 J·mol$^{-1}$; $\Delta S$ = 29.8 J·mol$^{-1}$·K$^{-1}$

100% crystallinity.

**Molecular Weight** 96.1718

**Wiswesser Line Notation** /*1Y1&2U2*/

**Evaluation** A

$T$(glass) = 198 K.

**$C_7H_{12}O_2$** (liq) 85KAR/ABD2

Butyl acrylate

**Phase Changes**

c/liq 209.5 K, $\Delta H$ = 17307 J·mol$^{-1}$; $\Delta S$ = 82.61 J·mol$^{-1}$·K$^{-1}$

**Molecular Weight** 128.1706

**Wiswesser Line Notation** 4OV1U1

**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, $\Delta H$ = 5840 J·mol$^{-1}$; $\Delta S$ = 18.52 J·mol$^{-1}$·K$^{-1}$

**Molecular Weight** 136.1195

**Wiswesser Line Notation** OV6 .LI

**Evaluation** A

**$C_7H_{13}NO$** (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, $\Delta H$ = 13775 J·mol$^{-1}$; $\Delta S$ = 44.4 J·mol$^{-1}$·K$^{-1}$

**Molecular Weight** 127.1835

**Wiswesser Line Notation** T8MVTJ

**Evaluation** B

**$C_7H_{13}O_2Tl$** (c) 76MEI/SEY

Thallium heptanoate

**Phase Changes**

c,II/c,I 299 K, $\Delta H$ = 2761 J·mol$^{-1}$; $\Delta S$ = 9.20 J·mol$^{-1}$·K$^{-1}$

c,I/liq 419 K, $\Delta H$ = 6276 J·mol$^{-1}$; $\Delta S$ = 15.1 J·mol$^{-1}$·K$^{-1}$

Solid-mesophase.

liq/liq 501 K, $\Delta H$ = 3138 J·mol$^{-1}$; $\Delta S$ = 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/LOP

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, $\Delta H$ = 2652 J·mol$^{-1}$; $\Delta S$ = 8.81 J·mol$^{-1}$·K$^{-1}$

c,I/liq 420.7 K, $\Delta H$ = 6302 J·mol$^{-1}$; $\Delta S$ = 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:

502.0 K; $\Delta H$ = 3301 J·mol$^{-1}$; $\Delta S$ = 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, $\Delta H$ = 1966 J·mol$^{-1}$; $\Delta S$ = 7.44 J·mol$^{-1}$·K$^{-1}$

c,V/c,IV 267.8 K, $\Delta H$ = 1167 J·mol$^{-1}$; $\Delta S$ = 4.36 J·mol$^{-1}$·K$^{-1}$

c,IV/c,III 271.7 K, $\Delta H$ = 1176 J·mol$^{-1}$; $\Delta S$ = 4.32 J·mol$^{-1}$·K$^{-1}$

c,III/c,II 296.2 K, $\Delta H$ = 2956 J·mol$^{-1}$; $\Delta S$ = 10.02 J·mol$^{-1}$·K$^{-1}$

c,II/c,I 300.9 K, $\Delta H$ = 2546 J·mol$^{-1}$; $\Delta S$ = 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, | $\Delta H$ = 1413 J·mol$^{-1}$ |
| | | $\Delta S$ = 5.24 J·mol$^{-1}$·K$^{-1}$ |
| c,III'/c,II | 271.8 K, | $\Delta H$ = 1413 J·mol$^{-1}$ |
| | | $\Delta S$ = 5.15 J·mol$^{-1}$·K$^{-1}$ |
| c,V/c,IV | 262.3 K, | $\Delta H$ = 2087 J·mol$^{-1}$ |
| | | $\Delta S$ = 7.98 J·mol$^{-1}$·K$^{-1}$ |
| c,IV/c,III | 267.9 K, | $\Delta H$ = 1214 J·mol$^{-1}$ |
| | | $\Delta S$ = 4.49 J·mol$^{-1}$·K$^{-1}$ |
| c,III/c,II | 272.4 K, | $\Delta H$ = 1588 J·mol$^{-1}$ |
| | | $\Delta S$ = 5.82 J·mol$^{-1}$·K$^{-1}$ |
| c,II/c,I | 300.96 K, | $\Delta H$ = 3009 J·mol$^{-1}$ |
| | | $\Delta S$ = 9.18 J·mol$^{-1}$·K$^{-1}$ |
| c,I/liq | 420.7 K, | $\Delta H$ = 6302 J·mol$^{-1}$ |
| | | $\Delta S$ = 15.0 J·mol$^{-1}$·K$^{-1}$ |
| c,I/mesophase. | | |
| c/liq | 502.0 K, | $\Delta H$ = 3301 J·mol$^{-1}$ |
| | | $\Delta S$ = 6.57 J·mol$^{-1}$·K$^{-1}$ |

Mesophase/isotropic liquid.
**Molecular Weight** 333.5485
**Wiswesser Line Notation** OV6 .TL
**Evaluation** A

**$C_7H_{14}$** (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 − 0.0054107773$T$ + 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) 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

**$C_7H_{14}O$** (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** VH1YY
**Evaluation** A

**$C_7H_{14}O$** (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 $S$ = 335.4 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq $\Delta H$ = 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

**$C_7H_{14}O_3$** (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 − 0.001197$T^2$ J·mol$^{-1}$·K$^{-1}$.
**Molecular Weight** 146.1858
**Wiswesser Line Notation** Q2OVX1&1&1
**Evaluation** C

**$C_7H_{16}$** (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, | $\Delta H$ = 793.7 J·mol$^{-1}$ |
| | | $\Delta S$ = 5.98 J·mol$^{-1}$·K$^{-1}$ |
| c,II/liq | 138.20 K, | $\Delta H$ = 7642.5 J·mol$^{-1}$ |
| | | $\Delta S$ = 55.30 J·mol$^{-1}$·K$^{-1}$ |
| c,I/liq | 138.75 K, | $\Delta H$ = 6846.3 J·mol$^{-1}$ |
| | | $\Delta S$ = 49.34 J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 100.2034
**Wiswesser Line Notation** 2X2&1&1
**Evaluation** A

**$C_7H_{16}$** (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) 37VOL
*n*-Heptane
**Heat Capacity** 298 K, $C_p$ = 223.0 J·mol$^{-1}$·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) 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 − 0.14490$T$ + 5.7813×10$^{-4}T^2$ − 4.1667×10$^{-7}T^3$ cal·mol$^{-1}$·K$^{-1}$.
**Phase Changes**
c/liq 182.55 K, $\Delta H$ = 14037 J·mol$^{-1}$
$\Delta S$ = 76.89 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 100.2034
**Wiswesser Line Notation** 7H
**Evaluation** A

**$C_7H_{16}$** (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 − 9.9628490$T$ + 0.054561085$T^2$ − 0.00013079634$T^3$ + 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) 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) 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) 82ZAR
*n*-Heptane
**Heat Capacity** 298 K, $C_p$ = 224.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 100.2034
Temperature range 298, 323, 363 K.
**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) 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) 84ZEG/SOM
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) 89VES/BAR
1-Heptanol
**Heat Capacity** 298.15 K $C_p$ = 270.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 116.2028
**Wiswesser Line Notation** Q7
**Evaluation** A

**$C_7H_{17}NSi$** (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, $\Delta H$ = 10623 J·mol$^{-1}$
$\Delta S$ = 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) 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, $\Delta H$ = 11113 J·mol$^{-1}$
$\Delta S$ = 78.99 J·mol$^{-1}$·K$^{-1}$
liq/g 460.58 K, $\Delta H$ = 40250 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 11113 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 10800 J·mol$^{-1}$
$\Delta S$ = 44.3 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 112.2144
**Wiswesser Line Notation** 1U1*R* &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

**$(C_8H_3D_5)_n$** (gls) 83LEB/SMI
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

**$C_8H_4Cl_2O_2$** (c) 79KAR/SAP
Terephthaloyl chloride
**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** 203.0244
**Wiswesser Line Notation** GVR DVG
**Evaluation** A

**$C_8H_4N_2$** (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, $\Delta H$ = 20000 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 20000 J·mol$^{-1}$
$\Delta S$ = 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

**$C_8H_4O_3$** (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

**$C_8H_5MnO_3$** (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 to 135 K, $\Delta S$ = <1 J·mol$^{-1}$·K$^{-1}$
"Abnormally" high heat capacity.
c/liq 350 K, $\Delta H$ = 19300 J·mol$^{-1}$
$\Delta S$ = 55 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 204.0637
**Wiswesser Line Notation** L5ØJ Ø-MN- -CO 3
**Evaluation** A

**$C_8H_6$** (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, $\Delta H$ = 9460 J·mol$^{-1}$
$\Delta S$ = 41.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 102.1354
**Wiswesser Line Notation** 1UU1R
**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

**$C_8H_7ClN_2O_2$** (c) 82CUE/SOL
2-Chloroisonitrosoacetanilide
**Phase Changes**
c/liq 429 K, $\Delta H$ = 29700 J·mol$^{-1}$
$\Delta S$ = 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

**$C_8H_8$** (liq) 43GUT/WES
Styrene
**Entropy** 298.15 K, $S$ = 237.6 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 242.47 K, $\Delta H$ = 10950 J·mol$^{-1}$
$\Delta S$ = 45.16 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, $\Delta H$ = 10950 J·mol$^{-1}$
$\Delta S$ = 45.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 104.1512
**Wiswesser Line Notation** 1U1R
**Evaluation** B

**$(C_8H_8)_n$** (gls) 83LEB/SMI
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*/

**$C_8H_8N_2O_2$** 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

**$C_8H_8O$** (liq) 86CHI/NGU
4,5-Dihydro-2,3-benzofuran
**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

**$C_8H_9NO$** (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

**$C_8H_9NO_3$** (c) 81LEB/RYA
*p*-Nitrophenetole; *p*-Nitroethoxybenzene
**Heat Capacity** $C_p$ = 246.2 J·mol$^{-1}$·K$^{-1}$
Temperature range 298 to 328 K.
Data given over temperature range.
**Molecular Weight** 167.1640
**Wiswesser Line Notation** WNR DO2
**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, $\Delta H$ = 17117.46 J·mol$^{-1}$
$\Delta S$ = 59.77 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 106.1670
**Wiswesser Line Notation** 1R D1
**Evaluation** A

**$C_8H_{10}N_4O_2$** (c) 80CES/STA
Caffeine
**Heat Capacity** 298 K, $C_p$ = 173.2 J·mol$^{-1}$·K$^{-1}$
Temperature range 300 to 392 K.
Unsmoothed experimental data and equation given.
$C_p$ = 41.4 + 0.104(T-298) cal·mol$^{-1}$·K$^{-1}$.
Data given at 298 *K* is an extrapolation by the author.
**Phase Changes**
c,II/c,I 426 K, $\Delta H$ = 940 J·mol$^{-1}$
$\Delta S$ = 2.2 J·mol$^{-1}$·K$^{-1}$
$\alpha$ to $\beta$ form.
c,I/liq 512 K, $\Delta H$ = 5600 J·mol$^{-1}$
$\Delta S$ = 10.9 J·mol$^{-1}$·K$^{-1}$
$\beta$ to liquid.
**Molecular Weight** 194.1926
**Wiswesser Line Notation** T56 BN DN FNVNVJ B1 F1 H1
**Evaluation** B
Data given for $\beta$ form. $\beta$ form is obtained by high temperature sublimation.

**$C_8H_{10}O$** (liq) 75FEN/HAR
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

**$C_8H_{10}O$** (c) 82POE/FAN
2,3-Dimethylphenol
**Phase Changes**
c/liq 346.0 K, $\Delta H$ = 21024 J·mol$^{-1}$
$\Delta S$ = 60.76 J·mol$^{-1}$·K$^{-1}$
**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·mol$^{-1}$
$\Delta S$ = 67.17 J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S$ = 59.26 J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S$ = 54.27 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 122.1664
**Wiswesser Line Notation** QR C1 D1
**Evaluation** A

**$C_8H_{10}O$** (c) 82POE/FAN
3,5-Dimethylphenol
**Phase Changes**
c/liq 336.8 K, $\Delta H$ = 17997 J·mol$^{-1}$
$\Delta S$ = 53.38 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 122.1664
**Wiswesser Line Notation** QR C1 E1
**Evaluation** A

**$C_8H_{10}O_3$** (c) 83GEI/NUR
*cis*-Cyclohexane-1,2-dicarboxylic anhydride
**Heat Capacity** 298.15 K, $C_p$ = 207.4 J·mol$^{-1}$·K$^{-1}$
Temperature range 12 to 330 K.
**Entropy** 298.15 K, $S$ = 202.4 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,III/c,II 304 K, $\Delta H$ = 5594 J·mol$^{-1}$
$\Delta S$ = 18.41 J·mol$^{-1}$·K$^{-1}$
Conformational transition.
c,II/c,I 310.5 K, $\Delta H$ = 845 J·mol$^{-1}$
$\Delta S$ = 2.72 J·mol$^{-1}$·K$^{-1}$
Conformational transition.
**Molecular Weight** 154.1652
**Wiswesser Line Notation** T56 BVOVTJ—C
**Evaluation** A

**$C_8H_{11}N$** (liq) 86STE/CHI
2,6-Dimethylaniline
**Heat Capacity** 298.15 K, $C_p$ = 238.86 J·mol$^{-1}$·K$^{-1}$
Temperature range 10 to 450 K.
**Entropy** 298.15 K, $S$ = 251.35 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 284.598 K
**Molecular Weight** 121.1816
**Wiswesser Line Notation** ZR B1 F1
**Evaluation** A

**$C_8H_{12}$** (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, $\Delta H$ = -393 J·mol$^{-1}$
c,I/liq 203.983 K, $\Delta H$ = 9828 J·mol$^{-1}$
$\Delta S$ = 48.24 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 108.1828
**Wiswesser Line Notation** L8 AU EUTJ
**Evaluation** A

**$C_8H_{12}N_2O_2$** (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, $\Delta H$ = 18640 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 18640 J·mol$^{-1}$
$\Delta S$ = 90.46 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 168.1950
**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.

**$C_8H_{12}N_4$** (c) 81LEB/RYA
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/GUT
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
$\Delta H$ sublimation = 76600 J·mol$^{-1}$;
temperature range: 288 to 313 K.

**$C_8H_{14}$** (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, $\Delta H$ = 635 J·mol$^{-1}$
$\Delta S$ = 3.34 J·mol$^{-1}$·K$^{-1}$
c,I/liq 259.15 K, $\Delta H$ = 1813 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 6336 J·mol$^{-1}$
$\Delta S$ = 35.2 J·mol$^{-1}$·K$^{-1}$
Glass transition.
c,I/liq 308 K, $\Delta H$ = 16760 J·mol$^{-1}$
$\Delta S$ = 54.4 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 110.1986
**Wiswesser Line Notation** /L8TJ A* B*/
**Evaluation** A

**$C_8H_{14}O$** (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

**$C_8H_{14}O_2$** (liq) 85KAR/ABD
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/ABD2
Butyl methacrylate
**Phase Changes**
c/liq 196.8 K, $\Delta H$ = 13947 J·mol$^{-1}$
$\Delta S$ = 70.87 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 142.1974
**Wiswesser Line Notation** 40VY1&U1
**Evaluation** A

**$C_8H_{14}O_4$** (liq) 86NIL/WAD
Ethyleneglycol dipropanoate
**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

**$C_8H_{15}NO_2$** (liq) 85KAR/ABD2
Dimethylaminoethyl methacrylate
**Phase Changes**
c/liq 237.7 K, $\Delta H = 16852$ J·mol$^{-1}$
$\Delta S = 70.90$ 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, $\Delta H = 2720$ J·mol$^{-1}$
$\Delta S = 5.44$ J·mol$^{-1}$·K$^{-1}$
Mesophase-isotropic.
c,I/liq 403 K, $\Delta H = 4686$ J·mol$^{-1}$
$\Delta S = 11.7$ J·mol$^{-1}$·K$^{-1}$
Solid-mesophase.
**Molecular Weight** 347.5753
**Wiswesser Line Notation** OV7 .TL
**Evaluation** B

**$C_8H_{16}$** (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

**$C_8H_{16}O$** (liq) 80DYA/VAS
Octanal; Caprylaldehyde
**Heat Capacity**
Temperature range 50 to 350 K.
**Phase Changes**
c,I/liq 247.72 K, $\Delta H = 25860$ J·mol$^{-1}$
$\Delta S = 104.4$ J·mol$^{-1}$·K$^{-1}$
98.01 mol% purity.
**Molecular Weight** 128.2138
**Wiswesser Line Notation** VH7
**Evaluation** B
Manuscript deposited in Cent. Sci. Res. Inst. Tech. Eng. Petrochemicals, July 27, 1979.

**$C_8H_{16}O$** (liq) 82DYA/VAS
Octanal; Caprylaldehyde
**Entropy** 298.15 K, $S = 365.4$ J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq $\Delta H = 26130$ J·mol$^{-1}$
**Molecular Weight** 128.2138
**Wiswesser Line Notation** VH7
**Evaluation** B

**$C_8H_{16}O$** (liq) 84VAS/PET
Octanal; Caprylaldehyde
**Heat Capacity** 298.15 K, $C_p = 259.58$ J·mol$^{-1}$·K$^{-1}$
Temperature range 10 to 350 K.
**Entropy** 298.15 K, $S = 365.45$ J·mol$^{-1}$·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/SHU
Isoamyl propionate
**Heat Capacity** 298.15 K, $C_p = 285.2$ 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** 2VO2Y
**Evaluation** C

**$C_8H_{16}O_2$** (liq) 84VAS/PET
Butyl butanoate
**Heat Capacity** 300 K, $C_p = 281.9$ J·mol$^{-1}$·K$^{-1}$
Temperature range 180 to 370 K.
**Phase Changes**
c/liq 181.68 K, $\Delta H = 14930$ J·mol$^{-1}$
$\Delta S = 82.2$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 144.2132
**Wiswesser Line Notation** 4OV3
**Evaluation** A

**$C_8H_{16}O_2$** (liq) 83GUS/KLI
Amyl propionate; Pentyl propionate
**Heat Capacity** 277.11 K, $C_p = 239.5$ J·mol$^{-1}$·K$^{-1}$
Temperature range 200 to 360 K.
Unsmoothed experimental datum.
$C_p$ given as 1.661 J·g$^{-1}$·K$^{-1}$.
**Molecular Weight** 144.2132
**Wiswesser Line Notation** 50V2
**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, $\Delta H = 19830$ J·mol$^{-1}$
$\Delta S = 93.5$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 144.2132
**Wiswesser Line Notation** 6OV1
**Evaluation** A

**$C_8H_{16}S$** (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.
$C_p = 282.50 + 3.340\times10^{-2}T + 8.582\times10^{-5}T2$.
**Molecular Weight** 144.2744
**Wiswesser Line Notation** SH8
**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

**$C_8H_{18}$** (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) 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) 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) 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) 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) 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) 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

**$C_8H_{18}N_2$** (c) 80BYS
1,1-Dimethylazoethane
**Phase Changes**

| | | |
|---|---|---|
| c,II/c,I | 242.6 *K* | $\Delta H$ = 4890 J·mol$^{-1}$ |
| | | $\Delta S$ = 20.2 J·mol$^{-1}$·K$^{-1}$ |
| c,I//liq | 258.6 *K* | $\Delta H$ = 10280 J·mol$^{-1}$ |
| | | $\Delta S$ = 39.7 J·mol$^{-1}$·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·mol$^{-1}$ |
| | | $\Delta S$ = 31.1 J·mol$^{-1}$·K$^{-1}$ |
| c,I//liq | 288.4 *K* | $\Delta H$ = 11520 J·mol$^{-1}$ |
| | | $\Delta S$ = 39.9 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 293 to 311 K.
**Phase Changes**
c/liq 405 K, $\Delta H$ = 25900 J·mol$^{-1}$
$\Delta S$ = 64.0 J·mol$^{-1}$·K$^{-1}$
liq/g 551 K
**Molecular Weight** 174.2424
**Wiswesser Line Notation** T6N DNTJ A2Q D2Q
**Evaluation** B
$\Delta H$ sublimation = 104100 J·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·mol$^{-1}$·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·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 13 to 350 K.
**Entropy** 298.15 K, $S$ = 347.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 130.2296
**Wiswesser Line Notation** Q1Y4&2
**Evaluation** A

**$C_8H_{18}O$** (liq) 78RYB/EME
Isooctyl alcohol; 2-Methyl-1-heptanol
**Heat Capacity** 303.15 K, $C_p$ = 327.8 J·mol$^{-1}$·K$^{-1}$
Temperature range 293.15 to 353.15 K.
$C_p$ given as 2517 J·kg$^{-1}$·K$^{-1}$.
**Molecular Weight** 130.2296
**Wiswesser Line Notation** Q1Y5&1
**Evaluation** C

**$C_8H_{18}O$** (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) 89VES/BAR
1-Octanol; *n*-Octyl alcohol; Capryl alcohol
**Heat Capacity** 298.15 K $C_p$ = 304.0 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 130.2296
**Wiswesser Line Notation** Q8
**Evaluation** A

**$C_8H_{18}O_3$** (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

**$C_8H_{18}O_5$** (liq) 82ZAR
Tetraethylene glycol
**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

**$C_8H_{19}N$** (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

**$(C_8H_{19}NSi)_n$** (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.

**$C_8H_{19}NSi$** (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, $\Delta H$ = 12900 J·mol$^{-1}$
$\Delta S$ = 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.

**$C_8H_{19}Cl_2NSiZn$** (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.

**$C_8H_{20}Br_4FeN$** (c) 88NAV/PUE
Tetraethylammonium tetrabromo ferrate
**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, $\Delta H$ = 2428 J·mol$^{-1}$
$\Delta S$ = 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 tetrachloro ferrate
**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,IIII 234.7 K, $\Delta H$ = 2203 J·mol$^{-1}$
$\Delta S$ = 8.06 J·mol$^{-1}$·K$^{-1}$
First order transition.
c,III/c,II 217.5 K
c,II/c,I 226.6 K, $\Delta H$ = 2295 J·mol$^{-1}$
$\Delta S$ = 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
**Phase Changes**
c/liq 180.47 K, $\Delta H$ = 12406 J·mol$^{-1}$
$\Delta S$ = 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) 85RAB/SHE
Tetraethyl germane
**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, $\Delta H$ = 12312 J·mol$^{-1}$
$\Delta S$ = 68.00 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 188.8360
**Wiswesser Line Notation** 2-GE-2&2&2
**Evaluation** A

**$C_8H_{20}N_4$** (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

**$C_8H_{20}Pb$** (liq) 54STA/WAR
Tetraethyl lead
**Phase Changes**
c/liq 142.94 K, $\Delta H$ = 8791 J·mol$^{-1}$
$\Delta S$ = 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) 89RAB/NIS2
Tetraethyllead
**Heat Capacity** 298.15 K, $C_p$ = 307.4 J·mol$^{-1}$·K$^{-1}$
Temperature Range 5–315 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 $\Delta H$ = 9110 J·mol$^{-1}$
$\Delta S$ = 64.43 J·mol$^{-1}$·K$^{-1}$
c,I/liq 139.41 K $\Delta H$ = 9091 J·mol$^{-1}$
$\Delta S$ = 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
**Phase Changes**
c/liq 189.36 K, $\Delta H$ = 13012 J·mol$^{-1}$
$\Delta S$ = 68.70 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 144.3315
**Wiswesser Line Notation** 2-SI-2&2&2
**Evaluation** B

**$C_8H_{20}Sn$** (liq) 54STA/WAR
Tetraethyl tin
**Phase Changes**
c/liq 142.14 K, $\Delta H$ = 9146 J·mol$^{-1}$
$\Delta S$ = 64.35 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 234.9360
**Wiswesser Line Notation** 2-SN-2&2&2
**Evaluation** B

**$C_8H_{24}Ag_{13}I_{15}N_2$** (c) 85LIN/ARM
Bis-(tetramethylammonium iodide) tridecasilver iodide
**Heat Capacity** 282.93 K, $C_p$ = 1076 J·mol$^{-1}$·K$^{-1}$
Temperature range 79 to 283 K.
Unsmoothed experimental datum.
**Phase Changes**
c,II/c,I 150 K, $\Delta S$ = 5.34 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 3454.1425
**Wiswesser Line Notation** 1K1&1&1&1 2 .AG I 13
**Evaluation** A

**$C_8H_{24}Cl_4FeN_2$** (c) 88RUI/LOP
Tetramethylammonium tetrachloroferrate
**Heat Capacity** 300 K, $C_p$ = 424 J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S$ = 3.68 J·mol$^{-1}$·K$^{-1}$
c,III/c,II 266.8 K, $\Delta H$ = 238.5 J·mol$^{-1}$
$\Delta S$ = 0.90 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 281.0 K, $\Delta H$ = 2179.9 J·mol$^{-1}$
$\Delta S$ = 8.34 J·mol$^{-1}$·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) manganese II
**Phase Changes**
c,II/c,I 371 K, $\Delta H$ = 2.4 J·mol$^{-1}$
$\Delta S$ = 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
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, $\Delta H$ = 308 J·mol$^{-1}$
$\Delta S$ = 1.75 J·mol$^{-1}$·K$^{-1}$
c,IV/c,III 268.65 K, $\Delta H$ = 233 J·mol$^{-1}$
$\Delta S$ = 0.83 J·mol$^{-1}$·K$^{-1}$
c,III/c,II 292.3 K, $\Delta H$ = 5.8 J·mol$^{-1}$
$\Delta S$ = 0.02 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 292.6 K, $\Delta H$ = 2079 J·mol$^{-1}$
$\Delta S$ = 7.98 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 345.0410
**Wiswesser Line Notation** 1K1&1&1 2 .MN G4
**Evaluation** A

**$C_8H_{23}N_5$** (liq) 88BOB/KAM
Tetraethylenepentamine
**Heat Capacity** 333 K, $C_p$ = 460 J·mol$^{-1}$K$^{-1}$
Temperature Range 333 to 513 K.
**Molecular Weight** 189.3032
**Wiswesser Line Notation** Z2M2M2M2Z
**Evaluation** D

**$C_8H_{24}Si_4O_4$** (liq) 81MEK/KAR
Octamethyltetrasiloxane
**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, $\Delta H$ = 23765 J·mol$^{-1}$
$\Delta S$ = 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

**$C_8H_{28}Ni_4Si$** (c) 81MEK/KAR
Octamethyltetrasilazane
**Heat Capacity** 298.15 K, $C_p$ = 569.9 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, $\Delta H$ = 25050 J·mol$^{-1}$
$\Delta S$ = 66.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 387.1947
**Wiswesser Line Notation** T8-SI-M-SI-M-SI-M-SI-
MTJ A1 A1 C1 C1 E1 E1 G1 G1

**$C_9H_6CrO_3$** (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.
$C_p = 38.17 + 2.37\times10^{-1}T + 3.77\times10^{-4}T^2 + 3.38\times10^{-7}T^3$ J·mol$^{-1}$·K$^{-1}$ (120 to 300 K).
$C_p$ value calculated from equation.
**Molecular Weight** 214.1406
**Wiswesser Line Notation** L6ØJ Ø-CR-- CO 3
**Evaluation** C ($C_p$), A (Phase changes)

**$C_9H_7Cu$** (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-1UU1R
**Evaluation** A

**$C_9H_7N$** (liq) 86STE/CHI
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 238.369 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·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 500 K.
**Entropy** 298.15 K, $S$ = 219.72 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 220.000 K, $\Delta H$ = 68.18 J·mol$^{-1}$
$\Delta S$ = 0.310 J·mol$^{-1}$·K$^{-1}$
c,I/liq 258.369 K, $\Delta H$ = 10662.90 J·mol$^{-1}$
$\Delta S$ = 41.27 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 129.1610
**Wiswesser Line Notation** T66 BNJ
**Evaluation** A

**$C_9H_7N$** (liq) 88STE/ARC
Isoquinoline
**Heat Capacity** 298.15 K, $C_p$ = 196.16 J·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 500 K. Values calculated from graphically extrapolated heat capacity values.
**Entropy** 298.15 K, $S$ = 215.98 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,III/c,II 221.000 K, $\Delta H$ = 0.00 J·mol$^{-1}$
c,II/c,I 275.000 K, $\Delta H$ = 0.00 J·mol$^{-1}$
c,I/liq 299.620 K, $\Delta H$ = 13544.17 J·mol$^{-1}$
$\Delta S$ = 45.20 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 10 to 400 K.
**Entropy** 298.15 K, $S$ = 171.06 J·mol$^{-1}$·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·mol$^{-1}$·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

**$C_9H_7O$** (liq) 86CHI/NGU
Chroman
**Heat Capacity** 298.15 K, $C_p$ = 214.00 J·mol$^{-1}$·K$^{-1}$
Temperature range 10 to 450 K.
**Entropy** 298.15 K, $S$ = 246.03 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 269.836 K
**Molecular Weight** 131.1537
**Wiswesser Line Notation** T66 BOJ

**Evaluation** A

**$C_9H_7O$** (liq) 86CHI/NGU
Isochroman
**Heat Capacity** 298.15 K, $C_p$ = 217.81 J·mol$^{-1}$·K$^{-1}$
Temperature range 10 to 450 K.
**Entropy** 298.15 K, $S$ = 247.04 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 277.503 K
**Molecular Weight** 131.1537
**Wiswesser Line Notation** T66 COJ
**Evaluation** A

**$C_9H_8MnO_3P$** (c) 82POI/SOU
3,4-Dimethylphosphoryl manganese tricarbonyl;
Dimethyl-3,4-phosphacymantrene
**Phase Changes**
c,II/c,I 275 K, $\Delta H$ = 190 J·mol$^{-1}$
$\Delta S$ = 0.69 J·mol$^{-1}$·K$^{-1}$
c,I/liq 300 K, $\Delta H$ = 19300 J·mol$^{-1}$
$\Delta S$ = 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) 86SIN/KUM
Cinnamic acid
**Phase Changes**
c/liq 406.15 K, $\Delta H$ = 22626 J·mol$^{-1}$
$\Delta S$ = 55.71 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 148.1610
**Wiswesser Line Notation** QV1U1R
**Evaluation** A

**$C_9H_8O_3$** (c) 83GEI/SAL
Endobicyclo[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.

**$C_9H_9FeN$** (c) 84CHH/POM
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, $\Delta H$ = 3000 J·mol$^{-1}$
$\Delta S$ = 15.0 J·mol$^{-1}$·K$^{-1}$
c,II/c,I′ 218 K, $\Delta H$ = −3800 J·mol$^{-1}$
$\Delta S$ = −17.4 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 187.0238
**Wiswesser Line Notation** T5NØJ Ø-FE-- ØL5ØJ
**Evaluation** A
Metastable phase.

**$C_9H_9FeN$** (c) 84CHH/POM
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, $\Delta H$ = 650 J·mol$^{-1}$
$\Delta S$ = 2.4 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 289.5 K, $\Delta H$ = 6748 J·mol$^{-1}$
$\Delta S$ = 23.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 187.0238
**Wiswesser Line Notation** T5NØJ Ø-FE-- ØL5ØJ
**Evaluation** A
Stable phase.

**$C_9H_9FeP$** (c) 84CHH/POM
Phosphaferrocene
**Phase Changes**
c,II/c,I 266 K, $\Delta H = 7330$ J·mol$^{-1}$
$\Delta S = 27.6$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 203.9909
**Wiswesser Line Notation** T5PØJ Ø-FE-- ØL5ØJ
**Evaluation** A
Stable phase.
A metastable phase transition is reported at $T = 210$ K.

**$C_9H_{10}$** (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, $\Delta H = 11924$ J·mol$^{-1}$
$\Delta S = 47.55$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 118.1780
**Wiswesser Line Notation** 1UY1&R
**Evaluation** B

**$(C_9H_{10})_n$** (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

**$C_9H_{10}N_2O_3$** (c) 82CUE/SOL
2-Methoxyisonitrosoacetanilide
**Phase Changes**
c/liq 422 K, $\Delta H = 27800$ J·mol$^{-1}$
$\Delta S = 65.9$ J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S = 18.1$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 194.1896
**Wiswesser Line Notation** QNU1VMR DO1
**Evaluation** D

**$C_9H_{10}O_2$** (c) 1889EYK
Phenylpropionic acid
**Phase Changes**
c/liq 321.6 K, $\Delta H = 15564$ J·mol$^{-1}$
$\Delta S = 48.4$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 150.1768
**Wiswesser Line Notation** QV2R
**Evaluation** C

**$C_9H_{10}O_2$** (c) 87LES/LIC
Phenyl glycidyl ether
**Heat Capacity** 298 K, $C_p = 278.7$ J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 330 K.
**Entropy** 298.15 K, $S = 274.9$ J·mol$^{-1}$·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.

**$C_9H_{11}N$** (liq) 89STE/CHI2
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* $\Delta H = 11813$ J·mol$^{-1}$
$\Delta S = 40.75$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 133.1926
**Wiswesser Line Notation** T66 BNT&J
**Evaluation** A

**$C_9H_{11}N$** (liq) 86STE/CHI2
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 $\Delta H = 9071.7$ J·mol$^{-1}$
$\Delta S = 40.75$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 133.1926
**Wiswesser Line Notation** T66 BN&TJ
**Evaluation** A

**$C_9H_{12}O$** (liq) 88BAG/GUR
2,5,6-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

**$C_9H_{12}O_2$** (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

**$C_9H_{14}O$** (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

**$C_9H_{14}O_2$** (liq) 85KAR/ABD2
Carbopropoxy methyl methacrylate
**Phase Changes**
c/liq 276.5 K, $\Delta H$ = 19867 J·mol$^{-1}$
**Molecular Weight** 154.2084
**Wiswesser Line Notation** 3OV1OVY1&U1
**Evaluation** A

**$C_9H_{14}O_6$** (liq) 83RAB/KHL
Triacetin; Glycerol 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, $\Delta H$ = 25800 J·mol$^{-1}$
$\Delta S$ = 93.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 218.2060
**Wiswesser Line Notation** 1OV1YOV1&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
**Heat Capacity** 298.15 K, $C_p$ = 389.0 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 218.2060
**Wiswesser Line Notation** 1VO1YOV1&1OV1
**Evaluation** A

**$C_9H_{17}O_2Tl$** (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

**$C_9H_{18}O$** (liq) 89VES/BAR
2,6-Dimethyl-4-heptanone; Diisobutylketone
**Heat Capacity** 298.15 K $C_p$ = 297.3 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 142.2406
**Wiswesser Line Notation** 1Y1&1V1Y1&1
**Evaluation** A

**$C_9H_{18}O$** (liq) 70HAR/HEA
5-Nonanone
**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) 82DYA/VAS
Nonanal; Pelargonaldehyde
**Entropy** 298.15 K, $S$ = 397.0 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq $\Delta H$ = 30510 J·mol$^{-1}$
**Molecular Weight** 142.2406
**Wiswesser Line Notation** VH8
**Evaluation** B

**$C_9H_{20}$** (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, $\Delta H$ = 9744.1 J·mol$^{-1}$
$\Delta S$ = 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 174.45K, $\Delta H$ = 7325.45 J·mol$^{-1}$
$\Delta S$ = 41.99 J·mol$^{-1}$·K$^{-1}$
c,I/liq 263.40 K, $\Delta H$ = 2332.6 J·mol$^{-1}$
$\Delta S$ = 8.86 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 128.2570
**Wiswesser Line Notation** 2X1&1&X1&1&1
**Evaluation** A

**$C_9H_{18}O$** (liq) 84VAS/PET
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/PET
Butyl 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, $\Delta H$ = 17600 J·mol$^{-1}$
$\Delta S$ = 92.94 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 158.2400
**Wiswesser Line Notation** 4OV4
**Evaluation** A

**$C_9H_{18}O_2$** (liq) 84VAS/PET
Amyl butyrate; 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, $\Delta H$ = 20010 J·mol$^{-1}$
$\Delta S$ = 99.81 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 158.2400
**Wiswesser Line Notation** 50V3
**Evaluation** A

**$C_9H_{18}O_4$** (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) 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, $\Delta H$ = 1272 J·mol$^{-1}$
Combined heats of transition for multiple phases.
c,I/liq 240.13 K, $\Delta H$ = 10033 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 483.7 J·mol$^{-1}$
$\Delta S$ = 2.32 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 210.4 K, $\Delta H$ = 810.4 J·mol$^{-1}$
$\Delta S$ = 3.85 J·mol$^{-1}$·K$^{-1}$
c,I/liq 240.10 K, $\Delta H$ = 10089.7 J·mol$^{-1}$
$\Delta S$ = 42.02 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 128.2570
**Wiswesser Line Notation** 2X2&2&2
**Evaluation** A

**$C_9H_{20}$** (liq) 82ZAR
*n*-Nonane
**Heat Capacity** 323 K, $C_p$ = 293.2 J·mol$^{-1}$·K$^{-1}$
Temperature range 323, 363 K.
**Molecular Weight** 128.2570
**Wiswesser Line Notation** 9H
**Evaluation** B

**$C_9H_{20}N_2O$** (c) 87DEL/FER
N,N′-Dibutylurea
**Phase Changes**
c,II/c,I 311.5 K, $\Delta H$ = 11100 J·mol$^{-1}$
$\Delta S$ = 35.6 J·mol$^{-1}$·K$^{-1}$
c/liq 346.9 K, $\Delta H$ = 14870 J·mol$^{-1}$
$\Delta S$ = 42.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 172.2698
**Wiswesser Line Notation** 4MVM4
**Evaluation** A

**$C_9H_{20}O_4$** (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.

**$C_9H_{21}N_3O_6CaCl_2$** (c) 80LOP/TEL
Trisarcosine 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** QV1M1 3 .C*A* G2
**Evaluation** C

**$C_9H_{24}Si_2$** (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, $\Delta H$ = 16058 J·mol$^{-1}$
$\Delta S$ = 71.76 J·mol$^{-1}$·K$^{-1}$
liq/g 444.52 K, $\Delta H$ = 43095 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 16498 J·mol$^{-1}$
$\Delta S$ = 61.42 J·mol$^{-1}$·K$^{-1}$
liq/g 476.55 K, $\Delta H$ = 45522 J·mol$^{-1}$
$\Delta S$ = 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·mol$^{-1}$
$\Delta S = 5.27$ J·mol$^{-1}$·K$^{-1}$
Lambda type transition in the metastable state.
c,II/c,I 251 K, $\Delta H = 4230$ J·mol$^{-1}$
$\Delta S = 16.83$ J·mol$^{-1}$·K$^{-1}$
Phase transition between stable L$T$ and stable H$T$ phases.
**Molecular Weight** 196.1150
**Wiswesser Line Notation** L5ØJ &1A-E/H-2 5Ø-FE--ØL5ØJ &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·mol$^{-1}$·K$^{-1}$
Temperature range 13 to 300 K.
**Entropy** 298.15 K, $S = 233.18$ J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,III/c,II 164.1 K, $\Delta H = 878$ J·mol$^{-1}$
$\Delta S = 5.27$ J·mol$^{-1}$·K$^{-1}$
Lambda transition.
Secondary $C_p$ maximum at 172 K.
c,II/c,I 251 K, $\Delta H = 4230$ J·mol$^{-1}$
$\Delta S = 16.83$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 196.1150
**Wiswesser Line Notation** L5ØJ &1A-E/H-2 5Ø-FE--ØL5ØJ &1A-E/H-2 5
**Evaluation** A
Data also given for the metastable phases over temperature range 10 to 250 K.

**$C_{10}H_2O_6$** (c) 77KAR/BAZ
Pyromellitic dianhydride
**Heat Capacity** 300 K, $C_p = 219.9$ J·mol$^{-1}$·K$^{-1}$
Temperature range 60 to 400 K.
**Entropy** 300 K, $S = 242.1$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 218.1222
**Wiswesser Line Notation** T565 DVOV JVOVJ
**Evaluation** B

**$C_{10}H_5Cu$** (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

**$C_{10}H_7Cl$** (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

**$C_{10}H_7Cl$** (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)

**$C_{10}H_7F$** (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) 82SYU/TUM
Naphthalene
**Phase Changes**
c/liq 354.1 K, $\Delta H = 19020$ J·mol$^{-1}$
$\Delta S = 53.7$ J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S = 219.3$ J·mol$^{-1}$·K$^{-1}$
c/g 298.15 K, $\Delta H = 72320$ J·mol$^{-1}$
$\Delta S = 242.6$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 128.1732
**Wiswesser Line Notation** L66J
**Evaluation** A

**$C_{10}H_8Cl$** (liq) 88COS/HUU
1-Chloronaphthalene
**Heat Capacity** 298.15 K, $C_p = 212.60$ J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 163.6262
**Wiswesser Line Notation** L66J BG
**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·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 450 K.
**Entropy** 298.15 K, $S$ = 174.66 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 366.5 K, $\Delta H$ = 15250 J·mol$^{-1}$
$\Delta S$ = 41.61 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 130.1890
**Wiswesser Line Notation** L737 B C 1A J BU EU IUTJ
**Evaluation** A

$C_{10}H_{10}$ (liq) 49PAR/HAT
*cis*-Decahydronaphthalene
**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, $\Delta H$ = 2209 J·mol$^{-1}$
$\Delta S$ = 9.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 130.1890
**Wiswesser Line Notation** L66TTJ -C
**Evaluation** B

$C_{10}H_{10}$ (liq) 49PAR/HAT
*trans*-Decahydronaphthalene
**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, $\Delta H$ = 3244 J·mol$^{-1}$
$\Delta S$ = 13.4 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 130.1890
**Wiswesser Line Notation** L66TTJ -T
**Evaluation** B

$C_{10}H_{10}Co$ (c) 75RAB/NIS
Cobaltocene
**Heat Capacity** 298.15 K, $C_p$ = 197.3 J·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 298.15 K.
**Entropy** 298.15 K, $S$ = 236.1 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 92 K, $\Delta H$ = 238 J·mol$^{-1}$
$\Delta S$ = 2.73 J·mol$^{-1}$·K$^{-1}$
Lambda transition between 70 to 140 *K* with a maximum at 92 K.
**Molecular Weight** 189.1222
**Wiswesser Line Notation** L5ØJ Ø-CO-- ØL5ØJ
**Evaluation** A
See also 78RAB/NIS.

$C_{10}H_{10}Co$ (c) 76POM/AZO
Cobaltocene
**Heat Capacity** 298.15 K
Temperature range 118 to 298 K. Data given graphically.
$C_p$=62.92–0.460T+6.07×10$^{-3}T^2$–9.53×10$^{-6}T^3$ (118 to 298 K).
$C_p$ value calculated from equation.
**Molecular Weight** 189.1222
**Wiswesser Line Notation** L5ØJ Ø-CO-- ØLTØJ
**Evaluation** C

$C_{10}H_{10}Cr$ (c) 75RAB/NIS
Chromocene
**Heat Capacity** 298.15 K, $C_p$ = 199.1 J·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 298.15 K.
**Entropy** 298.15 K, $S$ = 236.0 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 99.5 K, $\Delta H$ = 265 J·mol$^{-1}$
$\Delta S$ = 2.57 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** L5ØJ Ø-CR-- ØL5ØJ
**Evaluation** A
See also 78RAB/NIS.

$C_{10}H_{10}Cr$ (c) 76POM/AZO
Chromocene
**Heat Capacity** 298.15 K
Temperature range 121 to 298 K.
Data given graphically.
$C_p$ = −253.6 + 0.632$T$ + 33.52×10$^3T^{-1}$ 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** L5ØJ Ø-CR-- ØL5ØJ
**Evaluation** C($C_p$), A(Phase changes)

$C_{10}H_{10}Cr$ (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** L5ØJ Ø-CR-- ØL5ØJ
**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$^{-1}$
$\Delta H$ and $\Delta S$ 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** L5ØJ Ø-FE-- ØL5ØJ &PFFFFFF
**Evaluation** A

$C_{10}H_{10}Fe$ (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** L5ØJ Ø-FE-- ØL5ØJ
**Evaluation** A

**$C_{10}H_{10}Mn$** (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, $\Delta H$ = 41 J·mol$^{-1}$
$\Delta S$ = 0.63 J·mol$^{-1}$·K$^{-1}$
Lambda transition.
**Molecular Weight** 185.1270
**Wiswesser Line Notation** L5ØJ Ø-MN-- ØL5ØJ
**Evaluation** A
See also 78RAB/NIS.

**$C_{10}H_{10}N_2O_2$** (c) 82CUE/SOL
N-Ethanol isatoxine
**Phase Changes**
c/liq 505 K, $\Delta H$ = 28900 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 182 J·mol$^{-1}$
$\Delta S$ = 1.32 J·mol$^{-1}$·K$^{-1}$
Lambda transition.
**Molecular Weight** 188.8890
**Wiswesser Line Notation** L5ØJ Ø-NI-- ØL5ØJ
**Evaluation** A
See also 78RAB/NIS.

**$C_{10}H_{10}Ni$** (c) 76POM/AZO
Nickelocene
**Heat Capacity** 298.15 K
Temperature range 127 to 303 K.
Data given graphically.
$C_p = 87.705 - 0.649T + 5.86\times10^{-3}T^2 - 9.29\times10^{-6}T^3$ 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, $\Delta S$ = 5.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 188.8890
**Wiswesser Line Notation** L5ØJ Ø-NI-- ØL5ØJ
**Evaluation** $C(C_p)$, A(Phase changes)

**$C_{10}H_{10}O_2$** (c) 84BEK/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 $\Delta H$ = 82006 J·mol$^{-1}$
$\Delta H$ 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) 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, $\Delta H$ = 16945 J·mol$^{-1}$
$\Delta S$ = 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) 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.

**$C_{10}H_{10}Ru$** (c) 76POM/AZO
Ruthenocene
**Heat Capacity** 298.15 K
Temperature range 100 to 300 K.
Data given graphically.
$C_p = 74.33 + 2.59T - 1.50\times10^{-3}T^2 + 2.31\times10^{-5}T^3 - 4.35\times10^{-8}T^4$ J·mol$^{-1}$·K$^{-1}$ (100 to 300K).
**Molecular Weight** 231.2590
**Wiswesser Line Notation** L5ØJ Ø-RU- - ØL5ØJ
**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, $S$ = 340.2 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 130–200 K, $\Delta H$ = 196 J·mol$^{-1}$
$\Delta S$ = 1.21 J·mol$^{-1}$·K$^{-1}$
Lambda transition.
**Molecular Weight** 181.1305
**Wiswesser Line Notation** L5ØJ Ø-VA- - ØL5ØJ
**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, $\Delta H$ = 9660 J·mol$^{-1}$
$\Delta S$ = 40.0 J·mol$^{-1}$·K$^{-1}$
c,I/liq 304.8 K, $\Delta H$ = 2220 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 23000 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 7600 J·mol$^{-1}$
$\Delta S$ = 15.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 208.2164
**Wiswesser Line Notation** QVU1MR DO2
**Evaluation** D

**$C_{10}H_{12}O_2$** (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

**$C_{10}H_{12}N_2S$** (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, $\Delta H$ = 27614 J·mol$^{-1}$
$\Delta S$ = 73.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 192.2782
**Wiswesser Line Notation** 1U2MYMUS&R
**Evaluation** B

**$C_{10}H_{14}Si$** (liq) 77LEB/RAB2
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, $\Delta H$ = 12259 J·mol$^{-1}$
$\Delta S$ = 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/LEB
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, $\Delta H$ = 12300 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{10}H_{14}ZnO_4$** (c) 86GRI/LAZ
Zinc acetylacetonate
**Phase Changes**
c/liq 400.5 K, $\Delta H$ = 18200 J·mol$^{-1}$
$\Delta S$ = 45.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 263.5982
**Wiswesser Line Notation** D6O-ZN-O ADJ D1 F1
B-& BD6O-ZN-O ADJ D1 F1
**Evaluation** A

**$C_{10}H_{15}Cl$** (c) 88PAR/KAW
2-Chloroadamantane
**Phase Changes**
c,III/c,II 227 K, $\Delta H$ = 470 J·mol$^{-1}$
$\Delta S$ = 2.3 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 242 K, $\Delta H$ = 8300 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{10}H_{16}$** (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.
$C_s$ = 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

**$C_{10}H_{16}N_2ClO_4$** (c) 65CHI/NAK
Wurster's Blueperchlorate; 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, $\Delta H$ = 1709.6 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{10}H_{16}O$** (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) 88SAL/ABA
1-Hydroxyadamantane
**Phase Changes**
c,III/c,II 369.16 K, $\Delta H$ = 2500 J·mol$^{-1}$
$\Delta S$ = 6.77 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 529.16 K, $\Delta H$ = 7130 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 300 J·mol$^{-1}$
$\Delta S$ = 0.92 J·mol$^{-1}$·K$^{-1}$
c,III/c,II 391.16 K, $\Delta H$ = 3740 J·mol$^{-1}$
$\Delta S$ = 9.56 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 516.16 K, $\Delta H$ = 7750 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{10}H_{16}O$** (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) − S°(0) = 379.9 J·mol$^{-1}$·K$^{-1}$ for the highly elastic state.
**Phase Changes**
c/liq 328.8 K, $\Delta H$ = 24800 J·mol$^{-1}$
**Molecular Weight** 200.2340
**Wiswesser Line Notation** /*OV4VO4*/
**Evaluation** B
$T$(glass) = 199 K.

**$C_{10}H_{18}$** (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) 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

**$C_{10}H_{18}O_4$** (liq) 86NIL/WAD
Ethyleneglycol dibutanoate
**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

**$C_{10}H_{19}NO_2$** (liq) 85KAR/ABD2
Diethylaminoethyl methacrylate
**Phase Changes**
c/liq 207.5 K, $\Delta H$ = 13080 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 2411 J·mol$^{-1}$
$\Delta S$ = 10.39 J·mol$^{-1}$·K$^{-1}$
c,IV/c,III 288.6 K, $\Delta H$ = 599 J·mol$^{-1}$
$\Delta S$ = 2.08 J·mol$^{-1}$·K$^{-1}$
c,III/c,II 306.8 K, $\Delta H$ = 4240 J·mol$^{-1}$
$\Delta S$ = 13.89 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 327.4 K, $\Delta H$ = 3974 J·mol$^{-1}$
$\Delta S$ = 12.14 J·mol$^{-1}$·K$^{-1}$
c,I/liq 405.0 K, $\Delta H$ = 5670 J·mol$^{-1}$
$\Delta S$ = 13.97 J·mol$^{-1}$·K$^{-1}$
Solid-mesophase.
liq/liq 484.0 K, $\Delta H$ = 2552 J·mol$^{-1}$
$\Delta S$ = 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) 80BYS
2,2,5,5-Tetramethylhex-3-ene
**Phase Changes**
c,III/c,II 235.7 K, $\Delta H$ = 1210 J·mol$^{-1}$
$\Delta S$ = 5.13 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 243.5 K, $\Delta H$ = 4330 J·mol$^{-1}$
$\Delta S$ = 17.8 J·mol$^{-1}$·K$^{-1}$
c,I/liq 268.8 K, $\Delta H$ = 10250 J·mol$^{-1}$
$\Delta S$ = 38.1 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 140.2688
**Wiswesser Line Notation** 1X1&1&1U1X1&1&1
**Evaluation** A

**$C_{10}H_{20}BrFeN_2S_4$** (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, $\Delta H$ = 97.0 J·mol$^{-1}$
$\Delta S$ = 11.05 J·mol$^{-1}$·K$^{-1}$
Schottky type anomaly.
$\Delta H$ and $\Delta S$ values are the total of both transitions.
c,II/c,I 265.7 K, $\Delta H$ = 1960 J·mol$^{-1}$
$\Delta S$ = 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)

**$C_{10}H_{20}O$** (liq) 80DYA/VAS
Decanal; Capric aldehyde; Capraldehyde
**Heat Capacity**
Temperature range 50 to 350 K.
**Phase Changes**
c/liq 269.47 K, $\Delta H$ = 30600 J·mol$^{-1}$
$\Delta S$ = 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 $\Delta H$ = 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, $\Delta H$ = 29217 J·mol$^{-1}$
$\Delta S$ = 97.4 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 172.2668
**Wiswesser Line Notation** QV9
**Evaluation** C

**$C_{10}H_{22}$** (liq) 82ZAR
*n*-Decane
**Heat Capacity** 298 K, $C_p$ = 312.8 J·mol$^{-1}$·K$^{-1}$
Temperature range 298, 323, 363 K.
**Molecular Weight** 142.2838
**Wiswesser Line Notation** 10H
**Evaluation** B

**$C_{10}H_{22}$** (liq) 84GRO/ING
*n*-Decane
**Heat Capacity** 298.15 K, $C_p$ = 313.93 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 142.2838
**Wiswesser Line Notation** 10H
**Evaluation** B

**$C_{10}H_{22}$** (liq) 84ROU/GRO
*n*-Decane
**Heat Capacity** 298.15 K, $C_p$ = 314.21 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 142.2838
**Wiswesser Line Notation** 10H
**Evaluation** B

**$C_{10}H_{22}$** (liq) 85LAI/ROU
*n*-Decane
**Heat Capacity** 298.15 K, $C_p$ = 313.09 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 142.2838
**Wiswesser Line Notation** 10H
**Evaluation** B

**$C_{10}H_{22}$** (liq) 85LAI/WIL
*n*-Decane
**Heat Capacity** 298.15 K, $C_p$ = 313.09 J·mol$^{-1}$·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) 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) 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

**$C_{10}H_{22}N_4$** (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

**$C_{10}H_{25}N_5$** (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

**$C_{10}H_{22}S$** (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.
$C_p = 346.70 + 3.600\times10^{-2}T + 8.824\times10^{-5}T^2$.
**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, $\Delta H$ = 1312.5 J·mol$^{-1}$
$\Delta S$ = 5.38 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 193.7593
**Wiswesser Line Notation** 5M5 &GH
**Evaluation** A

**$C_{10}H_{24}CuN_6O_6$** (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

**$C_{10}H_{26}O_3Si_3$** (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 to300 K.
**Entropy** 298.15 K, $S$ = 616.9 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 195–210 K, $\Delta H$ = 131 J·mol$^{-1}$
$\Delta S$ = 0.946 J·mol$^{-1}$·K$^{-1}$
c,I/liq 260.03 K, $\Delta H$ = 9522 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{10}H_{28}Cl_4MnN_2$** (c) 75BOC/ARR
Tetrachlorobis-(pentylammonium) manganese II
**Phase Changes**

| | | |
|---|---|---|
| c,IV/c,III | 203 K, | $\Delta H$ = 53.2 J·mol$^{-1}$ |
| | | $\Delta S$ = 0.26 J·mol$^{-1}$·K$^{-1}$ |
| c,III/c,II | 208 K, | $\Delta H$ = 506.8 J·mol$^{-1}$ |
| | | $\Delta S$ = 2.43 J·mol$^{-1}$·K$^{-1}$ |
| c,II/c,I | 364 K, | $\Delta H$ = 3.6 J·mol$^{-1}$ |
| | | $\Delta S$ = 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, | $\Delta H$ = 441 J·mol$^{-1}$ |
| | | $\Delta S$ = 3.08 J·mol$^{-1}$·K$^{-1}$ |
| c,IV/c,III | 147.95 K, | $\Delta H$ = 499 J·mol$^{-1}$ |
| | | $\Delta S$ = 3.33 J·mol$^{-1}$·K$^{-1}$ |
| c,III/c,II | 249.95 K, | $\Delta H$ = 3584 J·mol$^{-1}$ |
| | | $\Delta S$ = 14.38 J·mol$^{-1}$·K$^{-1}$ |
| c,II/c,I | 349.05 K, | $\Delta H$ = 8672 J·mol$^{-1}$ |
| | | $\Delta S$ = 24.36 J·mol$^{-1}$·K$^{-1}$ |
| c,I/liq | 437 K, | $\Delta H$ = 6800 J·mol$^{-1}$ |

Solid-isotropic liquid.
**Molecular Weight** 383.5366
**Wiswesser Line Notation** 5ZH 2 .ZN G4

**$C_{11}H_{10}O_4$** (c) 84LEB/LEB
*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, | $\Delta H$ = 34000 J·mol$^{-1}$ |
| | | $\Delta S$ = 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/LEB
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·mol$^{-1}$ |
| | | $\Delta S$ = 8.01 J·mol$^{-1}$·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·mol$^{-1}$ |
| | | $\Delta S$ = 14.55 J·mol$^{-1}$·K$^{-1}$ |

$\Delta H$ and $\Delta S$ are total of c,IV/c,III; c,III/c,II; and c,II/c,I transitions.
**Molecular Weight** 344.0191
**Wiswesser Line Notation** L6ØJ Ø-FE-- ØL5ØJ &PFFFFFF
**Evaluation** A

**$C_{11}H_{12}O_2$** (liq) 84BEK/RUE
4-Carbomethoxyhomocubane
**Heat Capacity** 298 K, $C_p$ = 288 J·mol$^{-1}$·K$^{-1}$
$C_p$ given as 0.391 cal·K$^{-1}$·g$^{-1}$.
**Phase Changes**

| | | |
|---|---|---|
| liq/g | 303–343 K, | $\Delta H$ = 79956 J·mol$^{-1}$ |

Derived from vapor pressure measurements.
**Molecular Weight** 176.2146
**Wiswesser Line Notation** L444 B4 D5 4ABCD ITJ AVO1
**Evaluation** B

**$C_{11}H_{14}N_2$** (c) 81LEB/RYA
Gramine; 3-Dimethylaminomethyl indole
**Heat Capacity** $C_p$ = 283.5 J·mol$^{-1}$·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

**$C_{11}H_{16}Si$** (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, | $\Delta H$ = 11600 J·mol$^{-1}$ |
| | | $\Delta S$ = 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.

**$C_{11}H_{17}NO$** (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, $\Delta H$ = 108000 J·mol$^{-1}$
$\Delta S$ = 362.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 179.2614
**Wiswesser Line Notation** L66 B6/B-H/DI A B- C 1B ITJ BVZ
**Evaluation** A

**$C_{11}H_{20}$** (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, $\Delta H$ = 6359.7 J·mol$^{-1}$
$\Delta S$ = 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)

**$C_{11}H_{20}O_3Si_3$** (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, $\Delta H$ = 18293 J·mol$^{-1}$
$\Delta S$ = 80.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 284.5337
**Wiswesser Line Notation** T6-SI-O-SI-O-SI-OJ A1 A1 C1 C1 E1 ER
**Evaluation** A
Data given for glassy state from 5 to 226.8 K.
Glass transition at 150 K.

**$C_{11}H_{22}O$** (liq) 70HAR/HEA
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

**$C_{11}H_{24}O$** (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

**$C_{12}Cl_{10}$** (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) 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, $\Delta H$ = 0.18 J·mol$^{-1}$
$\Delta S$ = 0.009 J·mol$^{-1}$·K$^{-1}$
Lock-in transition.
c,II/c,I 36.8 K, $\Delta H$ = 4.61 J·mol$^{-1}$
$\Delta S$ = 0.128 J·mol$^{-1}$·K$^{-1}$
Twist transition.
**Molecular Weight** 164.2900
**Wiswesser Line Notation** RR &1A-E/H-2 &2A-E/H-2 5
**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, $\Delta H$ = 0.18 J·mol$^{-1}$
$\Delta S$ = 0.009 J·mol$^{-1}$·K$^{-1}$
Anamolous region: 18.5 to 22.5 K.
c,II/c,I 36.8 K, $\Delta H$ = 4.61 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{12}F_{10}$** (c) 87SAI/ATA
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

**$C_{12}H_7Cl_2NO_3$** (c) 81VOR/BOR
2,4-Dichloro-4'-nitrodiphenyl ether
**Phase Changes**
c/liq 343 K, $\Delta H$ = 2700 J·mol$^{-1}$
$\Delta S$ = 7.87 J·mol$^{-1}$·K$^{-1}$
liq/g 643 K, $\Delta H$ = 115900 J·mol$^{-1}$
$\Delta S$ = 180.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 284.0982
**Wiswesser Line Notation** WNR DOR BG DG
**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, $\Delta H$ = 24400 J·mol$^{-1}$
$\Delta S$ = 57.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 287.1600
**Wiswesser Line Notation** GR DSWR DG
**Evaluation** A

**$C_{12}H_8Cl_4Si_2$** (c) 74GEI/DZH
o,o'-Bis-trichlorosilylbiphenyl
**Heat Capacity**
Temperature range 12 to 370 K.
Deposited in VINITI, No 7671-73, 21 December 1973.
**Entropy** 298.15 K, $S$ = 348.4 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 289.5 K, $\Delta H$ = 57.7 J·mol$^{-1}$
$\Delta S$ = 0.20 J·mol$^{-1}$·K$^{-1}$
*trans*-cis conformational transition.
c,I/liq 339.18 K, $\Delta H$ = 20719 J·mol$^{-1}$
$\Delta S$ = 61.09 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 350.1782
**Wiswesser Line Notation** G-SI-GGR BR B-SI-GGG
**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, $\Delta H$ = 91200 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{12}H_8S$** (c) 83ORO/MRA
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 371.0 K) J·mol$^{-1}$·K$^{-1}$.
**Phase Changes**
c/liq 371.0 K, $\Delta H$ = 21580 J·mol$^{-1}$
$\Delta S$ = 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$^{-1}$.

**$C_{12}H_9Cl$** (c) 75GEI/DZH
*p*-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, $\Delta H$ = 13318 J·mol$^{-1}$
$\Delta S$ = 38.21 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 188.6561
**Wiswesser Line Notation** GR DR
**Evaluation** A
$T/_{\text{Debye}}$ = 91 K; see also 77GEI/KAR.

**$C_{12}H_9Cl_3Si$** (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, $\Delta H$ = 18569 J·mol$^{-1}$
$\Delta S$ = 49.80 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 287.6476
**Wiswesser Line Notation** G-SI-GGR DR
**Evaluation** A
See also 77GEI/KAR.

**$C_{12}H_{10}$** (c) 1889EYK
Biphenyl; Diphenyl
**Phase Changes**
c/liq 314.3 K, $\Delta H$ = 18945 J·mol$^{-1}$
$\Delta S$ = 60.3 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 154.2110
**Wiswesser Line Notation** RR
**Evaluation** C

**$C_{12}H_{10}$** (c) 79SMI
Biphenyl; Diphenyl
**Phase Changes**
c/liq 344.1 K, $\Delta H$ = 18800 J·mol$^{-1}$
$\Delta S$ = 54.6 J·mol$^{-1}$·K$^{-1}$
**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, $\Delta H$ = 19900 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 0.15 J·mol$^{-1}$
$\Delta S$ = 0.009 J·mol$^{-1}$·K$^{-1}$
Anomalous region: 15.3 to 18.3 K.
c,II/c,I 40.4 K, $\Delta H$ = 5.02 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 18580 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 0.15 J·mol$^{-1}$
$\Delta S$ = 0.009 J·mol$^{-1}$·K$^{-1}$
Lock-in transition.
c,II/c,I 40.4 K, $\Delta H$ = 5.02 J·mol$^{-1}$
$\Delta S$ = 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 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, $\Delta H$ = 2234.14 J·mol$^{-1}$
$\Delta S$ = 6.5307 J·mol$^{-1}$·K$^{-1}$
c/g 298.15 K $\Delta H$ = 81520 J·mol$^{-1}$
$\Delta S$ = 273.42 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 154.2110
**Wiswesser Line Notation** RR
**Evaluation** *A*

**$C_{12}H_{10}Cr$** (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** 206.2070
**Wiswesser Line Notation** L6ØJ Ø-CR-- ØL6ØJ
**Evaluation** A

**$C_{12}H_{10}N_2$** (c) 84VAN/BOU
*trans*-Azobenzene
**Heat Capacity** 300 K, $C_p$ = 229.3 J·mol$^{-1}$·K$^{-1}$
Temperature range 90 to 320 K.
**Phase Changes**
c/liq 341.03 K, $\Delta H$ = 22520 J·mol$^{-1}$
$\Delta S$ = 66.0 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 300 to 400 K.
**Phase Changes**
c,I/liq 341.06 K, $\Delta H$ = 22530 J·mol$^{-1}$
$\Delta S$ = 66.06 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 182.2244
**Wiswesser Line Notation** RNUNR -T
**Evaluation** A

**$C_{12}H_{10}N_2$** (c) 1889EYK
Azobenzene
**Phase Changes**
c/liq 342.2 K, $\Delta H$ = 22389 J·mol$^{-1}$
$\Delta S$ = 65.4 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 182.2244
**Wiswesser Line Notation** RNUNR
**Evaluation** C

**$C_{12}H_{10}O_2$** (c) 86SAI/ATA2
*p,p'*-Biphenol; 4,4'-Dihydroxybiphenyl
**Heat Capacity** 298.15 K, $C_p$ = 224.31 J·mol$^{-1}$·K$^{-1}$
Temperature range 3 to 315 K.
**Entropy** 298.15 K, $S$ = 220.57 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 186.2098
**Wiswesser Line Notation** QR DR DQ
**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, $\Delta H$ = -0.58 J·mol$^{-1}$
c,II/c,I 265.000 K, $\Delta H$ = -1.08 J·mol$^{-1}$
c,I/liq 377.496 K, $\Delta H$ = 19353.29 J·mol$^{-1}$
$\Delta S$ = 51.27 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 156.2268
**Wiswesser Line Notation** L66J C1 D1
**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** L6ØJ Ø-CR-- ØL6ØJ &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, $\Delta H$ = 1820 J·mol$^{-1}$
$\Delta S$ = 10.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 243.6758
**Wiswesser Line Notation** L6ØJ Ø-CR-- ØL6ØJ &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, $\Delta H$ = 1695 J·mol$^{-1}$
$\Delta S$ = 7.04 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 335.1273
**Wiswesser Line Notation** L6ØJ Ø-CR-- ØL6ØJ &I
**Evaluation** B

**$C_{12}H_{12}N_2O$** (c) 77KAR/BAZ
4,4'-Diaminodiphenylether
**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) 87LES/LIC
4,4′-Diaminodiphenyl oxide; 4,4′-Diaminodiphenyl 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

**$C_{12}H_{12}N_4O$** (c) 77KAR/RAB
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, $\Delta H$ = 25301 J·mol$^{-1}$
$\Delta S$ = 62.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 228.2532
**Wiswesser Line Notation** ZR BZ DOR CZ DZ
**Evaluation** C($C_p$),A,(S,Phase changes).

**$C_{12}H_{12}O_4$** (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, $\Delta H$ = 41000 J·mol$^{-1}$
$\Delta S$ = 93.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 220.2250
**Wiswesser Line Notation** L444 B4 D4 4ABCD HTJ AVO1 HVO1
**Evaluation** B

**$(C_{12}H_{12}O_4)_n$** (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

**$C_{12}H_{15}NO_2$** (liq) 85KAR/ABD2
Phenylaminoethyl methacrylate
**Phase Changes**
c/liq 297.5 K, $\Delta H$ = 25465 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 15270 J·mol$^{-1}$
$\Delta S$ = 54.44 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 160.2584
**Wiswesser Line Notation** L6TJ AR
**Evaluation** A

**$C_{12}H_{18}$** (c) 82ATA/GYO
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, $\Delta H$ = 990 J·mol$^{-1}$
$\Delta S$ = 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/FUJ
Hexamethylbenzene
**Phase Changes**
c,II/c,I 115.5 K, $\Delta H$ = 1103 J·mol$^{-1}$
$\Delta S$ = 9.55 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 162.2742
**Wiswesser Line Notation** 1R B1 C1 D1 E1 F1
**Evaluation** A

**$C_{12}H_{18}Be_4O_{13}$** (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, $\Delta H$ = 27196 J·mol$^{-1}$
$\Delta S$ = 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)

**$C_{12}H_{18}O_2$** (liq) 77KAR/SAP
Acetophenone diethyl ketal
**Heat Capacity** 298 K, $C_p$ = 210 J·mol$^{-1}$·K$^{-1}$
Temperature range 60 to 340 K.
$C_p$ data calculated 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.

**$C_{12}H_{20}O_6$** (liq) 86NIL/WAD
Tripropionin
**Heat Capacity** 298.15 K, $C_p$ = 481.3 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 260.2864
**Wiswesser Line Notation** 2VO1YOV2&1OV2
**Evaluation** A

**$C_{12}H_{22}$** (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, $\Delta H$ = 1540 J·mol$^{-1}$
c,III/c,II 267.5 K, $\Delta H$ = 740 J·mol$^{-1}$
c,II/c,I 273.5 K, $\Delta H$ = 7080 J·mol$^{-1}$
c,I/liq 277.2 K, $\Delta H$ = 6780 J·mol$^{-1}$
**Molecular Weight** 166.3058
**Wiswesser Line Notation** L6TJ A- AL6TJ
**Evaluation** A

**$C_{12}H_{22}O_2$** (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, $\Delta H$ = 24085 J·mol$^{-1}$
$\Delta S$ = 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/ABD2
Nonyl acrylate
**Phase Changes**
c/liq 236.5 K, $\Delta H$ = 23362 J·mol$^{-1}$
$\Delta S$ = 98.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 198.3046
**Wiswesser Line Notation** 9OV1U1
**Evaluation** A

**$C_{12}H_{22}O_6$** (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·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 330 K.
$C_p$ = 1.839 kJ·kg$^{-1}$·K$^{-1}$ at 298.15 K.
**Entropy** 298.15 K, $S$ = 471.1 J·mol$^{-1}$·K$^{-1}$
S° = 1.796 kJ·kg$^{-1}$·K$^{-1}$ at 298.15 K.
**Phase Changes**
gls/liq 207 K $\Delta H$ = 11565 J·mol$^{-1}$
$\Delta S$ = 55.87 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 330 K.
$C_p$ = 1.839 kJ·kg$^{-1}$·K$^{-1}$ at 298.15 K.
**Entropy** 298.15 K, $S$ = 527.0 J·mol$^{-1}$·K$^{-1}$
S° = 2.009 kJ·kg$^{-1}$·K$^{-1}$ at 298.15 K.
**Phase Changes**
c,I/liq 290.7 K, $\Delta H$ = 32709 J·mol$^{-1}$
$\Delta S$ = 112.5 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
One temperature.
$C_p$ given as 0.301 cal·g$^{-1}$·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) 03MAG
Maltose
**Heat Capacity** 298 K, $C_p$ = 461.2 J·mol$^{-1}$·K$^{-1}$
One temperature.
$C_p$ given as 0.322 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) 03MAG
Lactose, anhydrous; 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&C—B&BDEF
**Evaluation** D

$C_{12}H_{23}O_2Tl$ (c) 76MEI/SEY
Thallium *n*-dodecanoate
**Phase Changes**

| | | |
|---|---|---|
| c,III/c,II | 312 K, | $\Delta H$ = 3807 J·mol$^{-1}$ |
| | | $\Delta S$ = 12.1 J·mol$^{-1}$·K$^{-1}$ |
| c,II/c,I | 354 K, | $\Delta H$ = 2427 J·mol$^{-1}$ |
| | | $\Delta S$ = 6.69 J·mol$^{-1}$·K$^{-1}$ |
| liq/liq | 471 K, | $\Delta H$ = 1925 J·mol$^{-1}$ |
| | | $\Delta S$ = 4.10 J·mol$^{-1}$·K$^{-1}$ |

Mesophase-isotropic.

| | | |
|---|---|---|
| c,I/liq | 398 K, | $\Delta H$ = 5858 J·mol$^{-1}$ |
| | | $\Delta S$ = 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, | $\Delta H$ = 1829 J·mol$^{-1}$ |
| | | $\Delta S$ = 6.49 J·mol$^{-1}$·K$^{-1}$ |
| c,V/c,IV | 285.2 K, | $\Delta H$ = 2087 J·mol$^{-1}$ |
| | | $\Delta S$ = 7.32 J·mol$^{-1}$·K$^{-1}$ |
| c,IV/c,III | 293.6 K, | $\Delta H$ = 1413 J·mol$^{-1}$ |
| | | $\Delta S$ = 4.82 J·mol$^{-1}$·K$^{-1}$ |
| c,III/c,II | 312.3 K, | $\Delta H$ = 4490 J·mol$^{-1}$ |
| | | $\Delta S$ = 14.38 J·mol$^{-1}$·K$^{-1}$ |
| c,II/c,I | 356.6 K, | $\Delta H$ = 2054 J·mol$^{-1}$ |
| | | $\Delta S$ = 5.74 J·mol$^{-1}$·K$^{-1}$ |
| c,I/liq | 400.1 K, | $\Delta H$ = 5454 J·mol$^{-1}$ |
| | | $\Delta S$ = 13.64 J·mol$^{-1}$·K$^{-1}$ |

Solid-mesophase.

| | | |
|---|---|---|
| liq/liq | 471.6 K, | $\Delta H$ = 1971 J·mol$^{-1}$ |
| | | $\Delta S$ = 4.16 J·mol$^{-1}$·K$^{-1}$ |

Mesophase-isotropic liquid.
**Molecular Weight** 403.6825
**Wiswesser Line Notation** OV11 .TL
**Evaluation** A

$C_{12}H_{24}O_2$ (c) 86KAL/JAC
Butyl octadecanoate
**Phase Changes**

| | | |
|---|---|---|
| c,II/c,I | 288.4 K, | $\Delta H$ = 2220 J·mol$^{-1}$ |
| | | $\Delta S$ = 7.70 J·mol$^{-1}$·K$^{-1}$ |
| c,I/liq | 299.72 K, | $\Delta H$ = 37480 J·mol$^{-1}$ |
| | | $\Delta S$ = 121.5 J·mol$^{-1}$·K$^{-1}$ |

**Molecular Weight** 200.3204
**Wiswesser Line Notation** 7VO4
**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/GRO
*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) 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) 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) 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

**$C_{12}H_{26}O_5$** (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

**$C_{12}H_{27}O_4P$** (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, $\Delta H$ = 908 J·mol$^{-1}$
$\Delta S$ = 7.89 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 279.39 K, $\Delta H$ = 15950 J·mol$^{-1}$
$\Delta S$ = 57.38 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 221.8129
**Wiswesser Line Notation** 6M6 &GH
**Evaluation** A

**$C_{12}H_{28}S$** (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.
$C_p = 423.01 + 3.878\times10^{-2}\,T + 9.070\times10^{-5}\,T^2$.
**Molecular Weight** 204.4132
**Wiswesser Line Notation** SH12
**Evaluation** B

**$C_{12}H_{30}O_3Si_3$** (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 140–160 K, $\Delta H$ = 470 J·mol$^{-1}$
Glassy transition.
c,II/c,I 242.3 K, $\Delta H$ = 11730 J·mol$^{-1}$
$\Delta S$ = 48.41 J·mol$^{-1}$·K$^{-1}$
c,I/liq 283.41 K, $\Delta H$ = 11940 J·mol$^{-1}$
**Molecular Weight** 306.6237 $\Delta S$ = 42.1 J·mol$^{-1}$·K$^{-1}$
**Wiswesser Line Notation** T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 E2
**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, $\Delta H$ = 470 J·mol$^{-1}$
Glassy transition.
c,II/c,I 242.3 K, $\Delta H$ = 11700 J·mol$^{-1}$
$\Delta S$ = 48.4 J·mol$^{-1}$·K$^{-1}$
c,I/liq 283.24 K, $\Delta H$ = 11940 J·mol$^{-1}$
$\Delta S$ = 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 E2
**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 to300 K.
**Entropy** 298.15 K, $S$ = 680.8 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,III/c,II 160 K, $\Delta H$ = 462 J·mol$^{-1}$
$\Delta S$ = 2.9 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 242.3 K, $\Delta H$ = 11824 J·mol$^{-1}$
$\Delta S$ = 48.8 J·mol$^{-1}$·K$^{-1}$
c,I/liq 280.2 K, $\Delta H$ = 11424 J·mol$^{-1}$
$\Delta S$ = 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 E2

**$C_{12}H_{30}O_3Si_3$** (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, $\Delta H$ = 470.0 J·mol$^{-1}$
$\Delta S$ = 2.08 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 242.4 K, $\Delta H$ = 11730.8 J·mol$^{-1}$
$\Delta S$ = 48.39 J·mol$^{-1}$·K$^{-1}$
c,I/liq 283.41 K, $\Delta H$ = 11940.3 J·mol$^{-1}$
$\Delta S$ = 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 E2
**Evaluation** A

**$C_{12}H_{52}Cr_4N_{12}O_{18}S_3 \cdot 10H_2O$** (c) 72MOR/SEK
Hexahydroxyhexaethylenediamine chromium sulfate decahydrate
**Heat Capacity** 197.459 K, $C_p$ = 1001.82 J·mol$^{-1}$·K$^{-1}$
Temperature range 1.4 to 200 K.
Unsmoothed experimental datum.
**Molecular Weight** 1136.9284
**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·mol$^{-1}$
c,II/c,I 189.5 K, $\Delta H$ = 251 J·mol$^{-1}$
**Molecular Weight** 251.1116
**Wiswesser Line Notation** GR DVR DG
**Evaluation** B

**$C_{13}H_9N$** (c) 88STE/CHI
7,8-Benzoquinoline
**Heat Capacity** 298.15 K, $C_p$ = 206.36 J·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 500 K.
**Entropy** 298.15 K, $S$ = 213.20 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 324.104 K, $\Delta H$ = 14103 J·mol$^{-1}$
$\Delta S$ = 43.51 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 500 K.
**Entropy** 298.15 K, $S$ = 213.20 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 324.104 K, $\Delta H$ = 14103 J·mol$^{-1}$
$\Delta S$ = 43.51 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 6 to 450 K.
**Entropy** 298.15 K, $S$ = 205.87 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 500 K.
**Entropy** 298.15 K, $S$ = 205.91 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 354.0 K, $\Delta H$ = 20.79 J·mol$^{-1}$
$\Delta S$ = 0.059 J·mol$^{-1}$·K$^{-1}$
Extrapolated value.
c,I/liq 379.74 K, $\Delta H$ = 22831 J·mol$^{-1}$
$\Delta S$ = 60.12 J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 500 K.
**Entropy** 298.15 K, $S$ = 205.91 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 354.0 K, $\Delta H$ = 20.79 J·mol$^{-1}$
$\Delta S$ = 0.059 J·mol$^{-1}$·K$^{-1}$
Extrapolated value.
c,I/liq 379.74 K, $\Delta H$ = 22831 J·mol$^{-1}$
$\Delta S$ = 60.12 J·mol$^{-1}$·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, $\Delta H$ = 20682 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 20682 J·mol$^{-1}$
$\Delta S$ = 53.97 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 179.2208
**Wiswesser Line Notation** T C666 BNJ
**Evaluation** A

**$C_{13}H_{10}N_2$** (liq) 84LEB/BYK
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, $\Delta H$ = 18550 J·mol$^{-1}$
$\Delta S$ = 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 to 287.41 K.
$T$(glass) = 190 ± 1 K.

**$C_{13}H_{10}O$** (c) 1889EYK
Benzophenone
**Phase Changes**
c/liq 321.2 K, $\Delta H$ = 17669 J·mol$^{-1}$
$\Delta S$ = 55.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 182.2214
**Wiswesser Line Notation** RVR
**Evaluation** C

**$C_{13}H_{10}O$** (c) 83DEK/VAN
Benzophenone
**Heat Capacity** 300 K, $C_p$ = 224.80 J·mol$^{-1}$·K$^{-1}$
Temperature range 80 to345 K.
**Phase Changes**
c/liq 321.03 K, $\Delta H$ = 18194 J·mol$^{-1}$
$\Delta S$ = 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) J·mol$^{-1}$·K$^{-1}$.
$C_p$(liq) = 150.19 + 0.4576 ($T$/K) (280 to 350 K) J·mol$^{-1}$.

**$C_{13}H_{11}N$** (c) 86STE/CHI
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, $\Delta H$ = 17153.8 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 17153.71 J·mol$^{-1}$
$\Delta S$ = 47.32 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 181.2366
**Wiswesser Line Notation** T B656 HNJ H1
**Evaluation** A

**$C_{13}H_{12}$** (c) 1889EYK
Diphenylmethane
**Phase Changes**
c/liq 299.4 K, $\Delta H$ = 19050 J·mol$^{-1}$
**Molecular Weight** 168.2378
**Wiswesser Line Notation** R1R
**Evaluation** C

**$C_{13}H_{12}$** (c) 86CHI/ANN
Diphenylmethane
**Phase Changes**
c/liq $\Delta H$ = 19246 J·mol$^{-1}$
c/g $\Delta H$ = 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, $\Delta H$ = 57 J·mol$^{-1}$
$\Delta S$ = 0.39 J·mol$^{-1}$·K$^{-1}$
c,V/c,IV 160.6 K, $\Delta H$ = 1762 J·mol$^{-1}$
$\Delta S$ = 10.62 J·mol$^{-1}$·K$^{-1}$
c,IV/c,III 173.4 K, $\Delta H$ = 11 J·mol$^{-1}$
$\Delta S$ = 0.07 J·mol$^{-1}$·K$^{-1}$
c,III/c,II 187.1 K, $\Delta H$ = 31 J·mol$^{-1}$
$\Delta S$ = 0.17 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 219.0 K, $\Delta H$ = 57 J·mol$^{-1}$
$\Delta S$ = 0.27 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 424.4630
**Wiswesser Line Notation** L5ØJ Ø-FE-- ØL5ØJ &ZYZUS 3 &1/H-2 5 &14/H-2 5
**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·mol$^{-1}$
$\Delta S$ = 66.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 212.2506
**Wiswesser Line Notation** RNVNR
**Evaluation** A

**$C_{13}H_{14}N_2$** (c) 87LES/LIC
Bis(4-aminophenyl)methane
**Heat Capacity** 298 K, $C_p$ = 270.9 J·mol$^{-1}$·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/BAB
3,3′-Methylene bis(6-aminophenol)
**Heat Capacity** 298.15 K, $C_p$ = 281.2 J·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 470 K.
**Entropy** 298.15 K, $S$ = 284.6 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 230.2658
**Wiswesser Line Notation** ZR BQ D1R CQ DZ
**Evaluation** A

**$C_{13}H_{15}NO$** (liq) 86ACH/HAS
1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl)benzene
**Heat Capacity** 333 K, $C_p$ = 382 J·mol$^{-1}$·K$^{-1}$
Temperature range 333, 433 K.
$C_p$ = 1.9 J·g$^{-1}$·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.

**$C_{13}H_{20}O$** (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 B1U1V1C1 C1
**Evaluation** B

**$C_{13}H_{22}O_8$** (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$^{-1}$) = 0.023598$T$ - 2.835
**Molecular Weight** 306.3120
**Wiswesser Line Notation** /*O2O2OV4VO1YQ71O*/
**Evaluation** D
Authors did not provide formula for repeating unit of polymer; assumed: glycol-adipate-glycerol, as repeating unit.

**$C_{13}H_{24}O_2$** (c) 81LEB/EVS
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, $\Delta H$ = 18150 J·mol$^{-1}$
$\Delta S$ = 62.45 J·mol$^{-1}$·K$^{-1}$
c,I/liq 300.4 K, $\Delta H$ = 9060 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 46000 J·mol$^{-1}$
$\Delta S$ = 125 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 212.3314
**Wiswesser Line Notation** /*OV-14-*/
**Evaluation** A

**$C_{13}H_{26}O$** (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

**$C_{13}H_{28}O$** (c) 83MAS/STE
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, $\Delta H$ = 7200 J·mol$^{-1}$
$\Delta S$ = 24 J·mol$^{-1}$·K$^{-1}$
Solid-plastic.
c/liq 390.15 K, $\Delta H$ = 3430 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{14}H_9NO_2$** (c) 77KAR/BAZ
Phthalanilic acid
**Heat Capacity** 300 K, $C_p$ = 279.5 J·mol$^{-1}$·K$^{-1}$
Temperature range 60 to 400 K.
**Entropy** 300 K, $S$ = 322.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 223.2306
**Wiswesser Line Notation** QVR BVMR
**Evaluation** B

**$C_{14}H_{10}$** (c) 87RAI/SIN
Phenanthrene
**Phase Changes**
c/liq (373) K, $\Delta H$ = 18627 J·mol$^{-1}$
$\Delta S$ = 49.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 178.2330
**Wiswesser Line Notation** L B666J
**Evaluation** B

$C_{14}H_{10}$ (c) 88TOR/BAR
Phenanthrene
**Phase Changes**
liq/g 350 K, $\Delta H = 87240$ J·mol$^{-1}$
$\Delta S = 249.3$ J·mol$^{-1}$·K$^{-1}$
c/g 298.15 K, $\Delta H = 90900$ J·mol$^{-1}$.
$\Delta S = 304.9$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 178.2330
**Wiswesser Line Notation** L B666J
**Evaluation** A

$C_{14}H_{10}$ (c) 86CHI/ANN
Diphenylacetylene; Diphenylethyne
**Phase Changes**
c/liq $\Delta H = 20502$ J·mol$^{-1}$
c/g $\Delta H = 90374$ J·mol$^{-1}$
**Molecular Weight** 178.2330
**Wiswesser Line Notation** R1UU1R
**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·mol$^{-1}$
$\Delta S = 61.65$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 210.2318
**Wiswesser Line Notation** RVVR
**Evaluation** C

$C_{14}H_{10}O_2$ (c) 83DWO
Benzil; Diphenyl diketone
**Heat Capacity** 298.15 K, $C_p = 245.7$ J·mol$^{-1}$·K$^{-1}$
Temperature range 15 to 300 K.
**Entropy** 298.15 K, $S = 292.08$ J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 84.07 K, $\Delta H = 44.1$ J·mol$^{-1}$
$\Delta S = 0.52$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 210.2318
**Wiswesser Line Notation** RVVR
**Evaluation** A

$C_{14}H_{11}NO_3$ (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** 241.2458
**Wiswesser Line Notation** T56 BVNVJ CR
**Evaluation** B

$C_{14}H_{12}$ (c) 87CHI/HOS
9,10-Dihydrophenanthrene
**Heat Capacity** 298.15 K, $C_p = 243.08$ J·mol$^{-1}$·K$^{-1}$
Temperature range 10 to 350 K.
**Entropy** 298.15 K, $S = 229.29$ J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$.

$C_{14}H_{12}$ (c) 87CHI/HOS2
9,10-Dihydroanthracene
**Heat Capacity** 298.15 K, $C_p = 219.06$ J·mol$^{-1}$·K$^{-1}$
Temperature range 10 to 500 K.
**Entropy** 298.15 K, $S = 218.97$ J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 382.18 K, $\Delta H = 23840$ J·mol$^{-1}$
$\Delta S = 62.38$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 180.2488
**Wiswesser Line Notation** L C666&T&J
**Evaluation** A

$C_{14}H_{12}$ (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, $\Delta H = 27370$ J·mol$^{-1}$
$\Delta S = 68.8$ 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, $\Delta H = 27690$ J·mol$^{-1}$
$\Delta S = 69.6$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 180.2488
**Wiswesser Line Notation** R1U1R -T
**Evaluation** A

$(C_{14}H_{12}Ge)n$ (gls) 78LEB/RAB
Polyvinylenediphenylgermyl-$\alpha,\omega$-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** 252.8588
**Wiswesser Line Notation** /*-GE-R&R&1U1*/
**Evaluation** A
$T$(glass) = 237 K.

$(C_{14}H_{12}Si)_n$ (gls) 78LEB/RAB
Polyvinylenediphenylsilyl-$\alpha,\omega$-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** /*-SI-R&R&1U1*/
**Evaluation** A
$T$(glass) = 264 K.

$C_{14}H_{14}$ (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, $\Delta H = 19241$ J·mol$^{-1}$
$\Delta S = 68.78$ 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, $\Delta H$ = 2279.9 J·mol$^{-1}$
$\Delta S$ = 7.78 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 182.2646
**Wiswesser Line Notation** 1R BR B1
**Evaluation** A

$C_{14}H_{14}$ (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, $\Delta H$ = 2068.0 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 213 J·mol$^{-1}$
$\Delta S$ = 0.75 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 298.0 K, $\Delta H$ = 1344.2 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 2921 J·mol$^{-1}$
$\Delta S$ = 7.53 J·mol$^{-1}$·K$^{-1}$
c,I/liq 373.245 K, $\Delta H$ = 19157 J·mol$^{-1}$
$\Delta S$ = 51.33 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 182.2646
**Wiswesser Line Notation** L C666T&&J
**Evaluation** A

$C_{14}H_{14}$ (c,I) 88MES/FIN
1,2-Diphenylethane
**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, $\Delta H$ = 2247.55 J·mol$^{-1}$
$\Delta S$ = 8.23 J·mol$^{-1}$·K$^{-1}$
c,I/liq 324.348 K, $\Delta H$ = 22730.52 J·mol$^{-1}$
$\Delta S$ = 70.08 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 182.2646
**Wiswesser Line Notation** R2R
**Evaluation** A

$C_{14}H_{14}N_2O_3$ (c) 82JAI
p-Azoxyanisole; 4,4'-Dimethoxyazoxybenzene
**Phase Changes**
c,III/c,I 250.7 K, $\Delta H$ = 104.6 J·mol$^{-1}$
$\Delta S$ = 0.42 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 335.6 K
c,II/liq 377.5 K, $\Delta H$ = 23891 J·mol$^{-1}$
$\Delta S$ = 63.30 J·mol$^{-1}$·K$^{-1}$
Crystal II-nematic.
c,I/liq 388.0 K, $\Delta H$ = 30430 J·mol$^{-1}$
$\Delta S$ = 78.41 J·mol$^{-1}$·K$^{-1}$
Crystal I-nematic.
liq/liq 406.9 K, $\Delta H$ = 757 J·mol$^{-1}$
$\Delta S$ = 1.84 J·mol$^{-1}$·K$^{-1}$
Nematic-isotropic.
**Molecular Weight** 258.2762
**Wiswesser Line Notation** 1OR DNUNOR DO1
**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** L6ØJ A1 Ø-CR-- ØL6ØJ 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, $\Delta H$ = 2514.3 J·mol$^{-1}$
$\Delta S$ = 7.59 J·mol$^{-1}$·K$^{-1}$
c,I/liq 345.390 K, $\Delta H$ = 18341.6 J·mol$^{-1}$
$\Delta S$ = 53.10 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 186.2962
**Wiswesser Line Notation** L 666 T&TJ
**Evaluation** A

**$C_{14}H_{24}$** (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, $\Delta H$ = 11155 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 10481 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 11832 J·mol$^{-1}$
$\Delta S$ = 41.81 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 192.3436
**Wiswesser Line Notation** L B666TJ
**Evaluation** B
(tat) trans/anti/trans isomer

**$C_{14}H_{26}O$** (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, $\Delta H$ = 30548 J·mol$^{-1}$
$\Delta S$ = 121.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 226.3582
**Wiswesser Line Notation** 10OVY1&U1
**Evaluation** A

**$C_{14}H_{27}O_2Tl$** (c) 76MEI/SEY
Thallium tetradecanoate
**Phase Changes**
c,III/,cII 313 K, $\Delta H$ = 11715 J·mol$^{-1}$
$\Delta S$ = 37.2 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 371 K, $\Delta H$ = 3138 J·mol$^{-1}$
$\Delta S$ = 8.37 J·mol$^{-1}$·K$^{-1}$
c,I/liq 393 K, $\Delta H$ = 5439 J·mol$^{-1}$
$\Delta S$ = 13.4 J·mol$^{-1}$·K$^{-1}$
Solid-mesophase.
liq/liq 460 K, $\Delta H$ = 1632 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 15099 J·mol$^{-1}$
$\Delta S$ = 47.39 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 378.0 K, $\Delta H$ = 2877 J·mol$^{-1}$
$\Delta S$ = 7.65 J·mol$^{-1}$·K$^{-1}$
c,I/liq 396.3 K, $\Delta H$ = 6269 J·mol$^{-1}$
$\Delta S$ = 15.80 J·mol$^{-1}$·K$^{-1}$
Solid-mesomorphic liquid.
**Molecular Weight** 431.7361
**Wiswesser Line Notation** OV13 .TL
**Evaluation** A
Mesomorphic liquid-isotropic liquid phase change data also given:
460.7 K, $\Delta H$ = 1671 J·mol$^{-1}$,
$\Delta S$ = 3.66 J·mol$^{-1}$·K$^{-1}$.

**$C_{14}H_{30}$** (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) 84GRO/BEN
*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/ING
*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/GRO
*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) 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/LAI
*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) 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

$C_{14}H_{30}S$ (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.
$C_p = 480.72 + 4.157\times10^{-2}T + 9.310\times10^{-5}T^2$ (J·mol$^{-1}$·K$^{-1}$)
**Molecular Weight** 230.4510
**Wiswesser Line Notation** SH14
**Evaluation** B

$C_{14}H_{36}N_2CdCl_4$ (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, $\Delta H$ = 17630 J·mol$^{-1}$
$\Delta S$ = 71.38 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 316.74 K, $\Delta H$ = 5060 J·mol$^{-1}$
$\Delta S$ = 16.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 486.6738
**Wiswesser Line Notation** 7ZH 2 .CD G4
**Evaluation** A

$C_{14}H_{36}N_2MgCl_4$ (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, $\Delta H$ = 16930 J·mol$^{-1}$
$\Delta S$ = 68.2 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 313.8 K, $\Delta H$ = 10197 J·mol$^{-1}$
$\Delta S$ = 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) 77LEB/RAB4
4,4′-Diphenyl methane 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, $\Delta H$ = 27300 J·mol$^{-1}$
$\Delta S$ = 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)

$C_{15}H_{12}$ (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.
**Entropy** 298.15 K, $S$ = 244.55 J·mol$^{-1}$K$^{-1}$
**Phase Changes**
c,III/c,II 182.0 K, $\Delta H$ = 22.4 J·mol$^{-1}$
$\Delta S$ = 0.12 J·mol$^{-1}$·K$^{-1}$
Extrapolated value.
c,II/c,I 295.0 K, $\Delta H$ = 14039 J·mol$^{-1}$
$\Delta S$ = 43.21 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 192.2598
**Wisweeser Line Notation** L B666J C1
**Evaluation** A

$C_{15}H_{11}N_3O_7$ (c) 79FAR/SHA
Indene picric acid
**Phase Changes**
c/liq 366.7 K, $\Delta H$ = 25100 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 22.4 J·mol$^{-1}$
$\Delta S$ = 0.12 J·mol$^{-1}$·K$^{-1}$
Extrapolated value.
c,II/c,I 295 K, $\Delta H$ = 33.3 J·mol$^{-1}$
$\Delta S$ = 0.11 J·mol$^{-1}$·K$^{-1}$
Extrapolated value.
c,I/liq 324.925 K, $\Delta H$ = 14039 J·mol$^{-1}$
$\Delta S$ = 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) 71/SOR/KOS
Tris-(cyclopentadienylcobalt)disulfide
**Phase Changes**
c,II/c,I 192.5 K, $\Delta H$ = 5253.4 J·mol$^{-1}$
$\Delta S$ = 28.894 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 436.2031
**Wiswesser Line Notation** L5ØJ Ø-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** L5ØJ Ø-Y-- ØL5ØJ &ØL5ØJ
**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, $\Delta H$ = 30100 J·mol$^{-1}$
$\Delta S$ = 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) 86GRI/LAZ
Aluminum acetylacetonate
**Phase Changes**
c/liq 466.7 K, $\Delta H$ = 33700 J·mol$^{-1}$
$\Delta S$ = 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-& BD6O-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, $\Delta H$ = 34000 J·mol$^{-1}$
$\Delta S$ = 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

$C_{15}H_{26}O_6$ (liq) 86NIL/WAD
Tributyrin; Glyceryl tributyrate
**Heat Capacity** 298.15 K, $C_p$ = 555.3 J·mol$^{-1}$·K$^{-1}$
One temperature.
**Molecular Weight** 302.3668
**Wiswesser Line Notation** 3VO1YOV3&1OV3
**Evaluation** A

$C_{15}H_{28}O$ (liq) 88BAG/GUR
3,7,11-Trimethyl-1-dodecen-3-ol
**Heat Capacity** 313.15 K, $C_p$ = 574.4 J·mol$^{-1}$·K$^{-1}$
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
**Molecular Weight** 224.3856
**Wiswesser Line Notation** 1Y3Y3XQ1UU1
**Evaluation** B

$C_{15}H_{28}O_8$ (liq) 83SAN/CIO
Diethylene glycol-trimethylolpropane-adipate polymer
**Heat Capacity** 298.15 K, $C_p$ = 636 J·mol$^{-1}$·K$^{-1}$
Temperature Range 273.15 to 323.15 K
$C_p$(kJ kg$^{-1}$·K$^{-1}$) = 0.016882$T$ - 3.143
**Molecular Weight** 336.3814
**Wiswesser Line Notation** /*O2O2OV4VO2Y1Q&20*/
**Evaluation** D
Authors did not provide formula for repeating unit of polymer; assumed: glycol-adipate-trimethylolpropane, as repeating unit.

$C_{15}H_{32}$ (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

**$C_{15}H_{32}O_6$** (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

**$(C_{16}H_8D_8)_n$** (gls) 82LEB/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

**$(C_{16}H_{10}Ge)_n$** (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-1UU1&R&R*/
**Evaluation** B

**$C_{16}H_{11}N_3O_7$** (c) 79FAR/SHA
Naphthalene picric acid
**Phase Changes**
c/liq 426.2 K, $\Delta H$ = 34700 J·mol$^{-1}$
$\Delta S$ = 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/MIL
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, $\Delta H$ = 20100 J·mol$^{-1}$
$\Delta S$ = 62.80 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 276.8608
**Wiswesser Line Notation** 1UU1-GE-1UU1&R&R
**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, $\Delta H$ = 20100 J·mol$^{-1}$
$\Delta S$ = 62.80 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 276.8608
**Wiswesser Line Notation** 1UU1-GE-1UU1&R&R
**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 to393 K.
**Phase Changes**
c,II/c,I 363.7 K, $\Delta H$ = 1350 J·mol$^{-1}$
$\Delta S$ = 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.

**$C_{16}H_{12}Si$** (c) 77MIL/LEB
Diphenyldiethynylsilane
**Heat Capacity** 298.15 K, $C_p$ = 381.8 J·mol$^{-1}$·K$^{-1}$
Temperature range 10 to 326 K.
**Entropy** 298.15 K, $S$ = 411.3 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 209 K, $\Delta H$ = 22360 J·mol$^{-1}$
$\Delta S$ = 70.60 J·mol$^{-1}$·K$^{-1}$
Crystal-glass transition.
c,I/liq 316.72 K
**Molecular Weight** 232.3563
**Wiswesser Line Notation** 1UU1-SI-1UU1&R&R
**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·mol$^{-1}$·K$^{-1}$
Temperature range 0 to 330 K.
**Entropy** 298.15 K, $S$ = 330.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 269.2994
**Wiswesser Line Notation** T5NVOTJ AR D1OR
**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·mol$^{-1}$·K$^{-1}$
One temperature.
$C_p$ given as 0.290 cal·K$^{-1}$·g$^{-1}$.
**Molecular Weight** 208.3024
**Wiswesser Line Notation** L F6 C-12-6 *A* B F- F--&T&J
**Evaluation** A

**$C_{16}H_{18}$** (c) 83KRA/BEC
2,3-Dimethyl-2,3-diphenylbutane
**Heat Capacity** 298 K, $C_p$ = 283.4 J·mol$^{-1}$·K$^{-1}$
One temperature.
$C_p$ given as 0.322 Cal.K$^{-1}$.g$^{-1}$.
**Molecular Weight** 210.3182
**Wiswesser Line Notation** 1XR&XR
**Evaluation** B

**$C_{16}H_{20}CrI$** (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** L6ØJ A1 C1 Ø-CR-- ØL6ØJ A1 C1 &I
**Evaluation** B

**$C_{16}H_{20}CrI$** (liq) 72NIK/SAF
Bis(ethylbenzene)chromium iodide
**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** 391.2345
**Wiswesser Line Notation** L6ØJ A2 Ø-CR-- ØL6ØJ A2 &I
**Evaluation** B
Data also given for glassy phase from 60 to 190 K.

**$C_{16}H_{22}OSi_2$** (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.

**$C_{16}H_{22}O_3Si_3$** (liq) 87DZH/KUL2
1,1,3,3-Tetraethyl-5,5-diphenylcylotrisiloxane
**Heat Capacity** 298.15 K, $C_p$ = 629.6 J·mol$^{-1}$·K$^{-1}$
Temperature range 5 to 315 K.
**Entropy** 298.15 K, $S$ = 711.4 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 279.082 K, $\Delta H$ = 18374 J·mol$^{-1}$
$\Delta S$ = 66.01 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 346.6045
**Wiswesser Line Notation** T6-SI-O-SI-O-SI-OTJ A1 A1 C1 C1 ER ER
**Evaluation** A

**$C_{16}H_{22}O_4$** (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.

**$C_{16}H_{24}Si_8O_{12}$** (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, $\Delta H$ = 9200 J·mol$^{-1}$
$\Delta S$ = 40.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 633.0424
**Wiswesser Line Notation** XXXXXX
**Evaluation** C($C_p$), B(Phase changes)

**$C_{16}H_{31}O_2Tl$** (c) 76MEI/SEY
Thallium hexadecanoate
**Phase Changes**
liq/liq 450 K, $\Delta H$ = 1381 J·mol$^{-1}$
$\Delta S$ = 3.05 J·mol$^{-1}$·K$^{-1}$
Mesophase-isotropic.
c,II/c,I 327 K, $\Delta H$ = 10878 J·mol$^{-1}$
$\Delta S$ = 33.5 J·mol$^{-1}$·K$^{-1}$
c,I/liq 390 K, $\Delta H$ = 8786 J·mol$^{-1}$
$\Delta S$ = 22.2 J·mol$^{-1}$·K$^{-1}$
Solid-mesophase.
**Molecular Weight** 459.7897
**Wiswesser Line Notation** OV15 .TL
**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) 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) 82ZAR
*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) 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** A

$C_{16}H_{34}O$ (c) 1889EYK
*n*-Cetyl alcohol; 1-Hexadecanol
**Phase Changes**
c/liq 320 K, $\Delta H$ = 34727 J·mol$^{-1}$
$\Delta S$ = 108.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 242.4440
**Wiswesser Line Notation** Q16
**Evaluation** C

$C_{16}H_{34}S$ (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.
$C_p = 553.16 + 4.153\times10^{-2}T + 9.560\times10^{-5}T^2$.
**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

$C_{16}H_{36}ClN$ (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, $\Delta H$ = 33610 J·mol$^{-1}$
$\Delta S$ = 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

$C_{16}H_{40}O_4Si_4$ (liq) 87DZH/KUL
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, $\Delta H$ = 12219 J·mol$^{-1}$
$\Delta S$ = 58.69 J·mol$^{-1}$·K$^{-1}$
c,I/liq 213.35 K, $\Delta H$ = 13705 J·mol$^{-1}$
$\Delta S$ = 64.38 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 408.8316
**Wiswesser Line Notation** T8-SI-O-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 E2 G2 G2
**Evaluation** A

$C_{17}H_{12}$ (c) 79FAR/SHA
2,3-Benzofluorene
**Phase Changes**
c/liq 489.7 K, $\Delta H$ = 23400 J·mol$^{-1}$
$\Delta S$ = 47.8 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 216.2818
**Wiswesser Line Notation** L D6 B656 LHJ
**Evaluation** B

$C_{17}H_{12}$ (c) 79FAR/SHA
1,2-Benzofluorene
**Phase Changes**
c,II/c,I 399.9 K, $\Delta H$ = 3800 J·mol$^{-1}$
$\Delta S$ = 9.50 J·mol$^{-1}$·K$^{-1}$
c/liq 462.8 K, $\Delta H$ = 18400 J·mol$^{-1}$
$\Delta S$ = 39.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 216.2818
**Wiswesser Line Notation** L D6 B566 CHJ
**Evaluation** B

$C_{17}H_{14}N_2$ (c) 77LEB/RAB4
2,2-Bis(4-cyanatophenyl)propane
**Heat Capacity** 300 K, $C_p$ = 360 J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S$ = 74.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 246.3110
**Wiswesser Line Notation** NCR DX1&1&R DCN
**Evaluation** C($C_p$); A(Phase changes)

$C_{17}H_{14}N_2$ (c) 75LEB/ARO
2,2-Bis-(4-cyanatophenyl)propane
**Heat Capacity** 298.15 K, $C_p$ = 355.64 J·mol$^{-1}$·K$^{-1}$
Temperature range 0 to 420 K.
**Entropy** 298.15 K, $S$ = 391.2 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c/liq 355.83 K, $\Delta H$ = 26694 J·mol$^{-1}$
$\Delta S$ = 74.89 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 246.3110
**Wiswesser Line Notation** NCR DX1&1&R DCN
**Evaluation** A

**$(C_{17}H_{14}N_2O_2)_n$** (amorph) 75LEB/ARO
Poly[2,2-bis-(4-phenoxypropane)]2,4,6-triazine; Polycyanate
**Heat Capacity** 298.15 K, $C_p$ = 326.8 J·mol$^{-1}$·K$^{-1}$
Temperature range 0 to 420 K.
**Entropy** 298.15 K, $S$ = 325.9 J·mol$^{-1}$·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-dimethylaminopropylidene)-10-thioxanthene hydrochloride
**Phase Changes**
c/liq 294.85 K, $\Delta H$ = 28420 J·mol$^{-1}$
$\Delta S$ = 60.8 J·mol$^{-1}$·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).

**$C_{17}H_{36}$** (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

**$C_{18}H_8N_4$** (c) 79BOE/WES
Naphthalene-tetracyanoethylene
**Heat Capacity**
Temperature range 5 to 300 K.
Data graphically only.
**Phase Changes**
c,III/c,II 160 K, $\Delta S$ = 5.10 J·mol$^{-1}$·K$^{-1}$
Bifurcated peak.
Transition region 150 to 172.5 K.
c,II/c,I 222 K, $\Delta S$ = 5.02 J·mol$^{-1}$·K$^{-1}$
Extended transition.
Transition region 172.5 to 240K.
**Molecular Weight** 280.2880
**Wiswesser Line Notation** L66J &NC1U1CN
**Evaluation** A

**$C_{18}H_{11}N_3O_7$** (c) 79FAR/SHA
Acenaphthene picric acid
**Phase Changes**
c/liq 436.3 K, $\Delta H$ = 36000 J·mol$^{-1}$
$\Delta S$ = 82.5 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 381.3008
**Wiswesser Line Notation** L566 1A LT&&J &WNR BQ CNW ENW
**Evaluation** B

**$C_{18}H_{14}$** (c) 83CHA
*p*-Terphenyl
**Heat Capacity** 298.15 K, $C_p$ = 278.68 J·mol$^{-1}$·K$^{-1}$
Temperature range 4 to 580 K.
$C_p = 35.12 + 0.58825T + 0.0010062T^2 - 8.042\times10^{-7}T^3$
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, $\Delta H$ = 35300 J·mol$^{-1}$
$\Delta S$ = 72.5 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, $\Delta H$ = 41600 J·mol$^{-1}$
$\Delta S$ = 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) 79SMI
*p*-Terphenyl
**Phase Changes**
c/liq 486.3 K, $\Delta H$ = 35500 J·mol$^{-1}$
$\Delta S$ = 73.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 230.3086
**Wiswesser Line Notation** RR DR
**Evaluation** A

**$C_{18}H_{15}ClSi$** (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, $\Delta H$ = 26878 J·mol$^{-1}$
$\Delta S$ = 72.53 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 294.8550
**Wiswesser Line Notation** G-SI-R&R&R
**Evaluation** A

**$C_{18}H_{15}OP$** (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, $\Delta H$ = 23800 J·mol$^{-1}$
$\Delta S$ = 55.5 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, $\Delta H = 24220$ J·mol$^{-1}$
$\Delta S = 56.08$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 278.2897
**Wiswesser Line Notation** OPR&R&R
**Evaluation** A

**$C_{18}H_{15}O_4P$** (c) 86RAB/PET
Triphenyl phosphate
**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, $\Delta H = 29610$ J·mol$^{-1}$
$\Delta S = 91.80$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 326.2879
**Wiswesser Line Notation** RO 3 &PO
**Evaluation** A

**$C_{18}H_{15}P$** (c) 88KIR/DOM
Triphenylphosphine
**Phase Changes**
c/liq 354.4 K, $\Delta H = 19690$ J·mol$^{-1}$
$\Delta S = 55.56$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 262.2903
**Wiswesser Line Notation** RPR&R
**Evaluation** A

**$C_{18}H_{16}$** (liq) 78GOO/SCO
4b$\alpha$,4c$\beta$,5,9b$\beta$,9c$\alpha$,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

**$C_{18}H_{16}$** (liq) 78GOO/SCO
4b$\beta$,4c$\alpha$,9,9a$\alpha$,9b$\beta$,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

**$C_{18}H_{18}$** (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

**$C_{18}H_{18}ClNS$** (c) 83CHA/MAS
Chlorprothixene; 2-Chloro-9-(3-dimethylamino-propylidene)-10-thioxanthene
**Phase Changes**
c/liq 370.3 K, $\Delta H = 27820$ J·mol$^{-1}$
$\Delta S = 75.1$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 315.8663
**Wiswesser Line Notation** T C666 BS IYT EG IU3N1&1
**Evaluation** C

**$C_{18}H_{21}NO$** (liq) 75JAN/JAN
N-(4-Methoxybenzylidene)-*p*-(*n*-butyl)aniline
**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, $\Delta H = 18033$ J·mol$^{-1}$
$\Delta S = 61.04$ J·mol$^{-1}$·K$^{-1}$
Data also given for metastable modification:
294.0 K, $\Delta H = 14757$ J·mol$^{-1}$
$\Delta S = 50.21$ 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; $\Delta S = 1.962$ 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

**$C_{18}H_{22}N_2O$** (liq) 85SHA/ZHU
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, $\Delta H = 655$ J·mol$^{-1}$
$\Delta S = 1.84$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 282.3846
**Wiswesser Line Notation** 4R DNUNR DO2
**Evaluation** B

**$C_{18}H_{24}CrI$** (c) 72NIK/SAF
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, $\Delta H = 105$ J·mol$^{-1}$
$\Delta S = 0.40$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 419.2881
**Wiswesser Line Notation** L6ØJ A1 C1 D1 Ø-CR--ØL6ØJ A1 C1 D1 &I
**Evaluation** B

**$C_{18}H_{24}CrI$** (c) 72NIK/SAF
Bis(diisopropylbenzene)chromium iodide
**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** 419.2881
**Wiswesser Line Notation** L6ØJ AY DY Ø-CR-- ØL6ØJ AY DY &I
**Evaluation** B

**$C_{18}H_{28}Si_4O_4$** (c) 81MEK/KAR
1,1,3,3,5,5-Hexamethyl-7,7-diphenyltetrasiloxane
**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, $\Delta H$ = 42731 J·mol$^{-1}$
$\Delta S$ = 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 $\Delta H$ = 94977 J·mol$^{-1}$
**Molecular Weight** 246.4350
**Wiswesser Line Notation** 2R B2 C2 D2 E2 F2
**Evaluation** A

**$C_{18}H_{30}BaCa_2O_{12}$** (c) 55MOM/SEK
Barium dicalcium propionate
**Phase Changes**
c/liq 268.4 K, $\Delta H$ = 7284 J·mol$^{-1}$
$\Delta S$ = 27.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 655.9178
**Wiswesser Line Notation** OV1 6 .BE 4O
**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, $\Delta H$ = 4853 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 1067 J·mol$^{-1}$
$\Delta S$ = 13.4 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 282.6 K, $\Delta H$ = 667.8 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 1305 J·mol$^{-1}$
$\Delta S$ = 8.4 J·mol$^{-1}$·K$^{-1}$
c,I/liq 326.21 K, $\Delta H$ = 23502 J·mol$^{-1}$
$\Delta S_m$ = 23502/326.21 = 72.0 J·mol$^{-1}$·K$^{-1}$.
**Molecular Weight** 310.4326
**Wiswesser Line Notation** 2OXO2&1&R DX1&O2&O2
**Evaluation** A
$T$(glass) = 208.0 K, see also 78KAR/SAP.

**$C_{18}H_{30}O_4$** (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, $\Delta H$ = 1307 J·mol$^{-1}$
$\Delta S$ = 8.15 J·mol$^{-1}$·K$^{-1}$
c,I/liq 326.21 K, $\Delta H$ = 23500 J·mol$^{-1}$
$\Delta S$ = 72.04 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 310.4326
**Wiswesser Line Notation** 2OXO2&1&R DX1&O2&O2
**Evaluation** C($C_p$), A(S,Phase changes)
$T$(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, $\Delta H$ = 1307 J·mol$^{-1}$
$\Delta S$ = 8.14 J·mol$^{-1}$·K$^{-1}$
c,I/liq 326.61 K, $\Delta H$ = 23500 J·mol$^{-1}$
$\Delta S$ = 71.95 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 310.4326
**Wiswesser Line Notation** 2OXO2&1&R DX1&O2&O2
**Evaluation** A
Glass transition at $T$(glass) = 208 K.

**$C_{18}H_{32}O$** (liq) 88BAG/GUR
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

**$C_{18}H_{34}O_3$** (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;
$\Delta C_p$ = 0.55 J·g$^{-1}$·K$^{-1}$ for glass to supercooled liquid transition.
c/liq 264.87 K, $\Delta H$ = 17016 J·mol$^{-1}$
$\Delta S$ = 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.

**$C_{18}H_{35}O_2Tl$** (c) 76MEI/SEY
Thallium octadecanoate
**Phase Changes**
liq/liq 444 K, $\Delta H = 1381$ J·mol$^{-1}$
$\Delta S = 3.05$ J·mol$^{-1}$·K$^{-1}$
Mesophase-isotropic.
c,III/c,II 324 K, $\Delta H = 9623$ J·mol$^{-1}$
$\Delta S = 29.3$ J·mol$^{-1}$·K$^{-1}$
c,II/c,I 380 K, $\Delta H = 12134$ J·mol$^{-1}$
$\Delta S = 12.1$ J·mol$^{-1}$·K$^{-1}$
c,I/liq 385 K, $\Delta H = 5439$ J·mol$^{-1}$
$\Delta S = 14.2$ J·mol$^{-1}$·K$^{-1}$
Solid-mesophase.
**Molecular Weight** 487.8433
**Wiswesser Line Notation** OV17 .TL
**Evaluation** B

**$C_{18}H_{36}$** (c) 69BOR/DAL
Cyclooctadecane
**Phase Changes**
c,II/c,I 298 K, $\Delta H = 29288$ J·mol$^{-1}$
$\Delta S = 97.5$ J·mol$^{-1}$·K$^{-1}$
c/liq 346 K, $\Delta H = 9874$ J·mol$^{-1}$
$\Delta S = 28.4$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 252.4824
**Wiswesser Line Notation** L-18-TJ
**Evaluation** B

**$C_{18}H_{36}O$** (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

**$C_{18}H_{36}O_2$** (c) 1889EYK
Octadecanoic acid; Stearic acid
**Phase Changes**
c/liq 326.1 K, $\Delta H = 64643$ J·mol$^{-1}$
$\Delta S = 198$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 284.4812
**Wiswesser Line Notation** QV17
**Evaluation** C

**$C_{18}H_{36}O_2$** (c) 83BEC/ROU
Octadecanoic acid; Stearic acid
**Phase Changes**
c/liq 345, 346 K, $\Delta H = 62600$ J·mol$^{-1}$
$\Delta S = 181$ J·mol$^{-1}$·K$^{-1}$
First peak due to pre-melting or dissociation.
**Molecular Weight** 284.4812
**Wiswesser Line Notation** QV17
**Evaluation** B

**$C_{18}H_{38}$** (c) 55SCH/BUS
*n*-Octadecane
**Phase Changes**
c,I/liq 301.35 K, $\Delta H = 61379$ J·mol$^{-1}$
$\Delta S = 203.6$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 254.4982
**Wiswesser Line Notation** 18H
**Evaluation** B

**$C_{18}H_{38}$** (liq) 81HOE
*n*-Octadecane
**Heat Capacity** 325 K, $C_p = 568$ J·mol$^{-1}$·K$^{-1}$
Temperature range 300 to 500 K.
Cv = 2.20 J·g$^{-1}$·K$^{-1}$.
**Molecular Weight** 254.4982
**Wiswesser Line Notation** 18H
**Evaluation** B

**$C_{18}H_{38}$** (c) 85KOL/SYU
*n*-Octadecane
**Phase Changes**
c/liq 301.0 K, $\Delta H = 60760$ J·mol$^{-1}$
$\Delta S = 201.9$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 254.4982
**Wiswesser Line Notation** 18H
**Evaluation** A

**$C_{18}H_{38}O_7$** (liq) 82ZAR
Hexapropylene glycol
**Heat Capacity** 298 K, $C_p = 807.4$ J·mol$^{-1}$·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·mol$^{-1}$·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

**$C_{19}H_{13}N_3O_7$** (c) 79FAR/SHA
Fluorene picric acid
**Phase Changes**
c/liq 350.3 K, $\Delta H = 26800$ J·mol$^{-1}$
$\Delta S = 76.5$ J·mol$^{-1}$·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·mol$^{-1}$·K$^{-1}$
Temperature range 10 to 450 K.
**Entropy** 298.15 K, $S = 306.8$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 270.3330
**Wiswesser Line Notation** T56 BN DNJ CR DR
**Evaluation** A

**$C_{19}H_{16}N_2O$** (c) 74KAR/RAB
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

**$C_{19}H_{20}N_2O_3$** (c) 83FAN/POE

4-Propionyl-4′-*n*-butanoyloxyazobenzene

**Phase Changes**

c/liq 366 K, $\Delta H = 15021$ J·mol$^{-1}$
$\Delta S = 41.04$ 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 liquid phase change data also given: 392.65 K, $\Delta H = 10920$ J·mol$^{-1}$; 409.65 K, $\Delta H = 4100$ J·mol$^{-1}$; 428.65 K, $\Delta H = 753$ J·mol$^{-1}$.

**$C_{19}H_{22}ClNO$** (c) 82TSU/SOR2

*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, $\Delta H = 10880$ J·mol$^{-1}$
$\Delta S = 33.2$ J·mol$^{-1}$·K$^{-1}$

Crystal to intermediate phase $S_3$.

**Molecular Weight** 315.8419

**Wiswesser Line Notation** GR DNU1R DO6

**Evaluation** A

$S_3$-smectic B; smectic B-smectic A; smectic A-isotropic liquid phase change data also given: 333.90 K, $\Delta H = 12350$ J·mol$^{-1}$, $\Delta S = 37.0$ J·mol$^{-1}$·K$^{-1}$; 362.98 K, $\Delta H = 3390$ J·mol$^{-1}$, $\Delta S = 9.3$ J·mol$^{-1}$·K$^{-1}$; 370.38 K, $\Delta H = 5790$ J·mol$^{-1}$, $\Delta S = 15.6$ J·mol$^{-1}$·K$^{-1}$.

**$C_{19}H_{22}FNO$** (c) 82TSU/SOR3

*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, $\Delta H = 23220$ J·mol$^{-1}$
$\Delta S = 70.7$ J·mol$^{-1}$·K$^{-1}$

Crystal to smectic B.

**Molecular Weight** 299.3873

**Wiswesser Line Notation** FR DNU1R DO6

**Evaluation** A

Smectic B-smectic A; smectic A-nematic; nematic-isotropic liquid phase change data also given: 330.33 K, $\Delta H = 3050$ J·mol$^{-1}$, $\Delta S = 9.2$ J·mol$^{-1}$·K$^{-1}$; 334.88 K, $\Delta H = 3410$ J·mol$^{-1}$, $\Delta S = 10.2$ J·mol$^{-1}$·K$^{-1}$; 336.33 K, $\Delta H = 1170$ J·mol$^{-1}$, $\Delta S = 3.5$ J·mol$^{-1}$·K$^{-1}$.

**$C_{19}H_{23}NO$** (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, $\Delta H = 1553$ J·mol$^{-1}$
$\Delta S = 4.524$ J·mol$^{-1}$·K$^{-1}$

Nematic-isotropic.

c/liq 305.62 K, $\Delta H = 27090$ J·mol$^{-1}$
$\Delta S = 88.71$ 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,

**Entrop** 298.15 K, $\Delta S = 421.788$ J·mol$^{-1}$·K$^{-1}$

**Phase Changes**

c/nematic liq 305.62 K, $\Delta H = 27090$ J·mol$^{-1}$
$\Delta S = 88.71$ J·mol$^{-1}$·K$^{-1}$

Crystal-nematic

liq/liq 349.08 K, $\Delta H = 1553$ J·mol$^{-1}$
$\Delta S = 4.524$ J·mol$^{-1}$·K$^{-1}$

Nematic-isotropic

**Molecular Weight 281.3968**

**Wiswesser Line Notation** 4R DNUIR DO2

**Evaluation** A

**$C_{19}H_{23}NO$** (c) 82TSU/SOR

*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, $\Delta H = 192$ J·mol$^{-1}$
$\Delta S = 2.70$ J·mol$^{-1}$·K$^{-1}$

c,I/liq 321.63 K, $\Delta H = 309100$ J·mol$^{-1}$
$\Delta S = 96.1$ J·mol$^{-1}$·K$^{-1}$

Solid-isotropic liquid.

**Molecular Weight** 281.3968

**Wiswesser Line Notation** 6OR D1UNR

**Evaluation** A

**$C_{19}H_{40}$** (c) 55SCH/BUS

*n*-Nonadecane

**Phase Changes**

c,II/c,I 295.95 K, $\Delta H = 13807$ J·mol$^{-1}$
$\Delta S = 46.7$ J·mol$^{-1}$·K$^{-1}$

c,I/liq 305.15 K, $\Delta H = 45815$ J·mol$^{-1}$
$\Delta S = 150.1$ J·mol$^{-1}$·K$^{-1}$

**Molecular Weight** 268.5250

**Wiswesser Line Notation** 19H

**Evaluation** B

**$C_{19}H_{40}$** (c) 79CLA/LET

*n*-Nonadecane

**Phase Changes**

c,II/c,I 295.95 K, $\Delta H = 13665$ J·mol$^{-1}$
$\Delta S = 46.2$ J·mol$^{-1}$·K$^{-1}$

c,I/liq 303.95 K, $\Delta H = 47395$ J·mol$^{-1}$
$\Delta S = 155.9$ J·mol$^{-1}$·K$^{-1}$

**Molecular Weight** 268.5250

**Wiswesser Line Notation** 19H

**Evaluation** B

$C_{20}H_{10}N_4$ (c) 79BOE/WES
Naphthalene-tetracyanobenzene
**Heat Capacity**
Temperature range 30 to 80 K.
Data given graphically only.
**Phase Changes**
c,II/c,I 70 K, $\Delta S = 2.97$ J·mol$^{-1}$·K$^{-1}$
Transition extends over 50 K region, abruptly ending at 70 K.
**Molecular Weight** 306.3258
**Wiswesser Line Notation** L66J &NCR BCN DCN ECN
**Evaluation** A

$C_{20}H_{11}Cl_4NO_2$ (c) 87ECO/BER
AnthraceneTCNB; Anthracene-1,2,4,5-tetrachloro-3-nitrobenzene
**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, $\Delta H = 151$ J·mol$^{-1}$
$\Delta S = 0.71$ J·mol$^{-1}$·K$^{-1}$
Total enthalpy and entropy between 180 and 215 K.
**Molecular Weight** 439.1244
**Wiswesser Line Notation** WNR BG CG EG FG & L C666J
**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·mol$^{-1}$
$\Delta S = 28.8$ J·mol$^{-1}$·K$^{-1}$
c/liq 417.6 K, $\Delta H = 24300$ J·mol$^{-1}$
$\Delta S = 58.2$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 407.3386
**Wiswesser Line Notation** L C666J &WNR BQ CNW ENW
**Evaluation** B

$C_{20}H_{14}$ (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** L 6 H66 O66/GT 2AF T GH NHJ
**Evaluation** A

$C_{20}H_{14}$ (c) 79FAR/SHA
$\beta,\beta'$-Binaphthyl
**Phase Changes**
c/liq 461.2 K, $\Delta H = 38900$ J·mol$^{-1}$
$\Delta S = 84.4$ 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, $\Delta H = 7110$ J·mol$^{-1}$
$\Delta S = 15.86$ J·mol$^{-1}$·K$^{-1}$
c,II/c,I 488 K, $\Delta H = 40200$ J·mol$^{-1}$
$\Delta S = 62.38$ 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, $\Delta H = 22594$ J·mol$^{-1}$
$\Delta S = 55.0$ J·mol$^{-1}$·K$^{-1}$
Amorphous/crystal.
c/liq 534 K, $\Delta H = 51045$ J·mol$^{-1}$
$\Delta S = 95.6$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 318.3282
**Wiswesser Line Notation** T56 BVOT&J DR DQ DR DQ
**Evaluation** B

$C_{20}H_{16}Fe_2I_3$ (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, $\Delta H = 538$ J·mol$^{-1}$
$\Delta S = 1.77$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 748.7539
**Wiswesser Line Notation** L5ØJ Ø-FE- - ØL5ØJ A- AL5ØJØ-FE- - ØL5ØJ &I3
**Evaluation** A

$C_{20}H_{18}Sn$ (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,11,12,12a,12b-Octahydrodibenzo-[a,g]biphenylene
**Heat Capacity** 298.15 K, $C_p = 323.6$ J·mol$^{-1}$·K$^{-1}$
One temperature. $C_p$ given as 0.297 cal·g$^{-1}$.
**Molecular Weight** 260.3780
**Wiswesser Line Notation** L F6 C6 B466 &TTT&J
**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. $C_p$ given as 0.306 cal·g$^{-1}$.
**Molecular Weight** 260.3780
**Wiswesser Line Notation** L D6 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. $C_p$ given as 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, $\Delta H$ = 5110 J·mol$^{-1}$
$\Delta S$ = 16.7 J·mol$^{-1}$·K$^{-1}$
c,I/liq 334.05 K, $\Delta H$ = 23770 J·mol$^{-1}$
$\Delta S$ = 71.2 J·mol$^{-1}$·K$^{-1}$
Solid nematic.
**Molecular Weight** 306.4066
**Wiswesser Line Notation** NCR DNU1R DO6
**Evaluation** A
Nematic-isotropic liquid phase data also given:
375.10 K, $\Delta H$ = 1750 J·mol$^{-1}$,
$\Delta S$ = 3.2 J·mol$^{-1}$·K$^{-1}$
(Note: 1750/375.10 = 4.67 J·mol$^{-1}$·K$^{-1}$).

**$C_{20}H_{24}N_2O_3$** (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, $\Delta H$ = 573 J·mol$^{-1}$
$\Delta S$ = 1.54 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 340.4212
**Wiswesser Line Notation** 6VOR DNUNR DO1
**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 to385 K.
**Entropy** 298.15 K, $S$ = 448.95 J·mol$^{-1}$·K$^{-1}$
**Phase Changes**
c,II/c,I 317.5 K, $\Delta H$ = 5040 J·mol$^{-1}$
$\Delta S$ = 15.89 J·mol$^{-1}$·K$^{-1}$
Superheating phenomenon occurs at 324 K.
c,I/liq 334.26 K, $\Delta H$ = 25040 J·mol$^{-1}$
$\Delta S$ = 74.90 J·mol$^{-1}$·K$^{-1}$
Solid-nematic.
**Molecular Weight** 295.4236
**Wiswesser Line Notation** 60R D1UNR D1
**Evaluation** A
Nematic-isotropic liquid phase change data also given:
346.90 K, $\Delta H$ = 1370 J·mol$^{-1}$,
$\Delta S$ = 3.0 J·mol$^{-1}$·K$^{-1}$.

**$C_{20}H_{26}O$** (c) 79LEW/ENE

Northindrone
**Phase Changes**
c/liq 479 K, $\Delta H$ = 39600 J·mol$^{-1}$
$\Delta S$ = 82.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 282.4248
**Wiswesser Line Notation** L E5 B666 OV MUTJ E1 FQ F1UU1
**Evaluation** A

**$C_{20}H_{28}ZrO_6$** (c) 86GRI/LAZ

Zirconium acetylacetonate
**Phase Changes**
c/liq 470.8 K, $\Delta H$ = 50100 J·mol$^{-1}$
$\Delta S$ = 106.3 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 455.6576
**Wiswesser Line Notation** D6O-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

**$C_{20}H_{33}Cl_2FeN_6O$** (c) 85KAJ/SOR

Tris(2-picolylamine)iron chloride ethanolate
**Heat Capacity** 300 K, $C_p$ = 590 J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S$ = 50.59 J·mol$^{-1}$·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)

**$C_{20}H_{40}O$** (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** 296.5354
**Wiswesser Line Notation** 1Y3Y3Y3XQ1U1
**Evaluation** B

**$C_{20}H_{40}O$** (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** 296.5354
**Wiswesser Line Notation** 1Y3Y3Y3XQ1UU1
**Evaluation** B

**$C_{20}H_{41}NO$** (liq) 81ARU/DAU

4-Octyl-4'-heptyl-α-cyanostilbene
**Heat Capacity**
Temperature range 320 to 340 K.
Data given graphically.
**Molecular Weight** 311.5500
**Wiswesser Line Notation** 8OR D1U1R DYCN&6
**Evaluation** C
Smectic C-smectic A, 324.3 K;
smectic A-nematic, 337.3 K, $\Delta S$ = 1.66 J·mol$^{-1}$·K$^{-1}$;
nematic-isotropic liquid, 338.5 K, $\Delta S$ = 6.98 J·mol$^{-1}$·K$^{-1}$
phase change data given. Assume trans isomer.

**$C_{20}H_{42}$** (c) 55SCH/BUS

*n*-Eicosane
**Phase Changes**
c,II/c,I 309.35 K
c,I/liq 309.75 K, $\Delta H$ = 69873 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 69873 J·mol$^{-1}$
$\Delta S$ = 225.6 J·mol$^{-1}$·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·mol$^{-1}$
$\Delta S = 229.8$ J·mol$^{-1}$·K$^{-1}$
Relative error in determination ± 5%.
**Molecular Weight** 282.5518
**Wiswesser Line Notation** 20H
**Evaluation** B

$C_{20}H_{42}$ (c) 85KOL/SYU
*n*-Eicosane
**Phase Changes**
c/liq 308.8 K, $\Delta H = 67800$ J·mol$^{-1}$
$\Delta S = 219.6$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 282.5518
**Wiswesser Line Notation** 20H
**Evaluation** A

$C_{20}H_{42}$ (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

$C_{20}H_{42}S$ (liq) 82TUT/GAB
1-Eicosanethiol; *n*-Eicosanyl mercaptan
**Heat Capacity** 300 K, $C_p = 725.84$ J·mol$^{-1}$·K$^{-1}$
Temperature range 273 to 373 K.
$C_p = 702.70 + 4.703\times10^{-2}T + 10.040\times10^{-5}T^2$.
**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·mol$^{-1}$·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·mol$^{-1}$
$\Delta S = 158.97$ J·mol$^{-1}$·K$^{-1}$
$\Delta H$, $\Delta S$ combined data.
**Molecular Weight** 334.0273
**Wiswesser Line Notation** 10M10 &GH
**Evaluation** A

$C_{20}H_{48}Cl_4MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(decylammonium) manganese II
**Phase Changes**
c,III/c,II 309 K, $\Delta H = 1937$ J·mol$^{-1}$
$\Delta S = 6.3$ J·mol$^{-1}$·K$^{-1}$
c,II/c,I 437 K, $\Delta H = 16.8$ J·mol$^{-1}$
$\Delta S = 0.038$ J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 513.3626
**Wiswesser Line Notation** 10ZH 2 .MN G4
**Evaluation** A

$C_{20}.84H_{16}.66O_{0.62}$ (c) 78KAR/SAP
Polyphenylene PP-1
**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 use the repeating unit: $(C_{18}H_{12})_n$.

$C_{20}.84H_{16}.66O_{0.62}$ (c) 78KAR/SAP
Polyphenylene PP-2
**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 DR C* ER/
**Evaluation** C
WLN excludes ketal end groups and use 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) 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* H1- HT56 BN DOJ CR& C*/
**Evaluation** A

$C_{21}H_{15}N_3$ (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

$(C_{21}H_{16}N_2O_4)_n$ (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
$T$(glass) = 207.0 K.

**$C_{21}H_{24}N_2O_3$** (c) 83FAN/POE
4-Propionyl-4′-*n*-hexanoyloxyazobenzene
**Phase Changes**
c/liq 372.15 K, $\Delta H$ = 29790 J·mol$^{-1}$
Solid-smectic A.
**Molecular Weight** 352.4322
**Wiswesser Line Notation** 5VOR DNUNR DV2
**Evaluation** A
Smectic A-nematic; nematic-isotropic;
smectic A-smectic B (montropic phase) liquid
phase change data also given:
411.65 K, $\Delta H$ = 3933 J·mol$^{-1}$;
420.65 K, $\Delta H$ = 879 J·mol$^{-1}$;
361.65 K, $\Delta H$ = 2720 J·mol$^{-1}$.

**$C_{21}H_{24}O_4$** (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

**$C_{21}H_{24}Si_3O_3$** (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, $\Delta H$ = 47254 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 43769 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{21}H_{25}N$** (c) 83MAR/THO
Octylcyanobiphenyl
**Phase Changes**
liq/liq $\Delta H$ = 0.4 J·mol$^{-1}$
Smectic A− nematic.
liq/liq $\Delta H$ = 612 J·mol$^{-1}$
Nematic− isotropic.
c/liq $\Delta H$ = 25700 J·mol$^{-1}$
Solid-smectic A.
**Molecular Weight** 291.4352
**Wiswesser Line Notation** NCR DR D8
**Evaluation** D

**$C_{21}H_{25}N$** (liq) 82THO/MAR
Octylcyanobiphenyl
**Phase Changes**
c/liq 294.45 K, $\Delta H$ = 25700 J·mol$^{-1}$
$\Delta S$ = 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 0.4J·mol$^{-1}$.
liq/liq 313.91 K, $\Delta H$ = 612 J·mol$^{-1}$
$\Delta S$ = 1.95 J·mol$^{-1}$·K$^{-1}$
Nematic-isotropic.
**Molecular Weight** 291.4352
**Wiswesser Line Notation** NCR DR D8
**Evaluation** B

**$C_{21}H_{25}NO_5$** (c) 82RAC/MAS
4-Nitrophenyl-4′-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, $\Delta H$ = 34426 J·mol$^{-1}$
$\Delta S$ = 106.4 J·mol$^{-1}$·K$^{-1}$
Solid-smectic.
liq/liq 334.9 K, $\Delta H$ = 213 J·mol$^{-1}$
$\Delta S$ = 0.59 J·mol$^{-1}$·K$^{-1}$
Smectic-nematic.
liq/liq 341.2 K, $\Delta H$ = 448 J·mol$^{-1}$
$\Delta S$ = 1.3 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) 79BAT/BUK
4′-Nitrophenyl-4-*n*-octyloxybenzoate
**Phase Changes**
c,II/liq 323.2 K, $\Delta H$ = 34720 J·mol$^{-1}$
$\Delta S$ = 108 J·mol$^{-1}$·K$^{-1}$
liq/liq 334 K, $\Delta H$ = 90 J·mol$^{-1}$
$\Delta S$ = 0.30 J·mol$^{-1}$·K$^{-1}$
Smectic-A-nematic.
liq/liq 341 K, $\Delta H$ = 290 J·mol$^{-1}$
$\Delta S$ = 0.88 J·mol$^{-1}$·K$^{-1}$
Nematic-isotropic.
c,II/c,I 323 K
**Molecular Weight** 371.4322
**Wiswesser Line Notation** WNR DOVR DO8
**Evaluation** B

**$C_{21}H_{44}$** (c) 55SCH/BUS
*n*-Henicosane
**Phase Changes**
c,II/c,I 305.65 K, $\Delta H$ = 15481 J·mol$^{-1}$
$\Delta S$ = 50.6 J·mol$^{-1}$·K$^{-1}$
c,I/liq 313.35 K, $\Delta H$ = 47698 J·mol$^{-1}$
$\Delta S$ = 152.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 296.5786
**Wiswesser Line Notation** 21H
**Evaluation** B

$C_{22}H_{13}N_3O_7$ (c) 79FAR/SHA
Fluoranthene picric acid
**Phase Changes**
c,II/c,I 365.6 K, $\Delta H$ = 13800 J·mol$^{-1}$
$\Delta S$ = 37.7 J·mol$^{-1}$·K$^{-1}$
c/liq 462.4 K, $\Delta H$ = 24700 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 2900 J·mol$^{-1}$
$\Delta S$ = 6.5 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 456.6 K, $\Delta H$ = 1200 J·mol$^{-1}$
$\Delta S$ = 2.6 J·mol$^{-1}$·K$^{-1}$
c/liq 506.6 K, $\Delta H$ = 32600 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta S$ = 543.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 418.3619
**Wiswesser Line Notation** /*MVR BVQ DVQ EVMR DOR D*/
**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, $\Delta H$ = 32300 J·mol$^{-1}$
$\Delta S$ = 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/SAP
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** T56 BHOVT&J BR DVMZ& BR DVMZ
**Evaluation** A

$C_{22}H_{18}O_4$ (c) 84OZC/ASR
4,4'-Dipropanoyloxydiphenyldiacetylene
**Phase Changes**
c,III/c,II 351 K, $\Delta H$ = 586 J·mol$^{-1}$
$\Delta S$ = 1.674 J·mol$^{-1}$·K$^{-1}$
c,II/c,I 359 K, $\Delta H$ = 7530 J·mol$^{-1}$
$\Delta S$ = 20.96 J·mol$^{-1}$·K$^{-1}$
c,I/liq 430 K, $\Delta H$ = 19400 J·mol$^{-1}$
$\Delta S$ = 45.35 J·mol$^{-1}$·K$^{-1}$
Solid-nematic.
**Molecular Weight** 346.3818
**Wiswesser Line Notation** 2VOR D1UU2UU1R DOV2
**Evaluation** A
Nematic-isotropic liquid phase change data also given:
470 K, $\Delta H$ = 1380 J·mol$^{-1}$,
$\Delta S$ = 2.929 J·mol$^{-1}$·K$^{-1}$.

$C_{22}H_{20}N_2O_2$ (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

$C_{22}H_{26}$ (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

$C_{22}H_{26}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4'-*n*-heptanoyloxyazobenzene
**Phase Changes**
c/liq 365.15 K, $\Delta H$ = 24811 J·mol$^{-1}$
$\Delta S$ = 67.95 J·mol$^{-1}$·K$^{-1}$
Solid-smectic A.
**Molecular Weight** 366.4590
**Wiswesser Line Notation** 6VOR DNUNR DV2
**Evaluation** A
Smectic A-nematic; nematic-isotropic;
smectic A-montropic hexatic;
hexatic-montropic smectic B liquid phase change data also given:
414.65 K, $\Delta H$ = 5314 J·mol$^{-1}$;
416.65 K , $\Delta H$ = 920 J·mol$^{-1}$;
362.85 K, $\Delta H$ = 1590 J·mol$^{-1}$;
358.55 K, $\Delta H$ = 84 J·mol$^{-1}$.

$C_{22}H_{27}N$ (c) 83MAR/THO
Nonylcyanobiphenyl
**Phase Changes**
liq/liq 320.8 K, $\Delta H$ = 5 J·mol$^{-1}$
$\Delta S$ = 0.02 J·mol$^{-1}$·K$^{-1}$
Smectic A— nematic.
liq/liq 322.7 K, $\Delta H$ = 1200 J·mol$^{-1}$
$\Delta S$ = 3.7 J·mol$^{-1}$·K$^{-1}$
Nematic— isotropic.
c/liq $\Delta H$ = 34500 J·mol$^{-1}$
Solid— smectic A.
**Molecular Weight** 305.4620
**Wiswesser Line Notation** NCR DR D9
**Evaluation** D

**$C_{22}H_{28}N_2O_4Ni$** (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, $\Delta C_p$ = 172 J·mol$^{-1}$·K$^{-1}$.

**$C_{22}H_{28}O_2$** (c) 79LEW/ENE
Northindrone acetate
**Phase Changes**
c/liq 480 K, $\Delta H$ = 27300 J·mol$^{-1}$
$\Delta S$ = 56.9 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 324.4620
**Wiswesser Line Notation** L E5 B666 OV MUTJ E1 F1UU1 FOV1
**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, $\Delta H$ = 22680 J·mol$^{-1}$
$\Delta S$ = 75.70 J·mol$^{-1}$·K$^{-1}$
Solid-smectic G liquid transition.
liq/liq 325.72 K, $\Delta H$ = 7110 J·mol$^{-1}$
$\Delta S$ = 21.79 J·mol$^{-1}$·K$^{-1}$
Smectic G− nematic liquid transition.
liq/liq 342.48 K, $\Delta H$ = 1780 J·mol$^{-1}$
$\Delta S$ = 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.

**$C_{22}H_{42}O_4$** (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

**$C_{22}H_{44}$** (c) 69BOR/DAL
1,1,10,10-Tetramethylcyclooctadecane
**Phase Changes**
c/liq 359 K, $\Delta H$ = 39581 J·mol$^{-1}$
$\Delta S$ = 110 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 308.5896
**Wiswesser Line Notation** L-18-TJ A1 A1 J1 J1
**Evaluation** B

**$C_{22}H_{46}$** (c) 55SCH/BUS
*n*-Docosane
**Phase Changes**
c,II/c,I 316.15 K, $\Delta H$ = 28200 J·mol$^{-1}$
$\Delta S$ = 89.2 J·mol$^{-1}$·K$^{-1}$
c,I/liq 317.15 K, $\Delta H$ = 48953 J·mol$^{-1}$
$\Delta S$ = 154.4 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 310.6054
**Wiswesser Line Notation** 22H
**Evaluation** B

**$C_{22}H_{46}$** (c) 73COM
*n*-Docosane
**Phase Changes**
c,II/c,I 316.25 K, $\Delta H$ = 28200 J·mol$^{-1}$
$\Delta S$ = 89.2 J·mol$^{-1}$·K$^{-1}$
c,I/liq 317.25 K, $\Delta H$ = 48952 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 29505 J·mol$^{-1}$
$\Delta S$ = 93.6 J·mol$^{-1}$·K$^{-1}$
c,I/liq 316.05 K, $\Delta H$ = 47837 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{23}H_{15}N_3O_7$** (c) 79FAR/SHA
1,2-Benzfluorene picric acid
**Phase Changes**
c/liq 402.7 K, $\Delta H$ = 45600 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 33500 J·mol$^{-1}$
$\Delta S$ = 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) 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

**$C_{23}H_{17}N$** (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

**$C_{23}H_{28}N_2O_3$** (c) 83FAN/POE
4-Propionyl-4′-*n*-octanoyloxyazobenzene
**Phase Changes**
c/liq 369.65 K, $\Delta H$ = 27489 J·mol$^{-1}$
$\Delta S$ = 74.36 J·mol$^{-1}$·K$^{-1}$
Solid-smectic A.
**Molecular Weight** 380.4858
**Wiswesser Line Notation** 7VOR DNUNR DV2
**Evaluation** A
Smectic A-nematic; nematic-isotropic; smectic A-monotropic hexatic; hexatic-monotropic smectic B liquid phase change data also given:
416.15 K, $\Delta H$ = 5314 J·mol$^{-1}$;
416.65 K, $\Delta H$ = 1004 J·mol$^{-1}$;
359.85 K, $\Delta H$ = 1423 J·mol$^{-1}$;
353.75 K, $\Delta H$ = 42 J·mol$^{-1}$.

**$C_{23}H_{29}N$** (c) 83MAR/THO
Decylcyanobiphenyl
**Phase Changes**
liq/liq $\Delta H$ = 2830 J·mol$^{-1}$
Smectic A– isotropic.
c/liq $\Delta H$ = 36000 J·mol$^{-1}$
Solid– smectic A.
**Molecular Weight** 319.4888
**Wiswesser Line Notation** NCR DR D10
**Evaluation** D

**$C_{23}H_{31}NO$** (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, $\Delta H$ = 23290 J·mol$^{-1}$
$\Delta S$ = 75.98 J·mol$^{-1}$·K$^{-1}$
Solid-smectic G.
**Molecular Weight** 337.5040
**Wiswesser Line Notation** 60*R* D1UNR D4
**Evaluation** A
Smectic G-smectic B; smectic B-smectic A; smectic A-nematic; nematic-isotropic liquid phase change data given:
331.56 K, $\Delta H$ = 804 J·mol$^{-1}$, $\Delta S$ = 2.53 J·mol$^{-1}$·K$^{-1}$;
332.86 K, $\Delta H$ = 3370 J·mol$^{-1}$, $\Delta S$ = 10.14 J·mol$^{-1}$·K$^{-1}$;
343.24 K, $\Delta H$ = 3200 J·mol$^{-1}$, $\Delta S$ = 9.37 J·mol$^{-1}$·K$^{-1}$;
350.92 K, $\Delta H$ = 1890 J·mol$^{-1}$, $\Delta S$ = 5.37 J·mol$^{-1}$·K$^{-1}$.

**$C_{23}H_{31}NO$** (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

**$C_{23}H_{48}$** (c) 84SYU/TUM
Tricosane
**Phase Changes**
c/liq 319.7 K, $\Delta H$ = 76700 J·mol$^{-1}$
$\Delta S$ = 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) 55SCH/BUS
*n*-Tricosane
**Phase Changes**
c,II/c,I 313.65 K, $\Delta H$ = 21757 J·mol$^{-1}$
$\Delta S$ = 69.4 J·mol$^{-1}$·K$^{-1}$
c,I/liq 320.65 K, $\Delta H$ = 53974 J·mol$^{-1}$
$\Delta S$ = 168.3 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 324.6322
**Wiswesser Line Notation** 23H
**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, $\Delta H$ = 46900 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 32200 J·mol$^{-1}$
$\Delta S$ = 77.7 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 457.3984
**Wiswesser Line Notation** L D6 C666J &WNR BQ CNW ENW
**Evaluation** B

**$C_{24}H_{18}$** (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, $\Delta H$ = 33400 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 37800 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 1100 J·mol$^{-1}$
c,II/c,I 450–540 K, $\Delta H$ = 1000 J·mol$^{-1}$
c/liq 586.7 K, $\Delta H$ = 57600 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 414 J·mol$^{-1}$
$\Delta S$ = 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

**$C_{24}H_{20}BK$** (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 &-KA-
**Evaluation** B

**$C_{24}H_{20}BRb$** (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** L6ØJA- AL6ØJ Ø-CR--ØL6ØJA- AL6ØJ &I
**Evaluation** B

**$C_{24}H_{22}O_4$** (c) 84OZC/ASR
4,4′-Dibutanoyloxydiphenyldiacetylene
**Phase Changes**
c,V/c,IV 319 K, $\Delta H$ = 10400 J·mol$^{-1}$
$\Delta S$ = 32.51 J·mol$^{-1}$·K$^{-1}$
c,IV/c,III 368 K, $\Delta H$ = 1510 J·mol$^{-1}$
$\Delta S$ = 4.100 J·mol$^{-1}$·K$^{-1}$
c,III/c,II 400 K
c,II/c,I 408 K, $\Delta H$ = 12.5 J·mol$^{-1}$
$\Delta S$ = 0.2929 J·mol$^{-1}$·K$^{-1}$
c,II/c,II,c,II/c,I transitions combined.
c,I/liq 416 K, $\Delta H$ = 20100 J·mol$^{-1}$
$\Delta S$ = 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, $\Delta H$ = 1250 J·mol$^{-1}$,
$\Delta S$ = 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

**$C_{24}H_{28}O_2Si_3$** (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, $\Delta H$ = 22753 J·mol$^{-1}$
$\Delta S$ = 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) 83FAN/POE
4-Propionyl-4′-*n*-nonanoyloxyazobenzene
**Phase Changes**
c/liq 367.15 K, $\Delta H$ = 3017 J·mol$^{-1}$
$\Delta S$ = 8.22 J·mol$^{-1}$·K$^{-1}$
Solid-smectic A.
**Molecular Weight** 394.5126
**Wiswesser Line Notation** 8VOR DNUNR DV2
**Evaluation** A
Smectic A-isotropic; smectic A-monotropic hexatic;
hexatic-monotropic smectic B liquid phase change data also given:
417.15 K, $\Delta H$ = 7029 J·mol$^{-1}$;
361.05 K, $\Delta H$ = 1757J·mol$^{-1}$;
353.25 K, $\Delta H$ = 42 J·mol$^{-1}$.

**$C_{24}H_{31}N$** (c) 83MAR/THO
Undecylcyanobiphenyl
**Phase Changes**
liq/liq $\Delta H$ = 3800 J·mol$^{-1}$
Smectic A— isotropic.
c/liq $\Delta H$ = 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/ZHU
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, $\Delta H$ = 490 J·mol$^{-1}$
$\Delta S$ = 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/STR4
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, $\Delta H$ = 1928 J·mol$^{-1}$
$\Delta S$ = 10.1 J·mol$^{-1}$·K$^{-1}$
c,I/liq 281.40 K, $\Delta H$ = 38844 J·mol$^{-1}$
$\Delta S$ = 138.1 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 322.5326
**Wiswesser Line Notation** 11YR&R
**Evaluation** A
See also 60KAR/STR2.

**$C_{24}H_{38}O_4$** (c) 70MAR/RAB
Di-(2-ethylhexyl) *o*-phthalate
**Molecular Weight** 390.5618
**Wiswesser Line Notation** 4Y2&1OVR BVO1Y2&4
**Evaluation** B
$T$(glass) = 182.5 °C.

**$C_{24}H_{38}O_4$** (liq) 85RAB/NOV
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 transition 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/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, $\Delta H$ = 35171 J·mol$^{-1}$
$\Delta S$ = 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/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, $\Delta H$ = 44267 J·mol$^{-1}$
$\Delta S$ = 147.3 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 334.6274
**Wiswesser Line Notation** L6TJ AY11&- AL6TJ
**Evaluation** A

$C_{24}H_{50}$ (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

$C_{24}H_{50}$ (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.
Cv = 1.75 J·g$^{-1}$·K$^{-1}$.
**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

$C_{24}H_{56}Cl_4MnN_2$ (c) 87ZHA
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
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
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

$C_{24}H_{56}Cl_4N_2Zn$ (c) 88ZHA/YAN
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-Z 2 &GH 2 &-ZN- G2
**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
Northindrone 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
FOVX1&1&1 F1UU1
**Evaluation** A

$C_{25}H_{40}O_2Si_2$ (c) 79LEW/ENE
Northindrone 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
FO-SI-1&1&O-SI-1&1&1
**Evaluation** A

**$C_{25}H_{48}O_4$** (liq) 83BAB/RAB
Bis(2-ethylhexyl)azelaate; 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) 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

**$C_{26}H_{15}N_3O_7$** (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
$\beta,\beta'$-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

**$C_{26}H_{20}N_6O$** (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

**$C_{26}H_{26}O_4$** (c) 84OZC/ASR
4,4'-Dipentanoyloxydiphenyldiacetylene
**Phase Changes**
c,III/c,II 272 K
c,II/c,I 290 K, $\Delta H$ = 1240 J·mol$^{-1}$
$\Delta S$ = 4.309 J·mol$^{-1}$·K$^{-1}$
c,II/c,II, c,II/c,I transitions combined.
c,I/liq 405 K, $\Delta H$ = 24700 J·mol$^{-1}$
$\Delta S$ = 61.04 J·mol$^{-1}$·K$^{-1}$
Solid-nematic.
**Molecular Weight** 402.4891
**Wiswesser Line Notation** 4VOR D1UU2UU1R DOV4
**Evaluation** A
Nematic-isotropic liquid phase change data also given:
434 K, $\Delta H$ = 2300 J·mol$^{-1}$,
$\Delta S$ = 3.390 J·mol$^{-1}$·K$^{-1}$.

**$C_{26}H_{34}$** (c) 83KRA/BEC
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 A*R* A- AL8TJ AR
**Evaluation** B

**$C_{26}H_{34}N_2O_3$** (c) 83FAN/POE
4-Propionyl-4'-*n*-undecanoyloxyazobenzene
**Phase Changes**
c/liq 370.65 K, $\Delta H$ = 37489 J·mol$^{-1}$
$\Delta S$ = 101.1 J·mol$^{-1}$·K$^{-1}$
Solid-smectic A.
**Molecular Weight** 422.5662
**Wiswesser Line Notation** 10VOR DNUNR DV2
**Evaluation** A
Smectic A-isotropic liquid phase change data also given:
416.65 K, $\Delta H$ = 7573 J·mol$^{-1}$.

**$C_{26}H_{38}$** (c) 83KRA/BEC
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

$C_{26}H_{52}$ (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

$C_{26}H_{54}$ (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

$C_{26}H_{54}$ (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

$C_{27}H_{30}O_2$ (c) 79LEW/ENE
Northindrone 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 FOVR
**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.
**Molecular Weight** 436.5930
**Wiswesser Line Notation** 11VOR DNUNR DV2
**Evaluation** A
Smectic A-isotropic liquid phase change data also given:
416.15 K, $\Delta H = 7866$ J·mol$^{-1}$.

$C_{27}H_{38}O_2$ (c) 79LEW/ENE
Northindrone 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 FOV6 F1UU1
**Evaluation** A

$C_{27}H_{56}$ (c) 55SCH/BUS
*n*-Heptacosane
**Phase Changes**
c,II/c,I 320.25 K, $\Delta H = 28953$ J·mol$^{-1}$
$\Delta S = 90.4$ J·mol$^{-1}$·K$^{-1}$
c,I/liq 331.95 K, $\Delta H = 60417$ J·mol$^{-1}$
$\Delta S = 182.0$ 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, $\Delta H = 39300$ J·mol$^{-1}$
$\Delta S = 83.7$ 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
Picene picric acid
**Phase Changes**
c,II/c,I 391 K, $\Delta H = 3300$ J·mol$^{-1}$
$\Delta S = 8.4$ J·mol$^{-1}$·K$^{-1}$
c/liq 437.9 K, $\Delta H = 21300$ J·mol$^{-1}$
$\Delta S = 48.6$ 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
1,2,3,4-Dibenzanthracene picric acid
**Phase Changes**
c,II/c,I 446.5 K, $\Delta H = 6700$ J·mol$^{-1}$
$\Delta S = 15.0$ J·mol$^{-1}$·K$^{-1}$
c/liq 485.2 K, $\Delta H = 44800$ J·mol$^{-1}$
$\Delta S = 92.3$ 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
1,2,5,6-Dibenzanthracene picric acid
**Phase Changes**
c/liq 493.0 K, $\Delta H = 54000$ J·mol$^{-1}$
$\Delta S = 109.6$ 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; Polyvinlenediphenylsilyl,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-R7R&1U1-GE-R&R&1U1*/
**Evaluation** A
Average molecular weight, $n$ = 10,000

**$(C_{28}H_{24}GeSi)_n$** (gls) 78LEB/RAB
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.

**$C_{28}H_{30}O_4$** (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.
**Molecular Weight** 430.5426
**Wiswesser Line Notation** 5VOR D1UU2UU1R DOV5
**Evaluation** A
Nematic-isotropic liquid phase change data also given:
430 K, $\Delta H$ = 1710 J·mol$^{-1}$,
$\Delta S$ = 3.975 J·mol$^{-1}$·K$^{-1}$.

**$C_{28}H_{32}Cl_4N_2Zn$** (c) 82FER/SOC
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 temperaturephase.
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

**$C_{28}H_{32}Si_4O_4$** (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

**$C_{28}H_{38}N_2O_3$** (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.
**Molecular Weight** 450.6198
**Wiswesser Line Notation** 12VOR DNUNR DV2
**Evaluation** A
Smectic A-isotropic liquid phase change data also given:
416.65 K, $\Delta H$ = 8075 J·mol$^{-1}$;
$\Delta S$ = 19.4 J·mol$^{-1}$·K$^{-1}$.

**$C_{28}H_{40}O_4$** (liq) 81ARU/DAU
4-(2-Methylbutoxy)phenyl ester of 4-$n$-decycloxybenzoic acid (D)
**Molecular Weight** 440.6216
**Wiswesser Line Notation** 10OR DVOR DO1Y2&1
**Evaluation** C
Smectic C-smectic A, 323.7 K;
smectic A-isotropic liquid,
338.15 K, $\Delta S$ = 17.21 J·mol$^{-1}$·K$^{-1}$,
phase change data given.

**$C_{28}H_{58}$** (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

**$C_{28}H_{58}$** (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

**$C_{29}H_{40}N_2O_3$** (c) 83FAN/POE
4-Propionyl-4′-$n$-tetradecanoyloxyazobenzene
**Phase Changes**
c/liq 375.65 K, $\Delta H$ = 45898 J·mol$^{-1}$
$\Delta S$ = 122.2 J·mol$^{-1}$·K$^{-1}$
Solid-smectic A.
**Molecular Weight** 464.6466
**Wiswesser Line Notation** 13VOR DNUNR DV2
**Evaluation** A
Smectic A-isotropic liquid phase change data also given:
413.65 K, $\Delta H$ = 8117 J·mol$^{-1}$.

$C_{29}H_{60}$ (c) 55SCH/BUS
*n*-Nonacosane
**Phase Changes**
c,II/c,I 331.35 K, $\Delta H$ = 29706 J·mol$^{-1}$
$\Delta S$ = 89.7 J·mol$^{-1}$·K$^{-1}$
c,I/liq 336.55 K, $\Delta H$ = 66107 J·mol$^{-1}$
$\Delta S$ = 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

$(C_{30}H_{20}N_4O_6)_n$ (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

$C_{30}H_{22}$ (c) 79SMI
*p*-Quinquephenyl
**Phase Changes**
c/liq 659.6 K, $\Delta H$ = 42300 J·mol$^{-1}$
$\Delta S$ = 64.1 J·mol$^{-1}$·K$^{-1}$
Solid-nematic phase change.
liq/liq 688.1 K, $\Delta H$ = 922 J·mol$^{-1}$
$\Delta S$ = 1.34 J·mol$^{-1}$·K$^{-1}$
Nematic-isotropic phase change.
**Molecular Weight** 382.5038
**Wiswesser Line Notation** RR DR DR DR
**Evaluation** A

$C_{30}H_{34}O_4$ (c) 84OZC/ASR
4,4'-Diheptanoyloxydiphenyldiacetylene
**Phase Changes**
c,III/c,II 305 K
c,II/c,I 318 K, $\Delta H$ = 18900 J·mol$^{-1}$
$\Delta S$ = 60.67 J·mol$^{-1}$·K$^{-1}$
c,II/c,II, c,II/c,I transitions combined.
c,I/liq 402 K, $\Delta H$ = 25500 J·mol$^{-1}$
$\Delta S$ = 63.47 J·mol$^{-1}$·K$^{-1}$
Solid-nematic.
**Molecular Weight** 458.5962
**Wiswesser Line Notation** 6VOR D1UU2UU1R DOV6
**Evaluation** A
Nematic-isotropic liquid phase change data also given:
411 K, $\Delta H$ = 1170 J·mol$^{-1}$,
$\Delta S$ = 2.845 J·mol$^{-1}$·K$^{-1}$.

$C_{30}H_{42}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4'-*n*-pentadecanoyloxyazobenzene
**Phase Changes**
c/liq 376.65 K, $\Delta H$ = 51505 J·mol$^{-1}$
$\Delta S$ = 136.7 J·mol$^{-1}$·K$^{-1}$
Solid-smectic A.
**Molecular Weight** 478.6734
**Wiswesser Line Notation** 14VOR DNUNR DV2
**Evaluation** A
Smectic A-isotropic liquid phase change data also given:
412.15 K, $\Delta H$ = 8452 J·mol$^{-1}$;
$\Delta S$ = J·mol$^{-1}$·K$^{-1}$.

$C_{30}H_{46}$ (c) 83KRA/BEC
3,4-Dimethyl-3,4-bis(4-*tert*-butylphenyl)hexane
**Heat Capacity** 298 K, $C_p$ = 631.3 J·mol$^{-1}$·K$^{-1}$
One temperature.
$C_p$ given as 0.371 cal·K$^{-1}$·g$^{-1}$.
**Molecular Weight** 406.6934
**Wiswesser Line Notation** 1XR DX2&2&X2&2&R DX
**Evaluation** B

$C_{30}H_{62}$ (c) 55SCH/BUS
*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) 73COM
*n*-Triacontane
**Phase Changes**
c,II/c,I 335.25 K, $\Delta H$ = 37489 J·mol$^{-1}$
$\Delta S$ = 111.8 J·mol$^{-1}$·K$^{-1}$
c,I/liq 338.65 K, $\Delta H$ = 68827 J·mol$^{-1}$
$\Delta S$ = 203.2 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 422.8198
**Wiswesser Line Notation** 30H
**Evaluation** B

$C_{30}H_{62}$ (c) 81HOE
*n*-Triacontane
**Heat Capacity** 300 K, $C_p$ = 558 J·mol$^{-1}$·K$^{-1}$
Temperature range 300 to 500 K.
$C_v$ = 1.30 J·g$^{-1}$·K$^{-1}$.
**Molecular Weight** 422.8198
**Wiswesser Line Notation** 30H
**Evaluation** B

$C_{31}H_{44}N_2O_3$ (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.
**Molecular Weight** 492.7002
**Wiswesser Line Notation** 15VOR DNUNR DV2
**Evaluation** A
Smectic A-isotropic liquid phase change data also given:
410.65 K, $\Delta H$ = 8619 J·mol$^{-1}$;
$\Delta S$ = 21.0 J·mol$^{-1}$·K$^{-1}$.

$C_{31}H_{52}O_3$ (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

$(C_{32}H_{20}N_4)_n$ (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

$C_{32}H_2Ge$ (c) 75LEB/MIL3
1,1-Diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene
**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

$(C_{32}H_2Ge)_n$ (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

$C_{32}H_{38}Fe_3N_4O_{13}$ (c) 85OH/KAM
$\mu_3$-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
$\mu_3$-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- O &T6NJ
**Evaluation** A

$C_{32}H_{38}O_4$ (c) 84OZC/ASR
4,4′-Dioctanoyloxydinphenyldiacetylene
**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.
**Molecular Weight** 486.6498
**Wiswesser Line Notation** 7VOR D1UU2UU1R DOV7
**Evaluation** A
Nematic-isotropic liquid phase change data also given:
412 K, $\Delta H$ = 21800 J·mol$^{-1}$, $\Delta S$ = 5.272 J·mol$^{-1}$·K$^{-1}$.

$C_{32}H_{39}ClO_2$ (c) 79LEW/ENE
Northindrone-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 FOV5R DG
**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.
**Molecular Weight** 506.7270
**Wiswesser Line Notation** 16VOR DNUNR DV2
**Evaluation** A
Smectic A-isotropic liquid phase change data also given:
409.65 K, $\Delta H$ = 8703 J·mol$^{-1}$; $\Delta S$ = 21.2 J·mol$^{-1}$·K$^{-1}$.

$C_{32}H_{50}$ (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

**$C_{32}H_{66}$** (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.
$C_v$ = 1.77 J·g$^{-1}$·K$^{-1}$.
**Molecular Weight** 450.8734
**Wiswesser Line Notation** 32H
**Evaluation** B

**$C_{33}H_{34}O_2$** (c) 79LEW/ENE
Northindrone *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 FOV- AL6TJ
**Evaluation** A

**$C_{33}H_{34}O_2$** (c) 79LEW/ENE
Northindrone 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 FOVR DR
**Evaluation** A

**$C_{33}H_{40}O_2$** (c) 79LEW/ENE
Northindrone 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 FOVR D- AL6TJ
**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.
**Molecular Weight** 520.7538
**Wiswesser Line Notation** 17VOR DNUNR DV2
**Evaluation** A
Smectic A-isotropic liquid phase change data also given:
408.65 K, $\Delta H$ = 8954 J·mol$^{-1}$;
$\Delta S$ = 21.9 J·mol$^{-1}$·K$^{-1}$.

**$C_{33}H_{48}O_2$** (c) 79LEW/ENE
Northindrone *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 FOV2- AL6TJ D4
**Evaluation** A

**$(C_{34}H_{18}N_6O)_n$** (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.
**Molecular Weight** 514.7034
**Wiswesser Line Notation** 8VOR D1UU2UU1R DOV8
**Evaluation** A
Nematic-isotropic liquid phase change data also given:
401 K, $\Delta H$ = 14600 J·mol$^{-1}$,
$\Delta S$ = 3.640 J·mol$^{-1}$·K$^{-1}$.

**$C_{34}H_{54}$** (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

**$C_{34}H_{70}$** (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

**$C_{36}H_{18}$** (c) 79FAR/SHA
Decacyclene; Diacenaphtho[1,2-j:1′,2′-l]-fluoranthene
**Phase Changes**

| | | |
|---|---|---|
| c,II/c,I | 533 K | |
| c/liq | 562.0 K, | $\Delta H$ = 45200 J·mol$^{-1}$ |
| | | $\Delta S$ = 80.4 J·mol$^{-1}$·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

**$C_{36}H_{46}Fe_3N_4O_{13}$** (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·mol$^{-1}$·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·mol$^{-1}$,
$\Delta S$ = 13.71 J·mol$^{-1}$·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·mol$^{-1}$ |
| | | $\Delta S$ = 122.1 J·mol$^{-1}$·K$^{-1}$ |
| c,I/liq | 403 K, | $\Delta H$ = 42200 J·mol$^{-1}$ |
| | | $\Delta S$ = 104.6 J·mol$^{-1}$·K$^{-1}$ |

Solid-isotropic.
**Molecular Weight** 542.7570
**Wiswesser Line Notation** 9VOR D1UU2UU1R DOV9
**Evaluation** A

**$C_{36}H_{74}$** (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

**$C_{36}H_{74}$** (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)

**$C_{38}H_{28}B_2F_8FeN_8$** (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 NNØJ D1UNMR Ø-FE-- ØT B666 CN NNØJ 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 NNØJ D1UNMR Ø-FE-- ØT B666 CN NNØJ D1UNMR &G-O4 2
**Evaluation** A

**$C_{38}H_{36}O_4Si_4$** (c) 82KUL
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** 10OVR 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

**$C_{39}H_{30}N_6$** (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

**$C_{40}H_{54}O_4$** (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

**$C_{41}H_{72}O_2$** (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 E1FY1&3Y1&1 OV13
**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)

**$C_{42}H_{70}O_{35}\cdot 11H_2O$** (c) 87HAN/MAT

$\beta$-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$^{-1}$
$\Delta S$ = 61.9 J·mol$^{-1}$·K$^{-1}$

Solid-discotic.

liq/liq 472.6 K, $\Delta H$ = 8840 J·mol$^{-1}$
$\Delta S$ = 18.7 J·mol$^{-1}$·K$^{-1}$

Discotic-isotropic.

**Molecular Weight** 769.0236

**Wiswesser Line Notation** L6TJ AOV5 BOV5 COV5 DOV5 EOV5 FOV5

**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

**$C_{43}H_{76}O_2$** (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 E1FY1&3Y1&1 OV15

**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$^{-1}$
$\Delta S$ = 9.03 J·mol$^{-1}$·K$^{-1}$

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.

liq/liq 321.0 K, $\Delta H$ = 840 J·mol$^{-1}$
$\Delta S$ = 2.62 J·mol$^{-1}$·K$^{-1}$

Cholesteric-isotropic.

**Molecular Weight** 651.1100

**Wiswesser Line Notation** L E5 B666 LUTJ A1 E1FY1&3Y1&1 OV8U9

**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.

liq/liq 349.0 K, $\Delta H$ = 1800 J·mol$^{-1}$
$\Delta S$ = 5.16 J·mol$^{-1}$·K$^{-1}$

Smectic-cholesteric.

liq/liq 353.0 K, $\Delta H$ = 1700 J·mol$^{-1}$
$\Delta S$ = 4.82 J·mol$^{-1}$·K$^{-1}$

Cholesteric-isotropic.

**Molecular Weight** 653.1258

**Wiswesser Line Notation** L E5 B666 LUTJ A1 E1FY1&3Y1&1 OV17

**Evaluation** A

**$C_{48}H_{40}O_4Si_4$** (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.

**Molecular Weight** 847.1370

**Wiswesser Line Notation** 6OVR BVO6 CVO6 DVO6 EVO6 FVO6

**Evaluation** A(Phase changes), B($C_p$)

Mesophase-liquid phase transition data also given:

359.28 K, $\Delta H$ = 21540 J·mol$^{-1}$,
$\Delta S$ = 59.93 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, $S = 1514.3$ 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.
**Molecular Weight** 931.2978
**Wiswesser Line Notation** 7VOR BOV7 COV7 DOV7 EOV7 FOV7
**Evaluation** A
Columnar mesophase-isotropic liquid phase change data also given:
357.09 K, $\Delta H = 19220$ J·mol$^{-1}$,
$\Delta S = 53.77$ J·mol$^{-1}$·K$^{-1}$.

$C_{54}H_{96}O_{12}$ (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** H6TJ AOV7 BOV7 COV7 DOV7 EOV7 FOV7
**Evaluation** A

$C_{54}H_{98}O_{12}$ (liq) 75PHI/WAL
Poly(hexamethylene sebacate)
**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

$C_{54}H_{104}O_6$ (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$^{-1}$); $\beta$ (mp, 338 K) = 1393;
$\beta_1'$(mp, 335 K) 1518; $\beta_2'$(mp, 333 K) = 1621;
$\alpha$ (mp, 323 K) = 1759.
**Molecular Weight** 849.4120
**Wiswesser Line Notation** 16VO1YOV16&1OV16
**Evaluation** B

$C_{57}H_{110}O_6$ (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$^{-1}$); $\beta$ (mp, 345 K) = 1436;
$\beta_1'$(mp, 337 K) = 1544; $\beta_2'$(mp, 334 K) = 1615;
$\alpha$ (mp, 328 K) = 1846.
**Molecular Weight** 891.4924
**Wiswesser Line Notation** 17VO1YOV17&1OV17
**Evaluation** B

$C_{66}H_{96}O_{12}$ (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**
liq/liq 402.16 K, $\Delta H$ = 3626 J·mol$^{-1}$
$\Delta S$ = 9.02 J·mol$^{-1}$·K$^{-1}$
Discotic— isotropic.
c/liq 359.7 K, $\Delta H$ = 25440 J·mol$^{-1}$
$\Delta S$ = 71.12 J·mol$^{-1}$·K$^{-1}$
Solid II—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** 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.
liq/liq 461.8 K, $\Delta H$ = 10280 J·mol$^{-1}$
$\Delta S$ = 22.26 J·mol$^{-1}$·K$^{-1}$
Discotic-isotropic.
**Molecular Weight** 1105.6668
**Wiswesser Line Notation** L6TJ AOV9 BOV9 COV9 DOV9 EOV9 FOV9
**Evaluation** A

$C_{203}H_{288}O_{14}$ (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
**Wiswesser Line Notation**
**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
**Wiswesser Line Notation**
**Evaluation** A

## 8. Compound Name — Formula Index

### A



### B

| | |
|---|---|
| Bis(nitrato)(1,4,8,11-tetraazacyclotetradecane) copper (II) | $C_{10}H_{24}CuN_6O_6$ |
| Bis-pentylammonium tetrachloro zincate | $C_{10}H_{28}Cl_4N_2Zn$ |
| Bis(1,10-phenanthroline-2-carbaldehyde phenylhydrazone) iron(II) ditetrafluoroborate | $C_{38}H_{28}B_2F_8FeN_8$ |
| Bis(1,10-phenanthroline-2-carbaldehyde phenylhydrazone) iron(II) diperchlorate | $C_{38}H_{28}Cl_2FeN_8O_8$ |
| 2,2-Bis(phenyl-4-glycidoxy)propane | $C_{21}H_{24}O_4$ |
| 1,4-Bis(phenylglyoxaloyl)benzene | $C_{22}H_{14}O_4$ |
| Bis(tetradecylammonium)zinc tetrachloride | $C_{28}H_{32}Cl_4N_2Zn$ |
| Bis(tetraethylammonium) decahydrodecaborate | $C_{16}H_{50}B_{10}N_2$ |
| Bis(tetraethylammonium) dodecahydrododecaborate | $C_{16}H_{52}B_{12}N_2$ |
| Bis(tetramethylammonium iodide) trideca-silver iodide | $C_8H_{24}Ag_{13}I_{15}N_2$ |
| Bis(toluene)chromium iodide | $C_{14}H_{16}CrI$ |
| o,o′-Bis-trichlorosilylbiphenyl | $C_{12}H_8Cl_4Si_2$ |
| 1,3-Bis(trimethylsilyl)propane | $C_9H_{24}Si_2$ |
| Bis(m-xylene)chromium iodide | $C_{16}H_{20}CrI$ |
| 2,2′-Bitetralin | $C_{20}H_{22}$ |
| Bromo bis(N,N-diethyldithiocarbamate)iron (III) | $C_{10}H_{20}BrFeN_2S_4$ |
| Bromobenzene | $C_6H_5Br$ |
| 2-Bromobenzoic acid | $C_7H_5BrO_2$ |
| 3-Bromobenzoic acid | $C_7H_5BrO_2$ |
| 4-Bromobenzoic acid | $C_7H_5BrO_2$ |
| 1-Bromo-2-chloro-1,1,2-trifluoroethane | $C_2HBrClF_3$ |
| 2-Bromo-2-chloro-1,1,1-trifluoroethane | $C_2HBrClF_3$ |
| Bromoform | $CHBr_3$ |
| 2-Bromoiodobenzene | $C_6H_4BrI$ |
| 3-Bromoiodobenzene | $C_6H_4BrI$ |
| 4-Bromoiodobenzene | $C_6H_4BrI$ |
| 4-Bromophenol | $C_6H_5BrO$ |
| Bromotrifluoromethane | $CF_3Br$ |
| Bullvalene | $C_{10}H_{10}$ |
| Butadiene-propylene copolymer | $(C_7H_{12})_n$ |
| 1,4-Butanedinitrile | $C_4H_4N_2$ |
| 1,4-Butanedioic acid | $C_6H_{10}O_4$ |
| 1,4-Butanediol | $C_4H_{10}O_2$ |
| 1-Butanethiol | $C_4H_{10}S$ |
| 1-Butanol | $C_4H_{10}O$ |
| 2-Butanol | $C_4H_{10}O$ |
| *tert*-Butanol | $C_4H_{10}O$ |
| Butanone | $C_4H_8O$ |
| 2-Butenal | $C_4H_6O$ |
| 1-Butene | $C_4H_8$ |
| *cis*-2-Butene | $C_4H_8$ |
| *trans*-2-Butene | $C_4H_8$ |
| 2-*n*-Butoxy-1-ethanol | $C_6H_{14}O_2$ |
| 2-(2-Butoxyethoxy)ethanol | $C_8H_{18}O_3$ |
| *n*-Butyl acetate | $C_6H_{12}O_2$ |
| Butyl acrylate | $C_7H_{12}O_2$ |
| *n*-Butyl alcohol | $C_4H_{10}O$ |
| *sec*-Butyl alcohol | $C_4H_{10}O$ |
| *tert*-Butyl alcohol | $C_4H_{10}O$ |
| Butyl butanoate | $C_8H_{16}O_2$ |
| *n*-Butyl chloride | $C_4H_9Cl$ |
| *n*-Butyl ethanoate | $C_6H_{12}O_2$ |
| *n*-Butyl mercaptan | $C_4H_{10}S$ |
| Butyl methacrylate | $C_8H_{14}O_2$ |
| *n*-Butyl methanoate | $C_5H_{10}O_2$ |
| Butyl octadecanoate | $C_{12}H_{24}O_2$ |
| Butyl pentanoic acid | $C_9H_{18}O_2$ |
| Butyl urea | $C_5H_{12}N_2O$ |
| *tert*-Butyl urea | $C_5H_{12}N_2O$ |
| *tert*-Butylaldehyde | $C_5H_{10}O$ |
| 1,4-Butylene glycol-ethylene glycol-adipic acid oligomer | $C_{12}H_{22}O_6$ |
| Butylglycol | $C_6H_{14}O_2$ |
| $\tau$-Butyrolactone | $C_4H_6O_2$ |

## C

| | |
|---|---|
| Caffeine | $C_8H_{10}N_4O_2$ |
| Calcium oxalate mono-hydrate | $C_2CaO_4{\cdot}H_2O$ |
| Cane sugar | $C_{12}H_{22}O_{11}$ |
| Capraldehyde | $C_{10}H_{20}O$ |
| Capric acid | $C_{10}H_{20}O_2$ |
| Capric aldehyde | $C_{10}H_{20}O$ |
| $\epsilon$-Caprolactone | $C_6H_{10}O_2$ |
| Capryl alcohol | $C_8H_{18}O$ |
| Caprylaldehyde | $C_8H_{16}O$ |
| 4-Carbomethoxyhomocubane | $C_{11}H_{12}O_2$ |
| Carbon | C |
| Carbon, diamond | C |
| Carbon, graphite | C |
| Carbon tetrabromide | $CBr_4$ |
| Carbon tetrachloride | $CCl_4$ |
| Carbon tetrafluoride | $CF_4$ |
| Carbopropoxy methyl methacrylate | $C_9H_{14}O_2$ |
| 1,7-Carborane-12 | $C_2H_{12}B_{10}$ |
| *m*-Carborane | $C_2H_{12}B_{10}$ |
| 4-Carboxypentacyclo-[4.3.0.0$^{2,5}$.0$^{3,8}$.0$^{4,7}$]nonane | $C_{10}H_{10}O_2$ |
| Castor oil | $C_{18}H_{34}O_3$ |
| Catechol | $C_6H_6O_2$ |
| Cellulose nitrate | $(C_6H_8N_2O_9)_n$ |
| Cerium(III) oxalate | $C_6O_{12}Ce_2$ |
| *n*-Cetyl alcohol | $C_{16}H_{34}O$ |
| Cetane | $C_{16}H_{34}$ |
| 2-Chloro-1-(trichloromethyl)pyridine | $C_6H_3Cl_4N$ |
| Chloroacetic acid | $C_2H_3ClO_2$ |
| 2-Chloroadamantane | $C_{10}H_{15}Cl$ |
| Chlorobenzene | $C_6H_5Cl$ |
| *p*-Chlorobiphenyl | $C_{12}H_9Cl$ |
| Chlorobis(N,N-dimethyldithiocarbamate)iron(III) | $C_6H_{12}ClFeN_2S_4$ |
| 2-Chlorobromobenzene | $C_6H_4BrCl$ |
| 3-Chlorobromobenzene | $C_6H_4BrCl$ |
| 4-Chlorobromobenzene | $C_6H_4BrCl$ |
| 1-Chlorobutane | $C_4H_9Cl$ |
| Chloroethyl methacrylate | $C_6H_9ClO_2$ |
| Chloroform | $CHCl_3$ |
| 2-Chloroisonitrosoacetanilide | $C_8H_7ClN_2O_2$ |
| 1-Chloronaphthalene | $C_{10}H_7Cl$ |
| 2-Chloronaphthalene | $C_{10}H_7Cl$ |
| 1,2-Chloronitrobenzene | $C_6H_4ClNO_2$ |
| 2-Chlorophenol | $C_6H_5ClO$ |
| 3-Chlorophenol | $C_6H_5ClO$ |
| 4-Chlorophenol | $C_6H_5ClO$ |
| Chlorotrifluoroethylene | $C_2ClF_3$ |
| Chlorotrifluoroethene | $C_2ClF_3$ |
| Chlorotrimethylsilane | $C_3H_9ClSi$ |
| Cholesteryl oleate | $C_{45}H_{78}O_2$ |
| Cholesteryl myristate | $C_{41}H_{72}O_2$ |
| Cholesteryl palmitate | $C_{43}H_{76}O_2$ |
| Cholesteryl stearate | $C_{45}H_{80}O_2$ |
| Chroman | $C_9H_7O$ |
| Chromium acetylacetonate | $C_{15}H_{21}CrO_6$ |
| Chromocene | $C_{10}H_{10}Cr$ |
| Cinnamic acid | $C_9H_8O_2$ |
| Citral | $C_{10}H_{16}O$ |
| Citric acid monohydrate | $C_6H_8O_7{\cdot}H_2O$ |
| Citric acid | $C_6H_8O_7$ |

| | |
|---|---|
| Cobaltocene | $C_{10}H_{10}Co$ |
| Copper benzylacetylenide | $C_9H_7Cu$ |
| Copper butylacetylenide | $C_6H_9Cu$ |
| Copper (II) formate tetradeuterate | $C_2H_2CuO_4{\cdot}4D_2O$ |
| Copper (II) formate tetrahydrate | $C_2H_2CuO_4{\cdot}4H_2O$ |
| Copper phenylacetylenide | $C_8H_5Cu$ |
| Copper phenylethynylacetylenide | $C_{10}H_5Cu$ |
| Copper vinylacetylenide | $C_4H_3Cu$ |
| *o*-Cresol | $C_7H_8O$ |
| *m*-Cresol | $C_7H_8O$ |
| *p*-Cresol | $C_7H_8O$ |
| Crotonaldehyde | $C_4H_6O$ |
| Cyanamid | $CH_2N_2$ |
| Cyanoacetamide | $C_3H_4N_2O$ |
| α-Cyanopropionaldehyde | $C_4H_5NO$ |
| β-Cyanopropionaldehyde | $C_4H_5NO$ |
| Cyanuric acid | $C_3H_3N_3O_3$ |
| Cyclam | $C_{10}H_{24}N_4$ |
| β-Cyclodextrin undecahydrate | $C_{42}H_{70}O_{35}{\cdot}11H_2O$ |
| Cyclo-di-p-xylene | $C_{16}H_{16}$ |
| Cycloheptaamylose undecahydrate | $C_{42}H_{70}O_{35}{\cdot}11H_2O$ |
| *cis*-Cycloheptene | $C_7H_{12}$ |
| *cis*-Cyclohexane-1,2-dicarboxylic-anhydride | $C_8H_{10}O_3$ |
| Cyclohexane | $C_6H_{12}$ |
| 1,4-Cyclohexanedione | $C_6H_8O_2$ |
| Cyclohexanone | $C_6H_{10}O$ |
| (Cyclohexatriene)(cyclopentadienyl)-iron(II) hexafluorophosphate | $C_{11}H_{11}F_6FeP$ |
| Cyclohexene | $C_6H_{10}$ |
| Cyclohexene oxide | $C_6H_{10}O$ |
| Cyclohexylbenzene | $C_{12}H_{16}$ |
| Cyclooctadecane | $C_{18}H_{36}$ |
| Cycloocta-1,5-diene | $C_8H_{12}$ |
| Cyclooctane | $C_8H_{16}$ |
| Cyclooctene | $C_8H_{14}$ |
| Cyclopentadiene | $C_5H_6$ |
| Cyclopentadienyl manganese tricarboxyl | $C_8H_5MnO_3$ |
| Cymantrene | $C_8H_5MnO_3$ |

## D

| | |
|---|---|
| Decachlorobiphenyl | $C_{12}Cl_{10}$ |
| Decacyclene | $C_{36}H_{18}$ |
| Decafluorobiphenyl | $C_{12}F_{10}$ |
| *cis*-Decahydronaphthalene | $C_{10}H_{18}$ |
| *trans*-Decahydronaphthalene | $C_{10}H_{18}$ |
| Decanal | $C_{10}H_{20}O$ |
| Decane | $C_{10}H_{22}$ |
| *n*-Decane | $C_{10}H_{22}$ |
| 1-Decanethiol | $C_{10}H_{22}S$ |
| *cis*-Decalin | $C_{10}H_{18}$ |
| *trans*-Decalin | $C_{10}H_{18}$ |
| Decanoic acid | $C_{10}H_{20}O_2$ |
| *n*-Decyl mercaptan | $C_{10}H_{22}S$ |
| Decyl methacrylate | $C_{14}H_{26}O_2$ |
| Decylcyanobiphenyl | $C_{23}H_{29}N$ |
| Deuterotriglycine fluoroberyllate | $C_6D_{17}BeF_4N_3O_6$ |
| Deuterotriglycine sulfate | $C_6D_{17}N_3O_{10}S$ |
| Diacenaphtho[1,2-j:1′,2′-l]fluoranthene | $C_{36}H_{18}$ |
| *p*-Diacetylbenzene diethyl ketal | $C_{18}H_{30}O_4$ |
| 4,4′-Diaminodiphenyl ether | $C_{12}H_{12}N_2O$ |
| 4,4′-Diaminodiphenyl oxide | $C_{12}H_{12}N_2O$ |
| 4,4′-Diaminodiphenyl sulfone | $C_{12}H_{12}N_2O_2S$ |
| Diamond | C |
| 1,2-Diaminoethane | $C_2H_8N_2$ |
| 2,3-Diazabicyclo[2.2.2]oct-2-ene N-oxide | $C_6H_{10}N_2O$ |
| 6,7-Diazatricyclo[3.2.2.$0^{2,4}$]non-6-ene N-oxide | $C_7H_{10}N_2O$ |
| 1,2,3,4-Dibenzanthracene picric acid | $C_{28}H_{17}N_3O_7$ |
| 1,2,5,6-Dibenzanthracene picric acid | $C_{28}H_{17}N_3O_7$ |
| Dibenzothiophene | $C_{12}H_8S$ |
| 1,2-Dibromobenzene | $C_6H_4Br_2$ |
| 1,3-Dibromobenzene | $C_6H_4Br_2$ |
| 1,4-Dibromobenzene | $C_6H_4Br_2$ |
| 1,4-Dibromo-2,3-dichorohexa-fluorobutane | $C_4Br_2Cl_2F_6$ |
| 1,2-Dibromoethane | $C_2H_4Br_2$ |
| 1,6-Dibromo-2,3,5-trichloro-nonafluorohexane | $C_6Br_2Cl_3F_9$ |
| 1,2-Dibromotetrafluoroethane | $C_2Br_2F_4$ |
| 4,4′-Dibutanoyloxydi-phenyldiacetylene | $C_{24}H_{22}O_4$ |
| Di-*n*-butyl ether | $C_8H_{18}O$ |
| Di-*tert*-butyl ether | $C_8H_{18}O$ |
| 5,6-Dibutyl-5,6-bis(4-*tert*-butyl-phenyl)decane | $C_{38}H_{62}$ |
| Dibutyl phthalate | $C_{16}H_{22}O_4$ |
| Dibutyl *o*-phthalate | $C_{16}H_{22}O_4$ |
| N,N′-Dibutylurea | $C_9H_{20}N_2O$ |
| Dichloroacetic acid | $C_2H_2Cl_2O_2$ |
| 1,2-Dichlorobenzene | $C_6H_4Cl_2$ |
| 1,3-Dichlorobenzene | $C_6H_4Cl_2$ |
| 1,4-Dichlorobenzene | $C_6H_4Cl_2$ |
| *p*-Dichlorobenzene | $C_6H_4Cl_2$ |
| *p*-Dichlorobenzophenone | $C_{13}H_8Cl_2O$ |
| 1,4-Dichlorobutane | $C_4H_8Cl_2$ |
| 4,4′-Dichlorodiphenyl sulphone | $C_{12}H_8Cl_2O_2S$ |
| 1,2-Dichloroethane | $C_2H_4Cl_2$ |
| Dichloroethanoic acid | $C_2H_2Cl_2O_2$ |
| 1,6-Dichlorohexane | $C_6H_{12}Cl_2$ |
| Dichloromethane | $CH_2Cl_2$ |
| Dichlorodimethylsilane | $C_2H_6Cl_2Si$ |
| Dichloromethylvinylsilane | $C_3H_6Cl_2Si$ |
| 2,4-Dichloro-4′-nitrodiphenyl ether | $C_{12}H_7Cl_2NO_3$ |
| 2,3-Dichlorophenol | $C_6H_4Cl_2O$ |
| 2,4-Dichlorophenol | $C_6H_4Cl_2O$ |
| 2,5-Dichlorophenol | $C_6H_4Cl_2O$ |
| 2,6-Dichlorophenol | $C_6H_4Cl_2O$ |
| 3,4-Dichlorophenol | $C_6H_4Cl_2O$ |
| 3,5-Dichlorophenol | $C_6H_4Cl_2O$ |
| 1,2-Dicyanobenzene | $C_8H_4N_2$ |
| 1,4-Dicyanobenzene | $C_8H_4N_2$ |
| 1,1-Dicyclohexyldodecane | $C_{24}H_{46}$ |
| *endo*-Dicyclopentadiene | $C_{10}H_{12}$ |
| 4,4′-Didecanoyloxydiphenyl-diacetylene | $C_{36}H_{46}O_4$ |
| Di-*n*-decylammonium chloride | $C_{20}H_{44}ClN$ |
| 4,4′-Didodecanoyloxydiphenyl-diacetylene | $C_{40}H_{54}O_4$ |
| Diethanolamine | $C_4H_{11}NO_2$ |
| 4,4′-Diethanoyloxydiphenyldiacetylene | $C_{20}H_{14}O_4$ |
| Diethylaminoethyl methacrylate | $C_{10}H_{19}NO_2$ |
| 4,5-Diethyl-4,5-bis-(4-*tert*-butyl-phenyl)octane | $C_{32}H_{50}$ |
| Diethylene glycol | $C_4H_{10}O_3$ |
| Diethylene glycol-glycerol-adipate polymer | $C_{13}H_{22}O_8$ |
| Diethylene glycol-trimethylolpro-pane-adipate polymer | $C_{15}H_{28}O_8$ |
| Diethyleneimide oxide | $C_4H_9NO$ |
| Diethylenetriamine | $C_3H_{13}N_3$ |
| Di-(2-ethylhexyl)adipate | $C_{22}H_{42}O_4$ |
| Di-(2-ethylhexyl) *o*-phthalate | $C_{24}H_{38}O_4$ |
| Diethyl ketone | $C_5H_{10}O$ |
| Diethyl mercury | $C_4H_{10}Hg$ |
| 3,3-Diethylpentane | $C_9H_{20}$ |
| N,N-Diethylurea | $C_5H_{12}N_2O$ |
| 1,1-Diethylurea | $C_5H_{12}N_2O$ |
| 1,3-Diethylurea | $C_5H_{12}N_2O$ |
| Diethyl zinc | $C_4H_{10}Zn$ |
| Diethynyldiphenylgermane | $C_{16}H_{12}Ge$ |

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|---|---|
| 1,1-Diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene | $C_{32}H_{22}Ge$ |
| 1,2-Difluorobenzene | $C_6H_4F_2$ |
| 1,3-Difluorobenzene | $C_6H_4F_2$ |
| 1,4-Difluorobenzene | $C_6H_4F_2$ |
| 4,4′-Difluorobiphenyl | $C_{12}H_8F_2$ |
| 1,1-Difluoroethane | $C_2H_4F_2$ |
| Diformylhydrazine | $C_2H_4N_2O_2$ |
| Diglycine nitrate | $C_4H_{11}N_3O_7$ |
| Diglyme | $C_6H_{14}O_3$ |
| 4,4′-Diheptanoyloxydiphenyl-diacetylene | $C_{30}H_{34}O_4$ |
| 4,4′-Dihexanoyloxydiphenyl-diacetylene | $C_{28}H_{30}O_4$ |
| Di-*n*-hexylammonium chloride | $C_{12}H_{28}ClN$ |
| Di-*n*-hexyl sebacate | $C_{22}H_{42}O_4$ |
| 9,10-Dihydroanthracene | $C_{14}H_{12}$ |
| 4,5-Dihydro-2,3-benzofuran | $C_8H_8O$ |
| 2,5-Dihydrofuran clathrate hydrate | $C_4H_6O{\cdot}17H_2O$ |
| 9,10-Dihydrophenanthrene | $C_{14}H_{12}$ |
| 3,4-Dihydroxybenzaldehyde | $C_7H_6O_3$ |
| 1,2-Dihydroxybenzene | $C_6H_6O_2$ |
| 1,3-Dihydroxybenzene | $C_6H_6O_2$ |
| 1,4-Dihydroxybenzene | $C_6H_6O_2$ |
| 4,4′-Dihydroxybiphenyl | $C_{12}H_{10}O_2$ |
| 1,4-Dihydroxybutane | $C_4H_{10}O_2$ |
| 4,4′-Dihydroxydiphenyl-2,2-propane | $C_{15}H_{16}O_2$ |
| 1,2-Dihydroxyethane | $C_2H_6O_2$ |
| 1,5-Dihydroxy-3-oxapentane | $C_4H_{10}O_3$ |
| 1,2-Dihydroxypropane | $C_3H_8O_2$ |
| 3,5-Dihydroxytoluene monohydrate | $C_7H_8O_2{\cdot}H_2O$ |
| 1,2-Diiodobenzene | $C_6H_4I_2$ |
| 1,3-Diiodobenzene | $C_6H_4I_2$ |
| 1,4-Diiodobenzene | $C_6H_4I_2$ |
| Diisobutyl amine | $C_8H_{19}N$ |
| Diisobutyl ketone | $C_9H_{18}O$ |
| 1,6-Diisocyanatohexane | $C_8H_{12}N_2O_2$ |
| 1,1-Dimethylazoethane | $C_8N_{18}N_2$ |
| 1,1-Dimethylazoxyethane | $C_8H_{18}N_2O$ |
| 4,4′-Dimethoxyazoxybenzene | $C_{14}H_{14}N_2O_3$ |
| 1,1-Dimethoxy-3-cyanopropane | $C_6H_{11}NO_2$ |
| 2,2-Dimethoxypropane | $C_5H_{12}O_2$ |
| Dimethyl acetal of $\beta$-cyanopropion-aldehyde | $C_6H_{11}NO_2$ |
| Dimethylaminoethyl methacrylate | $C_8H_{15}NO_2$ |
| 3-Dimethylaminomethyl indole | $C_{11}H_{14}N_2$ |
| Dimethylaminopropylenediamine | $C_5H_{15}N_3$ |
| 2,6-Dimethylaniline | $C_8H_{11}N$ |
| 1,2-Dimethylbenzene | $C_8H_{10}$ |
| 1,4-Dimethylbenzene | $C_8H_{10}$ |
| 2,2′-Dimethylbiphenyl | $C_{14}H_{14}$ |
| 2,2-Dimethylbutane | $C_6H_{14}$ |
| 2,3-Dimethylbutane | $C_6H_{14}$ |
| 3,3-Dimethyl-2-butanone | $C_6H_{12}O$ |
| 2,3-Dimethyl-2,3-bis(4-*tert*-butyl-phenyl)butane | $C_{26}H_{38}$ |
| 3,4-Dimethyl-3,4-bis(4-*tert*-butyl-phenyl)hexane | $C_{30}H_{46}$ |
| 1,4-Dimethylcubane dicarboxylate | $C_{12}H_{12}O_4$ |
| 2,3-Dimethyl-2,3-diphenylbutane | $C_{16}H_{18}$ |
| N,N-Dimethylformamide | $C_3H_7NO$ |
| 2,6-Dimethyl-4-heptanone | $C_9H_{18}O$ |
| N,N′-Dimethylhydrazine | $C_2H_8N_2$ |
| N,N-Dimethylmethanamide | $C_3H_7NO$ |
| 2,3-Dimethylnaphthalene | $C_{12}H_{12}$ |
| 3,7-Dimethyl-6-octen-1-yn-3-ol | $C_{10}H_{16}O$ |
| 3,3-Dimethyl-2-oxabutane | $C_5H_{12}O$ |
| 3,4-Dimethylpentanal | $C_7H_{14}O$ |
| 2,3-Dimethylpentane | $C_7H_{16}$ |
| 3,3-Dimethylpentane | $C_7H_{16}$ |
| N,N-Dimethyl-2-pentylnonylamine | $C_{16}H_{35}N$ |
| 2,3-Dimethylphenol | $C_8H_{10}O$ |
| 2,4-Dimethylphenol | $C_8H_{10}O$ |
| 2,5-Dimethylphenol | $C_8H_{10}O$ |
| 2,6-Dimethylphenol | $C_8H_{10}O$ |
| 3,4-Dimethylphenol | $C_8H_{10}O$ |
| 3,5-Dimethylphenol | $C_8H_{10}O$ |
| 3,4-Dimethylphospholyl manganese tricarbonyl | $C_9H_8MnO_3P$ |
| Dimethyl *o*-phthalate | $C_{10}H_{10}O_4$ |
| N,N-Dimethyl-1,3-propanediamine | $C_5H_{14}N_2$ |
| 2,2-Dimethylpropanamide | $C_5H_{11}NO$ |
| 2-(1,2-Dimethylpropyl)-5,6-methylheptenal | $C_{14}H_{26}O$ |
| 2,3-Dimethylpyridine | $C_7H_9N$ |
| 2,4-Dimethylpyridine | $C_7H_9N$ |
| 2,5-Dimethylpyridine | $C_7H_9N$ |
| 2,6-Dimethylpyridine | $C_7H_9N$ |
| 3,4-Dimethylpyridine | $C_7H_9N$ |
| 3,5-Dimethylpyridine | $C_7H_9N$ |
| 2,4-Dimethylpyrrole | $C_6H_9N$ |
| 2,5-Dimethylpyrrole | $C_6H_9N$ |
| 1,1-Dimethyl-1-silacyclobutane | $C_5H_{12}Si$ |
| 6,10-Dimethyl-2-undecanone | $C_{13}H_{26}O$ |
| 6,10-Dimethyl-4,5,9-undecatrien-2-one | $C_{13}H_{20}O$ |
| 6,10-Dimethyl-3,5,9-undecatrien-2-one | $C_{13}H_{20}O$ |
| 1,3-Dimethyluracil | $C_6H_8N_2O_2$ |
| 1,1-Dimethylurea | $C_3H_8N_2O$ |
| 1,3-Dimethylurea | $C_3H_8N_2O$ |
| Dimethylzinc | $C_2H_6Zn$ |
| Dinitrile-2,2′-azodiisobutyric acid | $C_8H_{12}N_4$ |
| 1,2-Dinitrobenzene | $C_6H_4N_2O_4$ |
| 1,3-Dinitrobenzene | $C_6H_4N_2O_4$ |
| 1,4-Dinitrobenzene | $C_6H_4N_2O_4$ |
| 2,3-Dinitrophenol | $C_6H_4N_2O_5$ |
| 2,4-Dinitrophenol | $C_6H_4N_2O_5$ |
| 2,5-Dinitrophenol | $C_6H_4N_2O_5$ |
| 2,6-Dinitrophenol | $C_6H_4N_2O_5$ |
| 3,4-Dinitrophenol | $C_6H_4N_2O_5$ |
| 3,5-Dinitrophenol | $C_6H_4N_2O_5$ |
| 2,2-Dinitropropane | $C_3H_6N_2O_4$ |
| 4,4′-Dinonanoyloxydiphenyl diacetylene | $C_{34}H_{42}O_4$ |
| 4,4′-Dioctanoyloxydiphenyl-diacetylene | $C_{32}H_{38}O_4$ |
| Di-*n*-octylammonium chloride | $C_{16}H_{36}ClN$ |
| Dioctyl *o*-phthalate | $C_{24}H_{38}O_4$ |
| 1,4-Dioxane | $C_4H_8O_2$ |
| 1,3-Dioxane clathrate hydrate | $C_4H_8O_2{\cdot}17H_2O$ |
| 1,4-Dioxane-2,5-dione | $C_4H_4O_4$ |
| 3,6-Dioxaoctane | $C_6H_{10}O_2$ |
| 1,3-Dioxolan | $C_3H_6O_2$ |
| 1,3-Dioxolane clathrate hydrate | $C_3H_6O_2{\cdot}17H_2O$ |
| 2,5-Dioxopiperazine | $C_4H_6N_2O_2$ |
| 4,4′-Dipentanoyloxydiphenyldiacetylene | $C_{26}H_{26}O_4$ |
| Di-*n*-pentylammonium chloride | $C_{10}H_{24}ClN$ |
| Diphenyl | $C_{12}H_{10}$ |
| Diphenylacetylene | $C_{14}H_{10}$ |
| 1,2-Diphenylbenzimidazole | $C_{19}H_{14}N_2$ |
| 1,1′-Diphenyl-1,1′-bicyclohexane | $C_{24}H_{30}$ |
| 1,1′-Diphenyl-1,1′-bicyclooctane | $C_{26}H_{34}$ |
| 1,1′-Diphenyl-1,1′-bicyclopentane | $C_{22}H_{26}$ |
| Diphenylcarbodiimide | $C_{13}H_{10}N_2$ |
| Diphenyldiethynylsilane | $C_{16}H_{12}Si$ |
| Diphenyl diketone | $C_{14}H_{10}O_2$ |
| 1,1-Diphenyldodecane | $C_{24}H_{34}$ |
| 4′,4″-Diphenylenephthalidodicarboxylic acid dihydrazide | $C_{22}H_{18}N_4O_4$ |
| 1,2-Diphenylethane | $C_{14}H_{14}$ |
| Diphenylethyne | $C_{14}H_{10}$ |

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|---|---|
| Diphenylmethane | $C_{13}H_{12}$ |
| 4,4′-Diphenyl methane diisocyanate | $C_{15}H_{10}N_2O_2$ |
| 1,3-Diphenylurea | $C_{13}H_{12}N_2O$ |
| Dipiperazinylethane | $C_{10}H_{22}N_4$ |
| 4,4′-Dipropanoyloxydiphenyldiacetylene | $C_{22}H_{18}O_4$ |
| Dipropylamine | $C_6H_{15}N$ |
| 4,5-Dipropyl-4,5-bis(4-*tert*-butylphenyl)octane | $C_{34}H_{54}$ |
| Dipropylene glycol | $C_6H_{14}O_3$ |
| 1,3-Dithiane | $C_4H_8S_2$ |
| 1,4-Dithiane | $C_4H_8S_2$ |
| 4,4′-Diundecanoyloxydiphenyldiacetylene | $C_{38}H_{50}O_4$ |
| *n*-Docosane | $C_{22}H_{46}$ |
| *n*-Dodecane | $C_{12}H_{26}$ |
| 1-Dodecanethiol | $C_{12}H_{28}S$ |
| *n*-Dodecyl mercaptan | $C_{12}H_{28}S$ |
| Dodecylammonium tetrachloromanganate | $C_{24}H_{56}N_2MnCl_4$ |
| Dodecylammonium tetrachloromanganate (II) | $C_{24}H_{56}Cl_4MnN_2$ |
| Dodecylammonium tetrachlorozincate (II) | $C_{24}H_{56}Cl_4N_2Zn$ |
| *n*-Dotriacontane | $C_{32}H_{66}$ |
| Dulcite | $C_6H_{14}O_6$ |
| Dulcitol | $C_6H_{14}O_6$ |

## E

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|---|---|
| *n*-Eicosane | $C_{20}H_{42}$ |
| 1-Eicosanethiol | $C_{20}H_{42}S$ |
| *n*-Eicosanyl mercaptan | $C_{20}H_{42}S$ |
| Enanthal | $C_7H_{14}O$ |
| ζ-Enantholactam | $C_7H_{13}NO$ |
| Endobicyclo[2.2.1]-5-heptene-2,3-dicarboxylic acid anhydride | $C_9H_8O_3$ |
| Ethanal | $C_2H_4O$ |
| Ethanamide | $C_2H_5NO$ |
| Ethane | $C_2H_6$ |
| 1,2-Ethanediol | $C_2H_6O_2$ |
| Ethanoic acid | $C_2H_4O_2$ |
| N-Ethanol isatoxine | $C_{10}H_{10}N_2O_2$ |
| Ethanol | $C_2H_6O$ |
| 4-Ethoxy-4′-butylazobenzene | $C_{18}H_{22}N_2O$ |
| N-*p*-Ethoxybenzylidene-*p*′-butylaniline | $C_{19}H_{23}NO$ |
| 2-Ethoxyethanol acetate | $C_6H_{12}O_3$ |
| 2-Ethoxyisonitrosoacetanilide | $C_{10}H_{12}N_2O_3$ |
| 4-Ethoxyisonitrosoacetanilide | $C_{10}H_{12}N_2O_3$ |
| Ethyl acetate | $C_4H_8O_2$ |
| Ethyl alcohol | $C_2H_6O$ |
| 2-Ethylbiphenyl | $C_{14}H_{14}$ |
| Ethyl carbamate | $C_3H_7NO_2$ |
| Ethyl cyanoacetate | $C_5H_7NO_2$ |
| Ethyl-2,2-dimethylpropanoate | $C_7H_{14}O_2$ |
| Ethyl ethanoate | $C_4H_8O_2$ |
| 2-Ethylhexanol | $C_8H_{18}O$ |
| Ethyl phenyl ether | $C_8H_{10}O$ |
| Ethyl propanoate | $C_5H_{10}O_2$ |
| Ethyl propionate | $C_5H_{10}O_2$ |
| Ethyl *n*-propyl ether | $C_5H_{12}O$ |
| Ethyl urea | $C_3H_8N_2O$ |
| Ethylene | $C_2H_4$ |
| Ethylene butadiene copolymer | $(C_6H_{10})_n$ |
| Ethylenediamine | $C_2H_8N_2$ |
| Ethylene dibromide | $C_2H_4Br_2$ |
| Ethylene dichloride | $C_2H_4Cl_2$ |
| Ethylene glycol | $C_2H_6O_2$ |
| Ethylene glycol acetate | $C_4H_8O_3$ |
| Ethylene glycol diacetate | $C_6H_{10}O_4$ |
| Ethylene glycol dipropanoate | $C_8H_{14}O_4$ |
| Ethylene glycol dibutanoate | $C_{10}H_{18}O_4$ |
| Ethylene oxalate | $C_4H_4O_4$ |
| Ethylene oxide hydrate | $C_2H_4O{\cdot}7H_2O$ |
| Ethylidene difluoride | $C_2H_4F_2$ |
| Eugenol | $C_{10}H_{12}O_2$ |

## F

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|---|---|
| Ferrocene | $C_{10}H_{10}Fe$ |
| Ferrocene-$d_{10}$ | $C_{10}D_{10}Fe$ |
| Ferrocene-$d_{10}$ thiourea clathrate(1:3) | $C_{13}H_{12}D_{10}FeN_6S_3$ |
| Ferrocenium hexafluorophosphate | $C_{10}H_{10}F_6FeP$ |
| Fluoranthene picric acid | $C_{22}H_{13}N_3O_7$ |
| Fluorene picric acid | $C_{19}H_{13}N_3O_7$ |
| Fluorobenzene | $C_6H_5F$ |
| 2-Fluoronaphthalene | $C_{10}H_7F$ |
| 4-Fluorotoluene | $C_7H_7F$ |
| Fluorotrichloromethane | $CCl_3F$ |
| Formamide | $CH_3NO$ |
| Freon 11 | $CCl_3F$ |
| Freon 14 | $CF_4$ |
| Freon 113 | $C_2Cl_3F_3$ |
| Freon 152A | $C_2H_4F_2$ |
| Freon C318 | $C_4F_8$ |
| Fructose | $C_6H_{12}O_6$ |
| Fructose(D) | $C_6H_{12}O_6$ |

## G

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|---|---|
| Galactitol | $C_6H_{14}O_6$ |
| Galactose(D) | $C_6H_{12}O_6$ |
| Gallium triethyl | $C_6H_{15}Ga$ |
| Galvinoxyl hydrogalvinoxyl (6:1) radical | $C_{203}H_{288}O_{14}$ |
| Galvinoxyl hydrogalvinoxyl (9:1) radical | $C_{290}H_{411}O_{20}$ |
| Geranial | $C_{10}H_{16}O$ |
| α-Glucose(D) | $C_6H_{12}O_6$ |
| Glutamic acid | $C_5H_9NO_4$ |
| Glycerol | $C_3H_8O_3$ |
| Glycerol triacetate | $C_9H_{14}O_6$ |
| Glyceryl tributyrate | $C_{15}H_{26}O_6$ |
| Glyceryl trimargarate | $C_{54}H_{104}O_6$ |
| Glyceryl tristearate | $C_{57}H_{110}O_6$ |
| Glycolide | $C_4H_4O_4$ |
| Gramine | $C_{11}H_{14}N_2$ |
| Graphite | C |

## H

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|---|---|
| *n*-Henicosane | $C_{21}H_{44}$ |
| *n*-Heptacosane | $C_{27}H_{56}$ |
| *n*-Heptadecane | $C_{17}H_{36}$ |
| *n*-Heptaldehyde | $C_7H_{14}O$ |
| 2,2,4,4,6,8,8-Heptamethylnonane | $C_{16}H_{34}$ |
| 1,1,1,3,5,5,5-Heptamethyl-3-phenyltrisiloxane | $C_{11}H_{20}O_3Si_3$ |
| Heptanal | $C_7H_{14}O$ |
| *n*-Heptane | $C_7H_{16}$ |
| Heptanol | $C_7H_{16}O$ |
| 1-Heptanol | $C_7H_{16}O$ |
| 4-*n*-Heptoxyphenyl-4′-*n*-butylbenzoate | $C_{24}H_{32}O_3$ |
| *n*-Heptyl alcohol | $C_7H_{16}O$ |
| Hexachloroethane | $C_2Cl_6$ |
| *n*-Hexacosane | $C_{26}H_{54}$ |
| Hexadecafluoroheptane | $C_7F_{16}$ |
| *n*-Hexadecane | $C_{16}H_{34}$ |
| 1-Hexadecanethiol | $C_{16}H_{34}S$ |
| 1-Hexadecanol | $C_{16}H_{34}O$ |
| *n*-Hexadecyl mercaptan | $C_{16}H_{34}S$ |
| 2,4-Hexadiyne | $C_6H_6$ |
| Hexa-O-decanoyl-scyllo-inositol | $C_{66}H_{120}O_{12}$ |
| Hexaethylbenzene | $C_{18}H_{30}$ |
| 1,1,3,3,5,5-Hexaethylcyclotrisiloxane | $C_{12}H_{30}O_3Si_3$ |
| Hexaethylene glycol | $C_{12}H_{26}O_7$ |
| Hexafluorobenzene | $C_6F_6$ |
| Hexa-O-hexanoyl-scyllo-inositol | $C_{42}H_{72}O_{12}$ |

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| Hexahydroxyhexaethylenediamine chromium sulfate decahydrate | $C_{12}H_{52}Cr_4N_{12}O_{18}S_3 \cdot 10H_2O$ |
| Hexamethyldisilane | $C_6H_{18}Si_2$ |
| 1,6-Hexamethylene diisocyanate | $C_8H_{12}N_2O_2$ |
| 1,6-Hexamethylene diisocyanate polycyclotrimer | $(C_8H_{12}N_2O_2)_n$ |
| 1-Hexanol | $C_6H_{14}O$ |
| 2,3,6,7,10,11-Hexa-*n*-octanoyloxy-triphenylene | $C_{66}H_{96}O_{12}$ |
| 2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid I) | $C_{66}H_{96}O_{12}$ |
| 2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid II) | $C_{66}H_{96}O_{12}$ |
| 2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid III) | $C_{66}H_{96}O_{12}$ |
| Hexa-O-octanoyl-scyllo-inositol | $C_{54}H_{96}O_{12}$ |
| 4b$\alpha$,4c$\beta$,5,9b$\beta$,9c$\alpha$,10-Hexahydrocyclabuta[1,2-a:3,4-a']diindene | $C_{18}H_{16}$ |
| 4b$\beta$,4c$\alpha$,9,9a$\alpha$,9b$\beta$,10-Hexahydrocyclobuta[1,2-a:4,3-a']diindene | $C_{18}H_{16}$ |
| 1,1,3,3,5,5-Hexamethyl-1,3,5-trisilacyclohexane | $C_9H_{24}Si_3$ |
| 1,1,1,5,5,5-Hexamethyl-3,3-diphenyltrisiloxane | $C_{24}H_{28}O_2Si_3$ |
| 1,1,3,3,5,5-Hexamethyl-7,7-diphenyltetrasiloxane | $C_{18}H_{28}Si_4O_4$ |
| Hexamethylbenzene | $C_{12}H_{18}$ |
| Hexamethyldisilylmethane | $C_7H_{20}Si_2$ |
| 1,6-Hexamethylene diisocyanate | $C_8H_{12}N_2$ |
| Hexamethylphosphoramide | $C_6H_{18}N_3OP$ |
| Hexamethylphosphoric triamide | $C_6H_{18}N_3OP$ |
| *cis*-(5,12)-7,7,14,14-Hexamethyl-1,4,8,11-tetraazacyclotetradecane | $C_{16}H_{36}N_4$ |
| Hexamethyltrisilazane | $C_6H_{21}N_3Si_3$ |
| *n*-Hexane | $C_6H_{14}$ |
| 1,6-Hexanediol | $C_6H_{14}O_2$ |
| 1-Hexanethiol | $C_6H_{14}S$ |
| 1-Hexanol | $C_6H_{14}O$ |
| 2-Hexanone | $C_6H_{12}O$ |
| 3-Hexanone | $C_6H_{12}O$ |
| 1,1,3,3,5,5-Hexaphenyl-7,7-dimethyl-cyclotetrasiloxane | $C_{38}H_{36}O_4Si_4$ |
| Hexaphenylisomelamine | $C_{39}H_{30}N_6$ |
| Hexaphenylmelamine | $C_{39}H_{30}N_6$ |
| Hexapropylene glycol | $C_{18}H_{38}O_7$ |
| *n*-Hexatriacontane | $C_{36}H_{74}$ |
| 1-Hexene | $C_6H_{12}$ |
| *n*-Hexyl alcohol | $C_6H_{14}O$ |
| *n*-Hexyl ethanoate | $C_8H_{16}O_2$ |
| *n*-Hexyl mercaptan | $C_6H_{14}S$ |
| *p*-*n*-Hexyloxybenzylideneaniline | $C_{19}H_{23}NO$ |
| *p*-*n*-Hexyloxybenzylideneamino-*p'*-benzonitrile | $C_{20}H_{22}N_2O$ |
| *p*-*n*-Hexyloxybenzylideneamino-*p'*-chlorobenzene | $C_{19}H_{22}ClNO$ |
| *p*-*n*-Hexyloxybenzylideneamino-*p'*-fluorobenzene | $C_{19}H_{22}FNO$ |
| N-*p*-*n*-Hexyloxybenzylidene-*p'*-*n*-butylaniline | $C_{23}H_{31}NO$ |
| *p*-*n*-Hexyloxybenzylidene-*p'*-toluidine | $C_{20}H_{25}NO$ |
| 1-Hexynylcopper | $C_6H_9Cu$ |
| HMX | $C_4H_8N_8O_8$ |
| Homocubane-4-carboxylic acid | $C_{10}H_{10}O_2$ |
| Hydrazinium hydrogen oxalate | $C_2H_6N_2O_4$ |
| Hydroquinone | $C_6H_6O_2$ |
| 1-Hydroxyadamantane | $C_{10}H_{16}O$ |
| 2-Hydroxyadamantane | $C_{10}H_{16}O$ |
| 2-(2'-Hydroxyethoxy)ethyl pivalate | $C_9H_{18}O_4$ |
| 2-Hydroxyethyl-2',2'-dimethyl-propionate | $C_7H_{14}O_3$ |
| 2-Hydroxyethyl pivalate | $C_7H_{14}O_3$ |
| 2-Hydroxypropanoic acid (DL) | $C_3H_6O_3$ |
| m-Hydroxytoluene | $C_7H_8O$ |
| *o*-Hydroxytoluene | $C_7H_8O$ |
| p-Hydroxytoluene | $C_7H_8O$ |

## I

| | |
|---|---|
| Imidazole | $C_3H_4N_2$ |
| Indazole | $C_7H_6N_2$ |
| Indene picric acid | $C_{15}H_{11}N_3O_7$ |
| 3-Indole aldehyde | $C_9H_7NO$ |
| Indole | $C_8H_7N$ |
| meso-Inositol | $C_6H_{12}O_6$ |
| Iodobis(N,N-dimethyldithiocarbamato) iron (III) | $C_6H_{12}FeIN_2S_4$ |
| Iodomethane | $CH_3I$ |
| Iron (III) acetylacetonate | $C_{15}H_{21}FeO_6$ |
| Isoamyl propionate | $C_8H_{16}O_2$ |
| Isobutene | $C_4H_8$ |
| Isobutyl alcohol | $C_4H_{10}O$ |
| Isobutylmethylketone | $C_6H_{12}O$ |
| Isobutyric acid | $C_4H_8O_2$ |
| Isochroman | $C_9H_7O$ |
| 1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl)benzene | $C_{13}H_{15}NO$ |
| 1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl)benzene | $C_{13}H_{15}NO$ |
| Isonitrosoacetanilide | $C_8H_8N_2O_2$ |
| Isooctane | $C_8H_{18}$ |
| Isooctyl alcohol | $C_8H_{18}O$ |
| Isophytol | $C_{20}H_{40}O$ |
| Isopropyl methyl ketone | $C_5H_{10}O$ |
| Isopropyl nitrate | $C_3H_7NO_3$ |
| Isopropyl urea | $C_4H_{10}N_2O$ |
| Isoquinoline | $C_9H_7N$ |

## L

| | |
|---|---|
| Lactic acid (DL) | $C_3H_6O_3$ |
| Lactide (DL) | $C_6H_8O_4$ |
| Lactose, anhydrous | $C_{12}H_{22}O_{11}$ |
| Lead dicalcium propionate | $C_{18}H_{30}Ca_2O_{12}Pb$ |
| Leucine (L) | $C_6H_{13}NO_2$ |
| Lithium acetate dihydrate | $C_2H_3LiO_2 \cdot 2H_2O$ |
| Lithium butyrate | $C_4H_7LiO_2$ |
| Lithium n-heptanoate | $C_7H_{13}LiO_2$ |
| Lithium n-hexanoate | $C_6H_{11}LiO_2$ |
| Lithium n-pentanoate | $C_5H_9LiO_2$ |
| Lithium propionate | $C_3H_5LiO_2$ |

## M

| | |
|---|---|
| Magnesium acetate | $C_4H_6O_4Mg$ |
| Magnesium diethanoate tetrahydrate | $C_4H_6MgO_4 \cdot 4H_2O$ |
| Malononitrile | $C_3H_2N_2$ |
| Maleic anhydride | $C_4H_2O_3$ |
| Maltose | $C_{12}H_{22}O_{11}$ |
| Manganocene | $C_{10}H_{10}Mn$ |
| Mannitol | $C_6H_{14}O_6$ |
| Mannitol(D) | $C_6H_{14}O_6$ |
| Mannose(D) | $C_6H_{12}O_6$ |
| Manxane | $C_{11}H_{20}$ |
| Methacrylic acid | $C_4H_6O_2$ |
| *p*-Methacryloyloxybenzoic acid | $C_{11}H_{10}O_4$ |
| Methanamide | $CH_3NO$ |
| Methane | $CH_4$ |
| Methanol | $CH_4O$ |
| Methionine (DL) | $C_5H_{11}NO_2S$ |
| Methionine (L) | $C_5H_{11}NO_2S$ |
| Methoxybenzene | $C_7H_8O$ |
| N-(4-Methoxybenzylidene)-*p*-(*n*-butyl)-aniline | $C_{18}H_{21}NO$ |
| 2-Methoxyethanol acetate | $C_5H_{10}O_3$ |
| 2-Methoxyisonitrosoacetanilide | $C_9H_{10}N_2O_3$ |

| | |
|---|---|
| 4-Methoxyisonitrosoacetanilide | $C_9H_{10}N_2O_3$ |
| 2-Methoxy-1-propene | $C_4H_8O$ |
| 3-Methoxypropylamine | $C_4H_{11}NO$ |
| Methyl acrylate | $C_4H_6O_2$ |
| α-Methyl acrylic acid | $C_4H_6O_2$ |
| Methyl alcohol | $CH_4O$ |
| Methylammonium hexachloro-tellurate | $C_2H_{12}Cl_6Te$ |
| Methylammonium iodide | $CH_6IN$ |
| 4-Methylaniline | $C_7H_9N$ |
| N-Methylaniline | $C_7H_9N$ |
| 2-Methyl-2-butanol | $C_5H_{12}O$ |
| 3-Methyl-2-butanone | $C_5H_{10}O$ |
| 2-Methyl-1-butene | $C_5H_{10}$ |
| 2-Methyl-2-butene | $C_5H_{10}$ |
| 3-Methyl-1-butene | $C_5H_{10}$ |
| 2-Methyl-3-buten-2-ol | $C_5H_{10}O$ |
| 4-(2-Methylbutoxy)phenyl ester of 4-*n*-decycloxybenzoic acid (D) | $C_{28}H_{40}O_4$ |
| Methyl *n*-butyl ether | $C_5H_{12}O$ |
| Methyl *tert*-butyl ether | $C_5H_{12}O$ |
| Methyl carbamate | $C_2H_5NO_2$ |
| N-Methylcarbazole | $C_{13}H_{11}N$ |
| Methylchloroform | $C_2H_3Cl_3$ |
| Methyl cyanide | $C_2H_3N$ |
| Methylcyclohexane | $C_7H_{14}$ |
| 4-Methylcyclohexene | $C_7H_{12}$ |
| Methyl *n*-decyl ether | $C_{11}H_{24}O$ |
| 3,3'-Methylene bis(6-aminophenol) | $C_{13}H_{14}N_2O_2$ |
| Methylenecyclobutane | $C_5H_8$ |
| Methylene dichloride | $CH_2Cl_2$ |
| Methylene glycol acetate | $C_3H_6O_3$ |
| Methyl ester of nitroacetic acid | $C_3H_5NO_4$ |
| Methylethylethanolamine | $C_5H_{13}NO$ |
| Methyl ethyl ketone | $C_4H_8O$ |
| N-Methylformamide | $C_2H_5NO$ |
| Methyl formate | $C_2H_4O_2$ |
| 2-Methyl-1-heptanol | $C_8H_{18}O$ |
| 6-Methyl-5-hepten-2-one | $C_8H_{14}O$ |
| 3-Methylhexanal | $C_7H_{14}O$ |
| Methyl iodide | $CH_3I$ |
| Methyl methacrylate | $C_5H_8O_2$ |
| N-Methylmethanamide | $C_2H_5NO$ |
| Methyl methanoate | $C_2H_4O_2$ |
| Methyl 2-methylpropenoate | $C_5H_8O_2$ |
| Methyl nitroacetate | $C_3H_5NO_4$ |
| 2-Methyloxirane | $C_3H_6O$ |
| N-Methylpentanamide | $C_6H_{13}NO$ |
| 2-Methylpentane | $C_6H_{14}$ |
| 3-Methylpentane | $C_6H_{14}$ |
| 2-Methyl-1-pentanol | $C_6H_{14}O$ |
| 3-Methyl-2-pentanol | $C_6H_{14}O$ |
| 3-Methyl-3-pentanol | $C_6H_{14}O$ |
| 4-Methyl-2-pentanol | $C_6H_{14}O$ |
| 4-Methyl-2-pentanone | $C_6H_{12}O$ |
| Methyl perfluorobutanoate | $C_5H_3F_7O_2$ |
| 4-Methylphenanthrene | $C_{15}H_{12}$ |
| 2-Methylphenol | $C_7H_8O$ |
| 3-Methylphenol | $C_7H_8O$ |
| 4-Methylphenol | $C_7H_8O$ |
| 2-Methylpiperidine | $C_6H_{13}N$ |
| Methyl phenyl ether | $C_7H_8O$ |
| 2-Methylpropanamide | $C_4H_9NO$ |
| Methyl propanoate | $C_4H_8O_2$ |
| 2-Methylpropanoic acid | $C_4H_8O_2$ |
| 2-Methyl-1-propanol | $C_4H_{10}O$ |
| 2-Methyl-2-propanol | $C_4H_{10}O$ |
| 2-Methylpropene | $C_4H_8$ |
| Methyl propenoate | $C_4H_6O_2$ |
| Methyl propionate | $C_4H_8O_2$ |
| Methyl *n*-propyl ether | $C_4H_{10}O$ |
| 2-Methylpyridine | $C_6H_7N$ |
| 4-Methylpyridine | $C_6H_7N$ |
| N-Methylpyrrole | $C_5H_7N$ |
| 3-Methylpyrrolidine | $C_5H_{11}N$ |
| Methyl silicate | $C_4H_{12}O_4Si$ |
| α-Methylstyrene | $C_9H_{10}$ |
| Methyl trichlorothioacrylate | $C_4H_3Cl_3OS$ |
| Methyltriphenylphosphonium bis(7,7,8,8-tetracyanoquinodimethanide) | $C_{43}H_{26}N_8P$ |
| N-Methylvaleramide | $C_6H_{13}NO$ |
| 4-Methyoxy-4'-heptanoylazobenzene | $C_{20}H_{24}N_2O_3$ |
| Milk sugar | $C_{12}H_{22}O_{11}$ |
| Mixed valence iron oxo-centered complex with acetate and 3-methyl pyridine | $C_{36}H_{46}Fe_3N_4O_{13}$ |
| Monobutylurea | $C_5H_{12}N_2O$ |
| Mono-*tert*-butylurea | $C_5H_{12}N_2O$ |
| Monochloroacetic acid | $C_2H_3ClO_2$ |
| Monoethylurea | $C_3H_8N_2O$ |
| Monoisopropylurea | $C_4H_{10}N_2O$ |
| Monomethylurea | $C_2H_6N_2O$ |
| Monophenylurea | $C_7H_8N_2O$ |
| Monopropylurea | $C_4H_{10}N_2O$ |
| Morpholine | $C_4H_9NO$ |

## N

| | |
|---|---|
| Naphthalene picric acid | $C_{16}H_{11}N_3O_7$ |
| Naphthalene-tetracyanobenzene | $C_{20}H_{10}N_4$ |
| Naphthalene-tetracyanoethylene | $C_{18}H_8N_4$ |
| Naphthalene | $C_{10}H_8$ |
| Natural ricinoleic acid | $C_{18}H_{34}O_3$ |
| Nickelocene | $C_{10}H_{10}Ni$ |
| 3-Nitroaniline | $C_6H_6N_2O_2$ |
| 4-Nitroaniline | $C_6H_6N_2O_2$ |
| *p*-Nitroanisole | $C_7H_7NO_3$ |
| Nitrobenzene | $C_6H_5NO_2$ |
| 4-Nitrobenzoic acid | $C_7H_6NO_2$ |
| 4-Nitrochlorobenzene | $C_6H_4ClNO_2$ |
| *p*-Nitroethoxybenzene | $C_8H_9NO_3$ |
| 4-Nitromethoxybenzene | $C_7H_7NO_3$ |
| *p*-Nitrophenetole | $C_8H_9NO_3$ |
| 2-Nitrophenol | $C_6H_5NO_3$ |
| 3-Nitrophenol | $C_6H_5NO_3$ |
| 4-Nitrophenol | $C_6H_5NO_3$ |
| 4'-Nitrophenyl-4-*n*-octyloxybenzoate | $C_{21}H_{25}NO_5$ |
| 4-Nitrophenyl-4'-octyloxybenzoate | $C_{21}H_{25}NO_5$ |
| *n*-Nonacosane | $C_{29}H_{60}$ |
| *n*-Nonadecane | $C_{19}H_{40}$ |
| Nonanal | $C_9H_{18}O$ |
| *n*-Nonane | $C_9H_{20}$ |
| 5-Nonanone | $C_9H_{18}O$ |
| Nonylcyanobiphenyl | $C_{22}H_{27}N$ |
| Nonyl methacrylate | $C_{13}H_{24}O_2$ |
| Norbornadiene | $C_7H_8$ |
| Norbornane | $C_7H_{12}$ |
| Norbornene | $C_7H_{10}$ |
| Norleucine (DL) | $C_6H_{13}NO_2$ |
| Norleucine (L) | $C_6H_{13}NO_2$ |
| Northindrone 4-cyclohexylbenzoate | $C_{33}H_{40}O_2$ |
| Northindrone-6-(4-chlorophenyl)-hexanoate | $C_{32}H_{39}ClO_2$ |
| Northindrone acetate | $C_{22}H_{28}O_2$ |
| Northindrone benzoate | $C_{27}H_{30}O_2$ |
| Northindrone biphenyl-4-carboxylate | $C_{33}H_{34}O_2$ |
| Northindrone dimethylpropionate | $C_{25}H_{34}O_2$ |
| Northindrone heptanoate | $C_{27}H_{38}O_2$ |
| Northindrone pentamethyldisiloxyl ether | $C_{25}H_{40}O_2Si_2$ |
| Northindrone *trans*-3-(4-butylcyclo-hexyl)propionate | $C_{33}H_{48}O_2$ |
| Northindrone *trans*-4-hexylcyclo-hexylcarboxylate | $C_{33}H_{34}O_2$ |

| | |
|---|---|
| Northindrone | $C_{20}H_{26}O$ |
| Nortricyclene | $C_7H_{10}$ |
| Norvaline (L) | $C_5H_{11}NO_2$ |

## O

| | |
|---|---|
| *n*-Octacosane | $C_{28}H_{58}$ |
| *n*-Octadecane | $C_{18}H_{38}$ |
| 1-Octadecanethiol | $C_{18}H_{38}S$ |
| Octadecanoic acid | $C_{18}H_{36}O_2$ |
| Octadecylammonium cadmium tetrachloride | $C_{36}H_{80}CdCl_4N_2$ |
| *n*-Octadecyl mercaptan | $C_{18}H_{38}S$ |
| Octaethylcyclotetrasiloxane | $C_{16}H_{40}O_4Si_4$ |
| Octafluorocyclobutane | $C_4F_8$ |
| Octagen | $C_4H_8N_8O_8$ |
| Octagen($\alpha$) | $C_4H_8N_8O_8$ |
| Octagen($\beta$) | $C_4H_8N_8O_8$ |
| 1,2,3,4,5,6,7,8-Octahydroanthracene | $C_{14}H_{18}$ |
| 5,6,6a,6b,7,8,12b,12c-Octahydrodibenzo[a,i]biphenylene | $C_{20}H_{20}$ |
| 5,6,6a,6b,11,12,12a,12b-Octahydrodibenzo[a,g]biphenylene | $C_{20}H_{20}$ |
| 1,1,4,4,10,10,13,13-Octamethylcyclooctadecane | $C_{26}H_{52}$ |
| Octamethyltetrasiloxane | $C_8H_{24}Si_4O_4$ |
| Octamethyltetrasilazane | $C_8H_{28}Ni_4Si$ |
| Octanal | $C_8H_{16}O$ |
| *n*-Octane | $C_8H_{18}$ |
| 1-Octanethiol | $C_8H_{16}S$ |
| Octanol | $C_8H_{18}O$ |
| 1-Octanol | $C_8H_{18}O$ |
| Octaphenylcyclotetrasiloxane | $C_{48}H_{40}O_4Si_4$ |
| Octa(vinylsilasesquioxane) | $C_{16}H_{24}Si_8O_{12}$ |
| 4-Octyl-4′-heptyl-$\alpha$-cyanostilbene | $C_{20}H_{41}NO$ |
| *n*-Octyl alcohol | $C_8H_{18}O$ |
| *n*-Octyl mercaptan | $C_8H_{16}S$ |
| *n*-Octyl methacrylate | $C_{12}H_{22}O_2$ |
| Octylcyanobiphenyl | $C_{21}H_{25}N$ |
| Oenanthal | $C_7H_{14}O$ |
| Oligoethylene butylene glycol adipate | $C_{12}H_{22}O_6$ |
| Orcinol monohydrate | $C_7H_8O_2{\cdot}H_2O$ |
| 2-Oxadodecane | $C_{11}H_{24}O$ |
| 2-Oxahexane | $C_5H_{12}O$ |
| 3-Oxahexane | $C_5H_{12}O$ |
| Oxalyl fluoride | $C_2F_2O_2$ |
| 2-Oxapentane | $C_4H_{10}O$ |
| Oxolane | $C_4H_8O$ |
| $\mu_3$-Oxo-tris(pyridine)hexakis(acetato) iron(II)-diiron monopyridine | $C_{32}H_{38}Fe_3N_4O_{15}$ |

## P

| | |
|---|---|
| 2,2-Paracyclophane | $C_{16}H_{16}$ |
| Pelargonaldehyde | $C_9H_{18}O$ |
| *n*-Pentacosane | $C_{25}H_{52}$ |
| *n*-Pentadecane | $C_{15}H_{32}$ |
| Pentaerythritol | $C_5H_{12}O_4$ |
| 2,2,4,6,6-Pentamethylheptane | $C_{12}H_{26}$ |
| *n*-Pentanal | $C_5H_{10}O$ |
| 1-Pentanol | $C_5H_{12}O$ |
| *tert*-Pentanol | $C_5H_{12}O$ |
| 2-Pentanone | $C_5H_{10}O$ |
| 3-Pentanone | $C_5H_{10}O$ |
| Pentapropylene glycol | $C_{15}H_{32}O_6$ |
| 1-Pentene | $C_5H_{10}$ |
| *cis*-2-Pentene | $C_5H_{10}$ |
| *trans*-2-Pentene | $C_5H_{10}$ |
| *n*-Pentyl alcohol | $C_5H_{12}O$ |
| *tert*-Pentyl alcohol | $C_5H_{12}O$ |
| Pentyl butanoate | $C_9H_{18}O_2$ |
| Pentyl propionate | $C_8H_{16}O_2$ |
| *n*-Pentylamine | $C_5H_{13}N$ |
| Pentyldiamine manganese tetrachloride | $C_5H_{16}Cl_4Mn$ |
| 2-Pentylnonenal | $C_{14}H_{26}O$ |
| N-*p*-*n*-Pentyloxybenzylidene-*p*′-*n*-butylaniline | $C_{22}H_{29}NO$ |
| Perchlorobiphenyl | $C_{12}Cl_{10}$ |
| Perfluorobenzene | $C_6F_6$ |
| Perfluorobiphenyl | $C_{12}F_{10}$ |
| *n*-Perfluorobutane | $C_4F_{10}$ |
| Perfluoroheptane | $C_7F_{16}$ |
| *n*-Perfluorohexane | $C_6F_{14}$ |
| Perfluoromethyldiethylamine | $C_5F_{13}N$ |
| *n*-Perfluoropentane | $C_5F_{12}$ |
| Perfluorotriethylamine | $C_6F_{15}N$ |
| Perhydrophenanthrene | $C_{14}H_{24}$ |
| Perylene picric acid | $C_{26}H_{15}N_3O_7$ |
| Phenanthrene | $C_{14}H_{10}$ |
| Phenanthridine | $C_{13}H_9N$ |
| Phenol | $C_6H_6O$ |
| Phenolphthalein | $C_{20}H_{14}O_4$ |
| 1-Phenyl-1-cyclohexyldodecane | $C_{24}H_4O$ |
| Phenyl glycidyl ether | $C_9H_{10}O_2$ |
| Phenylacetylene | $C_8H_6$ |
| Phenylaminoethyl methacrylate | $C_{12}H_{15}NO_2$ |
| 1,3-Phenylenediamine | $C_6H_8N_2$ |
| Phenylhydrazine | $C_6H_8N_2$ |
| 3-Phenyl-5-phenoxymethyl-2-N-phenyliminooxazolidine | $C_{22}H_{20}N_2O_2$ |
| 3-Phenyl-5-phenoxymethyl-2-oxazolidinone | $C_{16}H_{15}NO_3$ |
| N-Phenylphthalimide | $C_{14}H_{11}NO_3$ |
| Phenylpropionic acid | $C_9H_{10}O_2$ |
| *o*-Phenylenepyrene picric acid | $C_{28}H_{15}N_3O_7$ |
| Phenyltrichlorogermane | $C_6H_5Cl_3Ge$ |
| Phenyltrichlorostannane | $C_6H_5Cl_3Sn$ |
| Phenyl-*o*-tolylmethane | $C_{14}H_{14}$ |
| Phenylurea | $C_7H_8N_2O$ |
| Phosphaferrocene | $C_9H_9FeP$ |
| Phthalanilic acid | $C_{14}H_9NO_2$ |
| Phthalic anhydride | $C_8H_4O_3$ |
| Phthalonitrile and *m*-phenylene diamine condensation product | $C_{28}H_{18}N_6$ |
| *o*-Phthalonitrile | $C_8H_4N_2$ |
| Phytone | $C_{18}H_{36}O$ |
| Picene picric acid | $C_{28}H_{17}N_3O_7$ |
| $\alpha$-Picoline | $C_6H_7N$ |
| Picric acid | $C_6H_3N_3O_7$ |
| Piperazine | $C_4H_{10}N_2$ |
| Piperidine | $C_5H_{11}N$ |
| $\alpha$-Piperidone | $C_5H_9NO$ |
| Pival aldehyde | $C_5H_{10}O$ |
| Polyacetylene | $(CH)_n$ |
| Polybenzimidazoloquinazole | $(C_{34}H_{18}N_6O)_n$ |
| Poly(2,2-bis-(4-phenoxypropane) 2,4,6-triazine | $(C_{17}H_{14}N_2)_n$ |
| *cis*-1,4-Polybutadiene | $(C_4H_6)n$ |
| *trans*-1,4-Polybutadiene | $(C_4H_6)n$ |
| Polybutylene glycol adipate | $(C_{10}H_{16}O_4)_n$ |
| Poly(butylene terephthalate) | $(C_{12}H_{12}O_4)_n$ |
| Poly-$\epsilon$-caprolactam | $(C_6H_{11}NO)_n$ |
| Poly-$\epsilon$-caprolactone | $(C_6H_{10}O_2)_n$ |
| Polycyanate | $(C_{17}H_{14}N_2O_2)_n$ |
| Poly(diethylsiloxane) | $(C_4H_{10}OSi)_n$ |
| Poly-1,1-diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene | $(C_{32}H_{22}Ge)_n$ |
| Poly-4,4′-dihydroxy-3,3′-isophthalamidodiphenylmethane | $(C_{21}H_{16}N_2O_4)_n$ |
| Poly(dimethylsiloxane) | $(C_2H_6OSi)_n$ |
| Poly-1,3-dioxolan | $(C_3H_6O_2)_n$ |
| Polydiphenyldiethynylgermanium | $(C_{16}H_{10}Ge)_n$ |

| | |
|---|---|
| Polydiphenyldiethynylgermanium | $(C_{16}H_{10}Ge)_n$ |
| Poly(*p,p'*-diphenylene oxide) pyromellitimide | $C_{22}H_{14}N_2O_7$ |
| Poly(*p,p'*-diphenylenephthalido)hydrazide | $(C_{30}H_{20}N_4O_6)_n$ |
| Poly(*p,p'*-diphenylenephthalido)-1,3,4-oxadiazole | $(C_{30}H_{16}N_4O_4)_n$ |
| Polyethylene | $(CH_2)_n$ |
| Polyethylene glycol | $(C_2H_4O)_n$ |
| Polyethylene oxalate | $(C_4H_4O_4)_n$ |
| Polyglycine I | $(C_2H_3NO)_n$ |
| Polyglycine II | $(C_2H_3NO)_n$ |
| Polyglycolide | $(C_4H_4O_4)_n$ |
| Poly(hexamethylene sebacate) | $(C_{38}H_{70}O_8)_n$ |
| 1-Polyhexene | $(C_6H_{12})_n$ |
| Polyisobutylene | $(C_4H_8)_n$ |
| Polyisocyanurate | $(C_{15}H_{10}N_2O_2)_n$ |
| Polymethacrylic acid | $(C_4H_6O_2)_n$ |
| Poly-*p*-methyacryloyloxybenzoic acid | $(C_{11}H_{10}O_4)_n$ |
| Poly(methyl methacrylate) | $(C_5H_8O_2)_n$ |
| Poly(α-methylstyrene) | $(C_9H_{10})_n$ |
| Polyoctenylene | $(C_8H_{14})_n$ |
| Polypentenamer | $(C_5H_8)_n$ |
| *cis*-Polypentenamer | $(C_5H_8)_n$ |
| *trans*-Polypentenamer | $(C_5H_8)_n$ |
| Polyphenylene PP-1 | $C_{20.84}H_{16.66}O_{0.62}$ |
| Polyphenylene PP-2 | $C_{20.84}H_{16.66}O_{0.62}$ |
| Poly-2,2'-*m*-phenylene)-5,5'-dibenzoxazole methane | $(C_{21}H_{12}N_2O_2)_n$ |
| Poly-[2,2'-(*p*-phenylene-1,1-diphenyl-5,5'-dibenzimidazole] | $(C_{32}H_{20}N_4)_n$ |
| Poly[2,2'-(1,4-phenylene)-7,7'-oxy-bis (3-phenylquinoxaline)] | $C_{34}H_{20}N_4O$ |
| Polypropylene, isotatic, amorphous | $(C_3H_6)_n$ |
| Polypropylene, isotatic, crystalline | $(C_3H_6)_n$ |
| Poly-[N-terphthalyl-bis-(N'-phenyl-*o*-diphenylamine)] | $(C_{32}H_{24}N_4O_2)_n$ |
| Polystyrene | $(C_8H_8)_n$ |
| Polystyrene-$d_3$ | $(C_8H_5D_3)_n$ |
| Polystyrene-$d_5$ | $(C_8H_3D_5)_n$ |
| Polystyrene-$d_8$ | $(C_8D_8)_n$ |
| Polystyrene-Polystyrene-$d_8$ | $(C_{16}H_8D_8)_n$ |
| Polytetrahydrofuran | $(C_4H_8O)_n$ |
| Polythene | $(CH_2)_n$ |
| Polytriazine | $(C_{24}H_{12}N_6)_n$ |
| Poly(tridecanolactone) | $(C_{13}H_{24}O_2)_n$ |
| Poly-N-(β-trimethylsilylethyl)azetidine | $(C_8H_{19}NSi)_n$ |
| Poly-N-(β-trimethylsilylethyl)ethylenimine | $(C_7H_{17}NSi)_n$ |
| Polyvinyl alcohol | $(C_2H_4O)_n$ |
| Polyvinyl chloride | $(C_2H_3Cl)_n$ |
| Polyvinyldimethylbenzylsilane | $(C_{11}H_{16}Si)_n$ |
| Polyvinyldimethylphenylsilane | $(C_{10}H_{14}Si)_n$ |
| Polyvinylenediphenylsilyl,germyl-α,ω-dihydride copolymer | $(C_{28}H_{24}GeSi)_n$ |
| Polyvinylenediphenylgermyl-α,ω-dihydride | $(C_{14}H_{12}Ge)_n$ |
| Polyvinylenediphenylsilyl-α,ω-dihydride | $(C_{14}H_{12}Si)_n$ |
| Polyvinylidene chloride | $(C_2H_2Cl_2)_n$ |
| Polyvinyltrimethylsilane | $(C_5H_{12}Si)_n$ |
| Potassium butyrate | $C_4H_7KO_2$ |
| Potassium 2-methylpropanoate | $C_4H_7KO_2$ |
| Potassium propionate | $C_3H_5KO_2$ |
| Potassium tetraphenyl boron | $C_{24}H_{20}BK$ |
| Propaldehyde | $C_3H_6O$ |
| Propanal | $C_3H_6O$ |
| *n*-Propane | $C_3H_8$ |
| 1,2-Propanediol | $C_3H_8O_2$ |
| 1,2,3-Propanetriol | $C_3H_8O_3$ |
| Propanoic acid | $C_3H_6O_2$ |
| 1-Propanol | $C_3H_8O$ |
| Propene | $C_3H_6$ |
| β-Propiolactone | $C_3H_4O_2$ |
| Propionic acid | $C_3H_6O_2$ |
| 4-Propionyl-4'-*n*-butanoyloxyazobenzene | $C_{19}H_{20}N_2O_3$ |
| 4-Propionyl-4'-*n*-decanoyloxyazobenzene | $C_{25}H_{32}N_2O_3$ |
| 4-Propionyl-4'-*n*-dodecanoyloxyazobenzene | $C_{27}H_{36}N_2O_3$ |
| 4-Propionyl-4'-*n*-heptadecanoyloxyazobenzene | $C_{32}H_{46}N_2O_3$ |
| 4-Propionyl-4'-*n*-heptanoyloxyazobenzene | $C_{22}H_{26}N_2O_3$ |
| 4-Propionyl-4'-*n*-hexadecanoyloxyazobenzene | $C_{31}H_{44}N_2O_3$ |
| 4-Propionyl-4'-*n*-hexanoyloxyazobenzene | $C_{21}H_{24}N_2O_3$ |
| 4-Propionyl-4'-*n*-nonanoyloxyazobenzene | $C_{24}H_{30}N_2O_3$ |
| 4-Propionyl-4'-*n*-octadecanoyloxyazobenzene | $C_{33}H_{48}N_2O_3$ |
| 4-Propionyl-4'-*n*-octanoyloxyazobenzene | $C_{23}H_{28}N_2O_3$ |
| 4-Propionyl-4'-*n*-pentadecanoyloxyazobenzene | $C_{30}H_{42}N_2O_3$ |
| 4-Propionyl-4'-*n*-tetradecanoyloxyazobenzene | $C_{29}H_{40}N_2O_3$ |
| 4-Propionyl-4'-*n*-tridecanoyloxyazobenzene | $C_{28}H_{38}N_2O_3$ |
| 4-Propionyl-4'-*n*-undecanoyloxyazobenzene | $C_{26}H_{34}N_2O_3$ |
| *n*-Propyl acetate | $C_5H_{10}O_2$ |
| *n*-Propyl alcohol | $C_3H_8O$ |
| Propyl ethanoate | $C_5H_{10}O_2$ |
| Propyl formate | $C_4H_8O_2$ |
| Propyl methanoate | $C_4H_8O_2$ |
| *n*-Propyl methyl ketone | $C_5H_{10}O$ |
| *n*-Propyl propanoate | $C_6H_{12}O_2$ |
| Propyl propionate | $C_6H_{12}O_2$ |
| Propyl urea | $C_4H_{10}N_2O$ |
| Propyldiammonium cadmium tetrachloride | $C_3H_{12}CdCl_4N_2$ |
| Propyldiammonium manganese tetrachloride | $C_3H_{12}Cl_4MnN_2$ |
| Propylene carbonate | $C_4H_6O_3$ |
| Propylene glycol | $C_3H_8O_2$ |
| Propylene oxide clathrate hydrate | $C_3H_6O{\cdot}17H_2O$ |
| Propylene oxide | $C_3H_6O$ |
| Propylene | $C_3H_6$ |
| Pyrazole | $C_3H_4N_2$ |
| Pyrene picric acid | $C_{22}H_{13}N_3O_7$ |
| Pyrocatechin | $C_6H_6O_2$ |
| Pyromellitic dianhydride | $C_{10}H_2O_6$ |
| α-Pyrrolidone | $C_4H_7NO$ |
| Pyrroyl manganese tricarbonyl | $C_7H_4MnNO_3$ |

## Q

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|---|---|
| Quadricyclane | $C_7H_8$ |
| *p*-Quaterphenyl | $C_{24}H_{18}$ |
| Quinoline | $C_9H_7N$ |
| *p*-Quinquephenyl | $C_{30}H_{22}$ |

## R

| | |
|---|---|
| Resorcin | $C_6H_6O_2$ |
| Resorcinol | $C_6H_6O_2$ |
| Ribose(D) | $C_5H_{10}O_5$ |
| Rochelle salt | $C_4H_4KNaO_6{\cdot}4H_2O$ |
| Rubidium tetraphenyl boron | $C_{24}H_{20}BRb$ |
| Ruthenocene | $C_{10}H_{10}Ru$ |

## S

| | |
|---|---|
| β-Selenodiglycol | $C_4H_{10}O_2Se$ |
| Selenophene chromium tricarbonyl | $C_7H_4CrO_3Se$ |
| Semicarbazide | $CH_5N_3O$ |
| Silver phenylacetylenide | $C_8H_5Ag$ |
| Sodium acetate | $C_2H_3NaO_2$ |
| Sodium acetate trihydrate | $C_2H_3NaO_2{\cdot}3H_2O$ |

| | |
|---|---|
| Sodium ethanoate | $C_2H_3NaO_2$ |
| Sodium formate | $CHNaO_2$ |
| Sodium methanoate | $CHNaO_2$ |
| Sodium potassium tartrate tetrahydrate | $C_4H_4KNaO_6{\cdot}4H_2O$ |
| Sodium propanoate | $C_3H_5NaO_2$ |
| Sorbitol(D) | $C_6H_{14}O_6$ |
| Squaric acid | $C_4H_2O_4$ |
| Stearic acid | $C_{18}H_{36}O_2$ |
| *trans*-Stilbene | $C_{14}H_{12}$ |
| Strontium dicalcium propionate | $C_{18}H_{30}Ca_2O_{12}Sr$ |
| Styphnic acid | $C_6H_3N_3O_8$ |
| Styrene | $C_8H_8$ |
| Styrene-$d_8$ | $C_8D_8$ |
| Succinonitrile | $C_4H_4N_2$ |
| Sucrose | $C_{12}H_{22}O_{11}$ |

## T

| | |
|---|---|
| Tellurophene chromium tricarbonyl | $C_7H_4CrO_3Te$ |
| Terephthaloyl chloride | $C_8H_4Cl_2O_2$ |
| *p*-Terphenyl | $C_{18}H_{14}$ |
| Terephthalodinitrile | $C_8H_4N_2$ |
| 3,3',4,4'-Tetraaminodiphenyl ether | $C_{12}H_{12}N_4O$ |
| 1,4,8,11-Tetraazacyclotetradecane | $C_{10}H_{24}N_4$ |
| Tetrabromomethane | $CBr_4$ |
| 1,2,4,5-Tetrachlorobenzene | $C_6H_2Cl_4$ |
| Tetrachlorobis-(butylammonium) manganese II | $C_8H_{24}Cl_4MnN_2$ |
| Tetrachlorobis-(decylammonium) manganese II | $C_{20}H_{48}Cl_4MnN_2$ |
| Tetrachlorobis-(deuteromethylammonium) manganese II | $C_2H_6Cl_4D_6MnN_2$ |
| Tetrachlorobis-(ethylammonium) manganese II | $C_4H_{16}Cl_4MnN_2$ |
| Tetrachlorobis-(methylammonium) manganese II | $C_2H_{12}Cl_4MnN_2$ |
| Tetrachlorobis-(pentylammonium) manganese II | $C_{10}H_{28}Cl_4MnN_2$ |
| Tetrachlorobis-(propylammonium) manganese II | $C_6H_{20}Cl_4MnN_2$ |
| 1,1,1,2-Tetrachlorodifluoroethane | $C_2Cl_4F_2$ |
| 1,1,2,2-Tetrachloroethane | $C_2H_2Cl_4$ |
| Tetrachloroethane | $C_2Cl_4$ |
| Tetrachloroethylene | $C_2Cl_4$ |
| Tetrachloromethane | $CCl_4$ |
| *n*-Tetracosane | $C_{24}H_{50}$ |
| Tetracyclo[3.2.0.0.$^{2,7}$.0$^{4,6}$]heptane | $C_7H_8$ |
| *n*-Tetradecane | $C_{14}H_{30}$ |
| 1-Tetradecanethiol | $C_{14}H_{30}S$ |
| *n*-Tetradecyl mercaptan | $C_{14}H_{30}S$ |
| Tetraethylammonium tetrabromoferrate | $C_8H_{20}Br_4FeN$ |
| Tetraethylammonium tetrachloroferrate | $C_8H_{20}Cl_4FeN$ |
| 1,1,3,3-Tetraethyl-5,5-dimethylcyclotrisiloxane | $C_{10}H_{26}O_3Si_3$ |
| 1,1,3,3-Tetraethyl-5,5-diphenylcylotrisiloxane | $C_{16}H_{22}O_3Si_3$ |
| Tetraethylene glycol | $C_8H_{18}O_5$ |
| Tetraethylenepentamine | $C_8H_23N_5$ |
| Tetraethylgermane | $C_8H_{20}Ge$ |
| Tetraethylgermanium | $C_8H_{20}Ge$ |
| Tetraethyllead | $C_8H_{20}Pb$ |
| Tetraethylmethane | $C_9H_{20}$ |
| Tetraethylsilicon | $C_8H_{20}Si$ |
| Tetraethyltin | $C_8H_{20}Sn$ |
| Tetrafluoromethane | $CF_4$ |
| 1,2,3,4-Tetrahydroanthracene | $C_{14}H_{14}$ |
| Tetrahydrofuran | $C_4H_8O$ |
| Tetrahydrofuran clathrate hydrate | $C_4H_8O{\cdot}17H_2O$ |
| Tetrahydro-1,4-isoxazine | $C_4H_9NO$ |
| *exo*-Tetrahydrodicyclopentadiene | $C_{10}H_{16}$ |
| 1,2,3,4-Tetrahydrophenanthrene | $C_{14}H_{14}$ |
| 1,2,3,4-Tetrahydroquinoline | $C_9H_{11}N$ |
| 5,6,7,8-Tetrahydroquinoline | $C_9H_{11}N$ |
| Tetramethylammonium hexacyanotrimethylenecyclopropanide | $C_{16}H_{12}N_7$ |
| Tetramethylammonium tetrachloroferrate | $C_8H_{24}Cl_4FeN_2$ |
| Tetramethylammonium tetrachloroferrate (III) | $C_4H_{12}Cl_4FeN$ |
| Tetramethylammonium tetrachloromanganate | $C_8H_{24}Cl_4MnN_2$ |
| Tetramethylammonium trichloromanganate(II) | $C_4H_{12}Cl_3MnN$ |
| 1,1,3,3-Tetramethyl-1,3-disilacyclobutane | $C_6H_{16}Si_2$ |
| 2,4,5,7-Tetramethyl-4,5-bis(4-*tert*-butylphenyl)octane | $C_{32}H_{50}$ |
| 1,1,10,10-Tetramethylcyclooctadecane | $C_{22}H_{44}$ |
| 1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane | $C_{16}H_{22}OSi_2$ |
| Tetramethyl germane | $C_4H_{12}Ge$ |
| 3,7,11,15-Tetramethyl-1-hexadecyn-3-ol | $C_{20}H_{40}O$ |
| 3,7,11,15-Tetramethyl-1-hexadecen-3-ol | $C_{20}H_{40}O$ |
| Tetramethylhex-3-ene | $C_{10}H_{20}$ |
| Tetramethyl lead | $C_4H_{12}Pb$ |
| 2,2,4,4-Tetramethyl-3-oxapentane | $C_8H_{18}O$ |
| 2,2,3,3-Tetramethylpentane | $C_9H_{20}$ |
| 2,2,4,4-Tetramethylpentane | $C_9H_{20}$ |
| N,N,N',N'-Tetramethyl-*p*-phenylenediamine perchlorate | $C_{10}H_{16}N_2ClO_4$ |
| Tetra(methylphenyl)tetrasiloxane | $C_{28}H_{32}Si_4O_4$ |
| Tetramethyl silicate | $C_4H_{12}O_4Si$ |
| Tetramethyl stannane | $C_4H_{12}Sn$ |
| Tetramethyl tin | $C_4H_{12}Sn$ |
| Tetramethylurea | $C_5H_{14}N_2O$ |
| 1,3,5,7-Tetranitro-1,3,5,7-tetrazocine($\alpha$) | $C_4H_8N_8O_8$ |
| 1,3,5,7-Tetranitro-1,3,5,7-tetrazocine($\beta$) | $C_4H_8N_8O_8$ |
| 1,3,5,7-Tetranitro-1,3,5,7-tetrazocine | $C_4H_8N_8O_8$ |
| Tetrapropylene glycol | $C_{12}H_{26}O_5$ |
| *n*-Tetratriacontane | $C_{34}H_{70}$ |
| Thallium acetate | $C_2H_3O_2Tl$ |
| Thallium butyrate | $C_4H_7O_2Tl$ |
| Thallium decanoate | $C_{10}H_{19}O_2Tl$ |
| Thallium dodecanoate | $C_{12}H_{23}O_2Tl$ |
| Thallium formate | $CHO_2Tl$ |
| Thallium heptanoate | $C_7H_{13}O_2Tl$ |
| Thallium hexadecanoate | $C_{16}H_{31}O_2Tl$ |
| Thallium hexanoate | $C_6H_{11}O_2Tl$ |
| Thallium nonanoate | $C_9H_{17}O_2Tl$ |
| Thallium octadecanoate | $C_{18}H_{35}O_2Tl$ |
| Thallium octanoate | $C_8H_{15}O_2Tl$ |
| Thallium pentanoate | $C_5H_9O_2Tl$ |
| Thallium propionate | $C_3H_5O_2Tl$ |
| Thallium tetradecanoate | $C_{14}H_{27}O_2Tl$ |
| Thioacetamide | $C_2H_5NS$ |
| Thiobenzamide | $C_7H_7NS$ |
| Thiocarbohydrazide | $CH_6N_4S$ |
| Thiophene chromium tricarbonyl | $C_7H_4CrO_3S$ |
| Thiophene | $C_4H_4S$ |
| Thiosemicarbazide | $CH_5N_3S$ |
| Thiourea | $CH_4N_2S$ |
| Thiourea nitrate | $CH_4N_2S{\cdot}HNO_3$ |
| Thymine | $C_5H_6N_2O_2$ |
| $\alpha$-Tocopherol | $C_{31}H_{52}O_3$ |

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|---|---|
| Toluene | $C_7H_8$ |
| *p*-Toluidine | $C_7H_9N$ |
| 1,2,4-Triazole | $C_2H_3N_3$ |
| Triacetin | $C_9H_{14}O_6$ |
| *n*-Triacontane | $C_{30}H_{62}$ |
| Triazine triol | $C_3H_3N_3O_3$ |
| 2,4,6-Tribromoaniline | $C_6H_3Br_3N$ |
| Tribromomethane | $CHBr_3$ |
| 2,4,6-Tribromophenol | $C_6H_3Br_3O$ |
| Tri-*tert*-butyl methanol | $C_{13}H_{28}O$ |
| Tri-*n*-butylphosphate | $C_{12}H_{27}O_4P$ |
| Tributyrin | $C_{15}H_{26}O_6$ |
| Trichloroacetic acid | $C_2HCl_3O_2$ |
| 1,2,4-Trichlorobenzene | $C_6H_3Cl_3$ |
| 1,1,1-Trichloroethane | $C_2H_3Cl_3$ |
| 1,1,2-Trichloroethane | $C_3H_3Cl_3$ |
| Trichloroethene | $C_2HCl_3$ |
| Trichloroethylene | $C_2HCl_3$ |
| Trichlorofluoroethene | $C_2ClF_3$ |
| Trichlorofluoroethylene | $C_2ClF_3$ |
| Trichloromethane | $CHCl_3$ |
| Trichloromethylsilane | $CH_3Cl_3Si$ |
| *p*-Trichlorosilylbiphenyl | $C_{12}H_9Cl_3Si$ |
| β-Trichlorosilylpropionitrile | $C_3H_4Cl_3Si$ |
| α,α,α-Trichlorotoluene | $C_7H_5Cl_3$ |
| 1,1,1-Trichlorotrifluoroethane | $C_2Cl_3F_3$ |
| 1,1,2-Trichlorotrifluoroethane | $C_2Cl_3F_3$ |
| Tricosane | $C_{23}H_{48}$ |
| *n*-Tricosane | $C_{23}H_{48}$ |
| Tricresyl phosphate | $C_{21}H_{21}O_4P$ |
| Tricyclopentadienyl yttrium | $C_{15}H_{15}Y$ |
| Tricyclo[2.2.1.0$^{2,6}$]heptane | $C_7H_{10}$ |
| Tricyclo[3.3.2.0$^{4,6}$]deca-2,7,9-triene | $C_{10}H_{10}$ |
| Tridecanolactone | $C_{13}H_{24}O_2$ |
| Triethanolamine | $C_6H_{15}NO_3$ |
| Triethanolamine borate | $C_6H_{12}BNO_3$ |
| Triethyl aluminum | $C_6H_{15}Al$ |
| Triethyl arsine | $C_6H_{15}As$ |
| Triethyl boron | $C_6H_{15}B$ |
| Triethylene glycol | $C_6H_{14}O_4$ |
| Triethylenetetramine | $C_6H_{18}N_4$ |
| Triethyl gallium | $C_6H_{15}Ga$ |
| Trifluoroacetyl fluoride | $C_2F_4O$ |
| α-(Trifluoromethoxy)-α,α-difluoromethyl acetate | $C_4H_3F_5O_3$ |
| 3-Trifluoromethylbenzoic acid | $C_7H_5F_3O_2$ |
| Trifluoromethyl (2-hydroxy-1-propenyl) ketone | $C_5H_5F_3O_2$ |
| 3-Trifluoromethyl nitrobenzene | $C_7H_4F_3NO_2$ |
| *m*-Trifluorotoluic acid | $C_7H_5F_3O_2$ |
| Triglycine fluoroberyllate-$d_x$ | $C_6D_{17}BeF_4N_3O_6$ |
| Triglycine fluoroberyllate, deuterated | $C_6D_{17}BeF_4N_3O_6$ |
| Triglycine fluoroberyllate | $C_6H_{17}BeF_4N_3O_6$ |
| Triglycine sulfate, deuterated | $C_6D_{17}N_3O_{10}S$ |
| Triglycine sulfate-triglycine selenate | $C_6H_{17}N_3O_{10}S{\cdot}C_6H_{17}N_3O_{10}Se$ |
| Triglycine sulfate | $C_6H_{17}N_3O_{10}S$ |
| 1,1,1-Trihydroxymethyl propane | $C_4H_{10}O_3$ |
| 1,2,3-Trihydroxypropane | $C_3H_8O_3$ |
| Trimargarin | $C_{54}H_{104}O_6$ |
| Trimethylaluminum | $C_3H_9Al$ |
| Trimethyl arsine | $C_3H_9As$ |
| 2,5,6-Trimethyl-2-cyclohexen-1-one | $C_9H_{14}O$ |
| 4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one | $C_{13}H_{20}O$ |
| 3,7,11-Trimethyl-1-dodecen-3-ol | $C_{15}H_{28}O$ |
| Trimethyl gallium | $C_3H_9Ga$ |
| Trimethylhydroquinone | $C_9H_{12}O_2$ |
| 6,10,14-Trimethyl-2-pentadecanone | $C_{18}H_{36}O$ |
| 6,10,14-Trimethyl-3,5-pentadecadien-2-one | $C_{18}H_{32}O$ |
| 2,2,4-Trimethylpentane | $C_8H_{18}$ |
| 2,5,6-Trimethylphenol | $C_9H_{12}O$ |
| *cis*-Tri(methylphenyl)trisiloxane | $C_{21}H_{24}Si_3O_3$ |
| *trans*-Tri(methylphenyl)trisiloxane | $C_{21}H_{24}Si_3O_3$ |
| N-(β-Trimethylsilylethyl) ethylenimine | $C_7H_{17}NSi$ |
| N-(β-Trimethylsilylethyl)azetidine | $C_8H_{19}NSi$ |
| 1,3,6-Trimethyluracil | $C_7H_{10}N_2O_2$ |
| 1,1,3-Trimethylurea | $C_4H_{10}N_2O$ |
| 2,4,6-Trinitrophenol | $C_6H_3N_3O_7$ |
| 2,4,6-Trinitroresorcinol | $C_6H_3N_3O_8$ |
| 1,3,5-Trioxane | $C_3H_6O_3$ |
| 2,5,8-Trioxanonane | $C_6H_{14}O_3$ |
| 1,3,5-Triphenylbenzene | $C_{24}H_{18}$ |
| Triphenylchlorosilane | $C_{18}H_{15}ClSi$ |
| Triphenylene picric acid | $C_{24}H_{15}N_3O_7$ |
| Triphenyl phenylethynyl tin | $C_{26}H_{20}Sn$ |
| Triphenyl phosphate | $C_{18}H_{15}O_4P$ |
| Triphenylphosphine | $C_{18}H_{15}P$ |
| Triphenylphosphine oxide | $C_{18}H_{15}OP$ |
| 2,4,6-Triphenylpyridine | $C_{23}H_{17}N$ |
| Triphenyl-s-triazine | $C_{21}H_{15}N_3$ |
| Triphenyl vinyl tin | $C_{20}H_{18}Sn$ |
| Tripropionin | $C_{12}H_{20}O_6$ |
| Tripropylaluminum | $C_9H_{21}Al$ |
| Tripropylene glycol | $C_9H_{20}O_4$ |
| Triptycene | $C_{20}H_{14}$ |
| Trisarcosine calcium chloride | $C_9H_{21}N_3O_6CaCl_2$ |
| Tris-(cyclopentadienylcobalt) disulfide | $C_{15}H_{15}Co_3S_2$ |
| Tris(2-picolylamine)iron chloride ethanolate | $C_{20}H_{33}Cl_2FeN_6O$ |
| Tristearin | $C_{57}H_{110}O_6$ |
| *anti,trans*-Truxane | $C_{18}H_{16}$ |
| *syn,trans*-Truxane | $C_{18}H_{16}$ |

## U

| | |
|---|---|
| 6-Undecanone | $C_{11}H_{22}O$ |
| Undecylcyanobiphenyl | $C_{24}H_{31}N$ |
| Urea | $CH_4N_2O$ |
| Urethane | $C_3H_7NO_2$ |

## V

| | |
|---|---|
| Valeral | $C_5H_{10}O$ |
| Valeraldehyde | $C_5H_{10}O$ |
| δ-Valerolactone | $C_5H_8O_2$ |
| Valeronitrile | $C_5H_9N$ |
| Vanadocene | $C_{10}H_{10}V$ |
| Vinyl chloride | $C_2H_3Cl$ |
| Vinyldimethylbenzylsilane | $C_{11}H_{16}Si$ |
| Vinyldimethylphenylsilane | $C_{10}H_{14}Si$ |
| Vinyltrimethylsilane | $C_5H_{12}Si$ |

## W

| | |
|---|---|
| Wurster's Blue perchlorate | $C_{10}H_{16}N_2ClO_4$ |

## X

| | |
|---|---|
| *p*-Xylene | $C_8H_{10}$ |
| Xylose(D) | $C_5H_{10}O_5$ |

## Z

| | |
|---|---|
| Zinc acetate | $C_4H_6O_4Zn$ |
| Zinc acetate dihydrate | $C_4H_6O_4Zn{\cdot}2H_2O$ |
| Zinc acetylacetonate | $C_{10}H_{14}ZnO_4$ |
| Zirconium acetylacetonate | $C_{20}H_{28}ZrO_6$ |

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# 10. Appendix: Errata for "Heat Capacities and Entropies of Organic Compounds in the Condensed Phase"

[J. Phys. & Chem. Ref. Data 13, Suppl. No.1, 286 pp. (1984)]

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The errata are arranged in the format shown below and are listed as found according to successive pages in the 1984 publication, J. Phys. Chem. Ref. Data **13**, Suppl. 1 (1984). After the page number for a specific erratum, which is shown on the extreme left side of the first line, information is provided regarding its location on a given page, such as: compound formula, compound name, reference squib, or other pertinent information. On the second line, the erratum appears as found in the publication. On the third line, one finds the correction. The last line offers a comment or explanation about the erratum.

| Errata Format | |
|---|---|
| Page | Formula/Name/Reference/Text |
| Incorrect | (as it appears) |
| Correct | (as it should be) |
| [comment regarding error] | |

Specific Errata

| | | |
|---|---|---|
| 6 | **5. Definitions**, 3rd paragraph, lines 3 and 4 | |
| Incorrect | ...and is referred to the midpoint of ... | |
| | ...$C_p = \Delta H/(T_2 - T_1)$, $(T_2 - T_1)/2$. | |
| Correct | ...and is referred to *as* the midpoint of ... | |
| | ...$C_p = \Delta H/(T_2 - T_1)$, $(T_1 + T_2)/2$. | |
| [missing word and formula error] | | |

| | | | |
|---|---|---|---|
| 10 | C | Graphite | 80TAY/GRO |
| Incorrect | Wiswesser Line Notation | ... | |
| Correct | Wiswesser Line Notation | C | |
| [WLN absent] | | | |

| | | | |
|---|---|---|---|
| 11 | $CCl_3F$ | Fluorotrichloromethane | 40BEN/MCH |
| Incorrect | Wiswesser Line Notation | GYGGF | |
| Correct | Wiswesser Line Notation | GXGGF | |
| [WLN error] | | | |

| | | | |
|---|---|---|---|
| 14 | $CHCl_2F$ | Dichlorofluoromethane | 40BEN/MCH |
| | $C_p$ = 112.6 J·mol$^{-1}$·K$^{-1}$ | | |
| [$C_p$ value in J·mol$^{-1}$·K$^{-1}$ repeated] | | | |

| | | | |
|---|---|---|---|
| 24 | $C_2Br_2F_4$ | 1,2-Dibromotetrafluoroethane | 82KOS/ZHO |
| Incorrect WLN | FXFFEXFFE | | |
| Correct WLN | FXFEXFFE | | |
| [WLN error] | | | |

| | | | |
|---|---|---|---|
| 32 | $(C_2H_3NO)_n$ | Polyglycine I | 81FIN/KUM |
| Incorrect molecular weight | 75.0670 | | |
| Correct molecular weight | 57.0518 | | |
| [numerical error] | | | |

| | | | |
|---|---|---|---|
| 32 | $(C_2H_3NO)_n$ | Polyglycine II | 81FIN/KUM |
| Incorrect molecular weight | 75.0670 | | |
| Correct molecular weight | 57.0518 | | |
| [numerical error] | | | |

| | | | |
|---|---|---|---|
| 33 | $C_2H_4Br_2$ | 1,2-Dibromoethane | 40PIT 2 |
| Incorrect | Phase Changes...c/I/liq... | | |
| Correct | Phase Changes...c,I/liq... | | |
| [typographical error] | | | |

| | | | |
|---|---|---|---|
| 42 | $C_2H_{12}CdCl_4N_2$ | Tetrachlorobis-(methylammonium) cadmium II | 81RAH/CLA |
| Incorrect WLN | CD ZI&2 G4 | | |
| Correct WLN | ZH&1 2 -CD- G4 | | |
| [WLN error] | | | |

| | | | |
|---|---|---|---|
| 42 | $C_2H_{12}Cl_4MnN_2$ | Tetrachloro-(methylammonium) manganese II | 82WHI/GRA |
| Incorrect WLN | MN Z1&2 G4 | | |
| Correct WLN | ZH&1 2 -MN- G4 | | |
| [WLN error] | | | |

| | | | |
|---|---|---|---|
| 43 | $C_{2.2}H_{6.5}N_2O$ | Urea-1-dodecene adduct | 72GAN/PAR |
| Incorrect WLN | 11U1 &ZVZ | | |
| Incorrect molecular weight | 77.8975 | | |
| Correct WLN | ZVZ &11U1 0.1060 | | |
| Correct molecular weight | 76.9884 | | |
| Mole ratio of 1-dodecene to urea = 0.1060 | | | |
| [WLN and molecular weight error] | | | |

| | | | |
|---|---|---|---|
| 43 | $C_{2.2}H_{6.6}N_2O$ | Urea-*n*-undecane adduct | 69COP/PAR |
| Incorrect WLN | ZVZ &11H | | |
| Incorrect molecular weight | 77.2496 | | |
| Correct WLN | ZVZ &11H 0.1104 | | |
| Correct molecular weight | 77.0892 | | |
| Mole ratio of *n*-undecane to urea = 0.1104 | | | |
| [WLN and molecular weight error] | | | |

| | | | |
|---|---|---|---|
| 43 | $C_{2.3}H_{6.7}N_2O$ | Urea-1-hexadecene adduct | 69COP/PAR |
| Incorrect WLN | 15U1 &ZVZ | | |
| Incorrect molecular weight | 79.3563 | | |
| Correct WLN | ZVZ &15U1 0.0860 | | |
| Correct molecular weight | 78.3911 | | |
| Mole ratio of 1-hexadecene to urea = 0.0860 | | | |
| [WLN and molecular weight error] | | | |

44 $C_{2.3}H_{6.7}N_2O$ Urea-1-decene adduct 69COP/PAR
Incorrect WLN ZVZ &9U1
Incorrect molecular weight 79.2721
Correct WLN ZVZ &9U1 0.1370
Correct molecular weight 78.3911
Mole ratio of 1-decene to urea = 0.1370
[WLN and molecular weight error]

44 $C_{2.4}H_{6.8}N_2O$ Urea-1-octadecene adduct 72GAN/PAR
Incorrect WLN 17U1 &ZVZ
Incorrect molecular weight 79.8893
Correct WLN ZVZ &17U1 0.0785
Correct molecular weight 79.6930
Mole ratio of 1-octadecene to urea = 0.0785
[WLN and molecular weight error]

44 $C_{2.4}H_{6.8}N_2O$ Urea-1-eicosene adduct 69COP/PAR
Incorrect WLN 19U1 &ZVZ
Incorrect molecular weight 79.6929
Correct WLN ZVZ &19U1 0.0704
Correct molecular weight 79.6930
Mole ratio of 1-eicosene to urea = 0.0704
[WLN and molecular weight error]

44 **$C_{2.4}H_{6.9}N_2O$** (c) 72GAN/PAR
Urea-1-tetradecene adduct; 1-Tetradecene-urea adduct
**Heat Capacity** 298.15 K $C_p$ = 30.9 cal·mol$^{-1}$·K$^{-1}$
129.2 J·mol$^{-1}$·K$^{-1}$
Temperature range 12–300 K. Values for one mole urea in adduct.
**Entropy** 298.15 K, $S$ = 34.7 cal·mol$^{-1}$·K$^{-1}$
145.1 J·mol−1·K$^{-1}$
Does not include possible zero-point entropy.
**Phase Changes**
Anomalous region 225–235 K,
with $\Delta H$ = 15 J·mol$^{-1}$ (urea) and $\Delta S$ = 0.067 J·mol$^{-1}$·K$^{-1}$.
c,II/c,I 256.6 K $\Delta H$ = 868.5 cal·mol$^{-1}$
3634 J·mol$^{-1}$
$\Delta S$ = 2.9 cal·mol$^{-1}$·K$^{-1}$
12.0 J·mol$^{-1}$·K$^{-1}$
**Molecular Weight** 80.0660
**Wiswesser Line Notation** ZVZ &13U1 0.1019
**Evaluation** B
[Data in 72GAN/PAR omitted from tables]

45 $C_3H_2N_2$ Malononitrile 68WES/WUL
Incorrect Reference 68WES/WUL
Correct Reference 68GIR/WES
[Incorrect reference citation; see also erratum for page 278]

52 $C_3H_6O$ 3-Propenol; Allyl alcohol 81REI
Incorrect 3-Propen-1-ol
Incorrect WLN Q1U2
Correct 2-Propen-1-ol
Correct WLN Q2U1

[nomenclature and WLN error]

54 $C_3H_7NO$ N,N-Dimethylmethanamide 66GEL
Incorrect 66GEL
Correct 61GEL
[reference error; see also erratum on page 277]

55 $C_3H_7NO_2$ 2-Aminopropanoic acid (L) 75DAU/DEL
Incorrect WLN ZYVQ -L
Correct WLN ZY1&VQ -L
[WLN error]

66 $C_4H_6KNaO_6.4H_2O$ Sodium potassium tartrate tetrahydrate 78TAT/MAT
Incorrect $C_4H_6KNaO_6{\cdot}4H_2O$
Incorrect Molecular Weight 284.2367
Correct $C_4H_4KNaO_6{\cdot}4H_2O$
Correct Molecular Weight 282.2209
[formula and molecular weight error]

68 $C_4H_7NO_4$ Aminosuccinic acid (L); Aspartic acid (L) 63HUT/COL 2
Incorrect WLN ZVYZ1VQ -L
Correct WLN QVYZ1VQ -L
[typographical error]

71 $C_4H_8O$ Butanal; n-Butryaldehyde 56PAR/KEN
Incorrect n-Butryaldehyde
Correct *n*-Butyraldehyde
[spelling error]

76 $C_4H_{10}$ Butane 40AST/MES
Incorrect $C_p$ = 13242 J·mol$^{-1}$·K$^{-1}$
Correct $C_p$ = 132.42 J·mol$^{-1}$·K$^{-1}$
[decimal point omitted]

83 $C_4H_{12}Pb$ Tetramethyllead 59GOO/SCO
Incorrect phase (c)
Correct phase (liq)
[$T_m$ = 242.9 K, hence, at 298.15 K, data for $C_p$ and $S$ for $C_4H_{12}Pb$ are for the liquid]
Incorrect entropy temperature 298.16 K
Correct entropy temperature 298.15 K
[transcription errors]

87 $C_5H_7N_2O_2$ Thymine 73ALV/BIL
Incorrect formula $C_5H_7N_2O_2$
Incorrect molecular weight 127.1225
Correct formula $C_5H_6N_2O_2$
Correct molecular weight 126.1146
[formula and molecular weight error]

87 $CH_7N_2O_2$ Thymine 78KIL2
Incorrect formula $C_5H_7N_2O_2$
Incorrect molecular weight 127.1225
Correct formula $C_5H_6N_2O_2$
Correct molecular weight 126.1146
[formula and molecular weight error]

91 $C_5H_8O_2$ Ethenyl ethanoate; Allyl acetate 81REI
Incorrect Ethenyl ethanoate
Correct 2-Propenyl ethanoate
[nomenclature error]

91 $(C_5H_8O_2)_n$ Polymethylmethacrylate 58SOC/TRA
Incorrect WLN /*X1&*VO1/
Correct WLN /*X1*1&VO1/
[WLN error]

93 $C_5H_{10}$ 1-Pentene 30PAR/HUF 2
Incorrect 1-Pentene
Incorrect WLN 4U1
Correct 2-Pentene
Correct WLN 3U2
[30PAR/HUF 2 measured 2-Pentene, liquid]

101 $C_5H_{12}O$ 2,2-Dimethyl-1-propanol; tert-Amyl alcohol 33PAR/HUF
Incorrect 2,2-Dimethyl-1-propanol; tert-Amyl alcohol
Incorrect WLN Q1X1&1&1
Correct 2-Methyl-2-butanol; *tert*-Amyl alcohol
Correct WLN QX1&1&2
[nomenclature and WLN errors]

| | | | |
|---|---|---|---|
| 103 | $C_5H_{12}S$ | 2-Methyl-2-butanethiol; tert-Amyl mercaptan | 74MES/FIN |
| Incorrect | 2-Methyl-2-butanethiol; tert-Amyl mercaptan..... | | |
| Correct | 3-Methyl-2-butanethiol | | |

[nomenclature error; 74MES/FIN measured six mercaptans among which were both 3-methyl-1-butanethiol and 3-methyl-2-butanethiol]

| | | | |
|---|---|---|---|
| 104 | $C_5H_{14}N_2$ | | 82DZH/KAR2 |
| | N,N-Dimethyl-1,3-propanediamine | | |
| Incorrect | Molecular weight | 130.1924 | |
| Incorrect | WLN | Z3NI&1 | |
| Correct | Molecular weight | 102.1790 | |
| Correct | WLN | Z3N1&1 | |

[Molecular weight and WLN errors]

| | | | |
|---|---|---|---|
| 108 | $C_6H_3N_3O_6$ | 1,3,5-Trinitrobenzene | 80RAD/RAD |
| Incorrect | Molecular weight | 181.4487 | |
| Correct | Molecular weight | 213.1064 | |

[Molecular weight error]

| | | | |
|---|---|---|---|
| 108 | $C_6H_3N_3O_7$ | 2,4,6-Trinitrophenol; Picric acid | 24TAY/RIN |
| Incorrect | $C_p$ = 57.3 cal·mol$^{-1}$K$^{-1}$ 223.9 J·mol$^{-1}$·K$^{-1}$ | | |
| Correct | $C_p$ = 57.3 cal·mol$^{-1}$·K$^{-1}$ 239.7 J·mol$^{-1}$·K$^{-1}$ | | |

[numerical error]

| | | | |
|---|---|---|---|
| 110 | $C_6H_4O_3$ | Phthalic anhydride | 36PAR/TOD |
| Incorrect | $C_6H_4O_3$ | | |
| Incorrect | Molecular Weight | 124.0958 | |
| Correct | $C_8H_4O_3$ | | |
| Correct | Molecular Weight | 148.1178 | |

| | | | |
|---|---|---|---|
| 110 | $C_6H_5Br$ | Bromobenzene | 81REI |
| Incorrect | WLN | BR | |
| Correct | WLN | ER | |

[WLN error]

| | | | |
|---|---|---|---|
| 116 | $C_6H_6N_2O_2$ | 3-Nitroaniline | 26AND/LYN |
| Incorrect (c/liq) temperature | | 285.0 K | |
| Correct (c/liq) temperature | | 385.0 K | |

[temperature error]

| | | | |
|---|---|---|---|
| 129 | $C_6H_{12}S$ | Cyclohexanethiol; Cyclohexyl mercaptan | 67MES/TOD |
| Incorrect | $C_p$ = 6.04 cal·mol$^{-1}$·K$^{-1}$ | | |
| Correct | $C_p$ = 46.04 cal·mol$^{-1}$ ·K$^{-1}$ | | |

[numerical error]

| | | | |
|---|---|---|---|
| 130 | $C_6H_{13}N_3O_8S$ | Triglycine sulfate | 68AGU/TEL |
| Incorrect formula | | $C_6H_{13}N_3O_8S$ | |
| Incorrect Mol. Wt. | | 287.2440 | |
| Incorrect WLN | | Z1VM1VM1VQ &WSQQ | |
| Correct formula | | $C_6H_{17}N_3O_{10}S$ | |
| Correct Mol. Wt. | | 323.2804 | |
| Correct WLN | | Z1VQ 3 &WSQQ | |

[error in formula, molecular weight, and WLN]

| | | | |
|---|---|---|---|
| 131 | $C_6H_{13}N_3O_8S$ | Triglycine sulfate | 80RAM/CER |
| Incorrect | $C_p$ = | 90.6 cal·mol$^{-1}$·K$^{-1}$ 379.1 J·mol$^{-1}$·K$^{-1}$ | |
| Incorrect | formula | $C_6H_{13}N_3O_8S$ | |
| Incorrect | Mol. Wt. | 287.2440 | |
| Incorrect | WLN | Z1VM1VM1VQ &WSQQ | |
| Correct | $C_p$ = | 102.0 cal·mol$^{-1}$K$^{-1}$ 426.7 J·mol$^{-1}$K$^{-1}$ | |
| Correct | formula | $C_6H_{17}N_3O_{10}S$ | |
| Correct | Mol. Wt. | 323.2804 | |
| Correct | WLN | Z1VQ 3 &WSQQ | |

[error in $C_p$, formula, molecular weight, and WLN]

| | | | |
|---|---|---|---|
| 136 | $C_6H_{15}In$ | Triethylindium | 73MAS/NOV |

[Data entry appears twice]

| | | | |
|---|---|---|---|
| 136 | $C_6H_{16}CdCl_4N_2$ | Tetrachlorobis-(2-propeneammonium) cadmium II | 82WHI/STA |
| Incorrect | WLN | CD Z2U1&2 G4 | |
| Correct | WLN | Z2U1 2 -CD- G4 | |

[WLN error]

| | | | |
|---|---|---|---|
| 137 | $C_6H_{20}CdCl_4N_2$ | Tetrachlorobis-(*n*-propylammonium) cadmium II | 81WHI/GRA |
| Incorrect WLN | | CD Z3&2 G4 | |
| Correct WLN | | Z3H 2 -CD- G4 | |

[WLN error]

| | | | |
|---|---|---|---|
| 137 | $C_6H_{20}Cl_4MnN_2$ | Tetrachlorobis-(*n*-propylammonium) manganese II | 81WHI/GRA |
| Incorrect WLN | | MN Z3&2 G4 | |
| Correct WLN | | Z3H 2 -MN- G4 | |

[WLN error]

| | | | |
|---|---|---|---|
| 141 | $C_7H_6O_2$ | Benzoic acid | 53GIN/FUR |
| Incorrect temperature range | | 14-570 K | |
| Correct temperature range | | 14-410 K | |

[numerical error]

| | | | |
|---|---|---|---|
| 157 | $C_8F_{16}$ | Perfluorodimethylcyclohexane | 57YAR/KAY |
| Incorrect WLN | | L6TJ AXFFF AF BF CF DF EF FF XXFFF XF | |
| Correct WLN | | L6TJ AXFFF AF BF CF DF EF FF XXFFF XF XF XF XF | |

[WLN error]

| | | | |
|---|---|---|---|
| 158 | $C_8H_8$ | Styrene | 50KUR |
| Incorrect | $C_p$ = 23.56 J·mol$^{-1}$·K$^{-1}$ | | |
| Correct | $C_p$ =235.6 J·mol$^{-1}$·K$^{-1}$ | | |

[numerical error]

| | | | |
|---|---|---|---|
| 165 | $C_8H_{12}$ | Cycloocta-1,5-diene | 75LEB/TSV |

[75LEB/TSV absent from bibliography; see erratum for page 282]

173 $C_8H_{18}O$ 2-Methyl-1-heptanol 31CLI/AND
Incorrect WLN QY5&1
Correct WLN Q1Y5&1
[WLN error]

179 $C_9H_{14}O_2$ Glyceryl triacetate 79FUC
Incorrect $C_9H_{14}O_2$
Incorrect Molecular Weight 154.2084
Correct $C_9H_{14}O_6$
Correct Molecular Weight 218.2060
[formula and molecular weight error]

191 $C_{10}H_{20}$ Diethylcyclohexane 63GUD/CAM
Incorrect $C_p$ = 62.2 cal·mol$^{-1}$·K$^{-1}$
Incorrect temperature range 313-424 K
Correct $C_p$ = 62.6 cal·mol$^{-1}$·K$^{-1}$
Correct temperature range 313-423 K
[numerical errors]

197 $C_{11}H_{26}N_2O$ Urea-*n*-decane adduct 65PEM/PAR
Incorrect spelling Value of aduct with...
Incorrect formula $C_{11}H_{26}N_2O$
Incorrect molecular weight 202.3392
Incorrect WLN ZVZ &10H
Correct spelling Value of adduct with...
Correct formula $C_{2.1}H_{6.5}N_2O$
Correct molecular weight 75.7876
Correct WLN ZVZ 10H 0.1149
Mole ratio of *n*-decane to urea = 0.1149
[spelling, formula, molecular weight, and WLN errors]

199 $C_{12}H_9N$ (c) Carbazole 80RAD/RAD
Heat Capacity 298.15 K $C_p$ = 45.6 cal·mol$^{-1}$·K$^{-1}$
190.8 J·mol$^{-1}$·K$^{-1}$

Temperature range 180-410 *K*
$C_p = 54.87 + 0.2328T + 7.477 \times 10^{-4}T^2$
Phase Changes
c/liq 521.1 K $\Delta H$ = 6501 cal·mol$^{-1}$·K$^{-1}$
27200 J·mol$^{-1}$·K$^{-1}$
Molecular Weight 167.2098
Wiswesser Line Notation T B656 HMJ
Evaluation B
[Carbazole is in the name-formula index and bibliography, but not in the table of data for $C_p$, $S$, and phase changes. Data for carbazole should appear after data for $C_{12}H_9Cl_3Si$, *p*-Trichlorosilylbiphenyl]

203 $C_{12}H_20$ Tetracyclo[6.2.1.1$^{3,6}$]dodecane 62GOL/BEL
Incorrect Tetracyclo[6.2.1.1$^{3,6}$]dodecane
Incorrect WLN L D595 A D-TJ
Correct Tricyclo[6.2.1.1$^{3,6}$]dodecane
Correct WLN L59 D5 A D-TJ
[nomenclature error, also in 62GOL/BEL]

204 $C_{12}H_{22}O_2$ Dimethoxydecalin 63GUD/CAM
Incorrect $C_{12}H_{22}O_2$ Dimethoxydecalin
Incorrect Molecular Weight 198.3046
Incorrect WLN L66TJ XO1 XO1
Correct $C_{12}H_{18}$ Dimethanodecalin
Correct Molecular Weight 162.2742
Correct WLN L D5 C555 A D-TJ
[errors in formula, name, molecular weight, and WLN]

209 $C_{13}H_{30}N_2O$ Urea-*n*-dodecane adduct 65PEM/PAR
Incorrect spelling Value of aduct with...
Incorrect formula $C_{13}H_{30}N_2O$
Incorrect molecular weight 230.3928
Incorrect WLN ZVZ &12H
Correct spelling Value of adduct with...
Correct formula $C_{2.2}H_{6.3}N_2O$
Correct mol. wt. 76.7871
Correct WLN ZVZ &12H 0.09714
Mole ratio of *n*-dodecane to urea = 0.09714
[spelling, formula, molecular weight, and WLN errors]

209 $C_{13}H_{30}N_2O$ Urea-*n*-dodecane adduct 65PEM/PAR
Incorrect spelling Value of aduct with...
Incorrect formula $C_{13}H_{30}N_2O$
Incorrect mol. wt. 230.3928
Incorrect WLN ZVZ &12H
Correct spelling Value of adduct with
Correct formula $C_{2.2}H_{6.3}N_2O$
Correct mol. wt. 76.7871
Correct WLN ZVZ &12H 0.09714
Mole ratio of *n*-dodecane to urea = 0.09714
[spelling, formula, molecular weight, and WLN errors]

211 $C_{14}H_{10}O_2$ Benzil; Diphenyl diketone 77DWO/FUC
Incorrect .....data given graphicallyonly.
Correct .....data given graphically only.
[space missing]

224 $C_{17}H_{38}N_2O$ Urea-*n*-hexadecane adduct 65PEM/PAR
Incorrect formula $C_{17}H_{38}N_2O$
Incorrect mol. wt. 286.5000
Incorrect WLN ZVZ &16H
Correct formula $C_{2.3}H_{6.7}N_2O$
Correct mol. wt. 78.3914
Correct WLN ZVZ &16H 0.08057
Mole ratio on *n*-hexadecane to urea = 0.08057
[formula, molecular weight, and WLN errors]

224 $C_{18}H_{12}$ Naphthacene 80WON/WES
[80WON/WES not in bibliography; see erratum for page 285]

229-230 $C_{19}H_{21}ClNO$ *p-n*-Hexyloxybenzylideneamino-*p'*-chlorobenzene 77TSU/SOR
Incorrect WLN GR DNU1UR DO6
Correct WLN GR DNUYR DO6
[WLN error]

231 $C_{20}H_{12}$ Perylene 80WON/WES
[80WON/WES not in bibliography; see erratum for page 285]

232 $C_{20}H_{40}Br_2N_2$ 1,2-Bis(triallylammonium)ethane bromide 74BUR/VER
[data entry out of place; should follow data entry for $C_{20}H_{38}HgO_4$ Mercuric decanoate 78ADE]

234 $C_{21}H_{46}N_2O$ Urea-*n*-eicosane adduct 65PEM/PAR
Incorrect spelling Value for aduct with...
Incorrect formula $C_{21}H_{46}N_2O$
Incorrect mol. wt. 342.6072
Incorrect WLN ZVZ 20H
Correct spelling Value for adduct with...
Correct formula $C_{2.3}H_{6.8}N_2O$
Correct mol. wt. 78.4922
Correct WLN ZVZ &20H 0.06712
Mole ratio of *n*-eicosane to urea = 0.06712
[spelling, formula, molecular weight, and WLN errors]

236 $C_{24}H_{12}$ Coronene 80WON/WES
[80WON/WES not in bibliography; see erratum for page 285]

245 $C_{38}H_{72}O_4$ Di-*n*-tetradecyl sebacate 76PHI/MAT
Incorrect $C_{38}H_{72}O_4$
Incorrect Molecular Weight 592.9844
Correct $C_{38}H_{74}O_4$
Correct Molecular Weight 595.0002
[formula and molecular weight error]

245 $C_{41}H_{72}O_2$ Cholestryl myristate 67BAR/POR
Incorrect ...temperature range 270-270 K
Correct ...temperature range 270-370 K
[numerical error]

246 $C_{43}H_{26}N_8P$ Methyltriphenylphosphonium-bis(7,7,8,8-tetracyanoquinodomethanide) 77KOS/SOR 2
Incorrect Methyldiphenylphosphonium-bis(7,7,8,8-tetracyanoquinodomethanide)
Correct Methyldiphenylphosphonium-bis(7,7,8,8-tetracyanoquinodimethanide)
[nomenclature error]

250 **8. Compound Name - Formula Index**
Incorrect n-Butryaldehyde...
Correct *n*-Butyraldehyde...
[spelling error]

253 **8. Compound Name - Formula Index**
Incorrect Dimethoxydecalin ..... $C_{12}H_{22}O_2$
Correct Dimethanodecalin ..... $C_{12}H_{18}$
[error in name and formula]

253 **8. Compound Name - Formula Index**
Incorrect 2,2-Dimethyl-1-propanol ..... $C_5H_{12}O$
Correct .....
[delete entry]

254 **8. Compound Name - Formula Index**
Incorrect Ethenyl ethanoate ..... $C_5H_8O_2$
Correct 2-Propenyl ethanoate ..... $C_5H_8O_2$
[nomenclature error, relocate corrected name alphabetically]

254 **8. Compound Name - Formula Index**
Incorrect Freon 12 ..... $CHClF_2$
Correct Freon 12 ..... $CCl_2F_2$
[formula error]

255 **8. Compound Name - Formula Index**
Incorrect Glyceryl triacetate ..... $C_9H_{14}O_2$
Correct Glyceryl triacetate ..... $C_9H_{14}O_6$
[formula error]

257 **8. Compound Name - Formula Index**
Incorrect .....
Correct 2-Methyl-2-butanethiol ..... $C_5H_{12}S$
[name and formula omitted]

257 **8. Compound Name - Formula Index**
Incorrect 3-Metgylcyclohexanone
Correct 3-Methylcyclohexanone
[nomenclature error]

258 **8. Compound Name - Formula Index**
Incorrect Methyltriphenylphosphonium bis(7,7,8,8-tetracyanoquinodomethanide...
Correct Methyltriphenylphosphonium bis(7,7,8,8-tetracyanoquinodimethanide)...
[nomenclature error]

259 **8. Compound Name - Formula Index**
Incorrect Phthalic anhydride ..... $C_6H_4O_3$
Correct Phthalic anhydride ..... $C_8H_4O_3$
[formula error]

260 **8. Compound Name - Formula Index**
Incorrect 3-Propen-1-ol
Correct 2-Propen-1-ol
[numerical error]

260 **8. Compound Name - Formula Index**
Incorrect Sodium potassium tartrate tetrahydrate... ...$C_4H_6KNaO_6.4H_2O$
Correct Sodium potassium tartrate tetrahydrate... ...$C_4H_4KNaO_6.4H_2O$
[numerical error]

261 **8. Compound Name - Formula Index**
Incorrect Tetracyclo[6,2,1,$1^{3,6}$]dodecane...
Correct Tricyclo[6.2.1.$1^{3,6}$]dodecane...
[nomenclature error, relocate corrected name alphabetically]

262 **8. Compound Name - Formula Index**
Incorrect $C_6H_{13}N_3O_8S$ Triglycine sulfate
Correct $C_6H_{17}N_3O_{10}S$ Triglycine sulfate
[formula error]

262 **9. Compound Name - Formula Index**
Incorrect formula Urea-*n*-decane adduct $C_{11}H_{26}N_2O$
Incorrect formula Urea-*n*-dodecane adduct $C_{13}H_{30}N_2O$
Incorrect formula Urea-*n*-eicosnae adduct $C_{21}H_{46}N_2O$
Incorrect formula Urea-*n*-hexadecane adduct $C_7H_{38}N_2O$
Correct formula Urea-*n*-decane adduct $C_{2.1}H_{6.5}N_2O$
Correct formula Urea-*n*-dodecane adduct $C_{2.2}H_{6.3}N_2O$
Correct formula Urea-*n*-eicosane adduct $C_{2.3}H_{6.8}N_2O$
Correct formula Urea-*n*-hexadecane adduct $C_{2.3}H_{6.7}N_2O$
[formula error]

262 **8. Compound Name - Formula Index**
Incorrect name .....
Correct name Urea-1-tetradecene adduct $C_{2.4}H_{6.9}N_2O$
[compound name omitted from index]

265 **9. Bibliography**
Incorrect 31BLA/LET
Correct 31BLA/LEI
[tyopgrphical error]

265 **9. Bibliography**
Incorrect 31FIO/GIN ...881-800 (1931).
Correct 31FIO/GIN ...881-900 (1931).
[typographical error]

267 **9. Bibliography**
Incorrect 40AST/MES ...1917-1933 (1940).
Correct 40AST/MES ...1917-1923 (1940).
[numerical error]

267 **9. Bibliography**
Incorrect 40MES/AST ...J. Am. Chem. Soc. **62**, 887-890 (1940).
Correct 40MES/AST ...J. Am. Chem. Soc. **62**, 886-890 (1940).
[numerical error]

270 **9. Bibliography**
Incorrect 51SUG ...Bull. Chem. Soc. Japan **34**, 426-433 (1961).
Correct 61SUG ...Bull. Chem. Soc. Japan **34**, 426-433 (1961).
[numerical error]

271 **9. Bibliography**
Incorrect 52SCO/FIN ...functions, **74**, 2478-2483 (1952).
Correct 52SCO/FIN ...functions, J. Am. Chem. Soc. **74**, 2478-2483 (1952).
[journal citation absent]

271 **9. Bibliography**
Incorrect 53RAT/GWI ...5629 (1953).
Correct 53RAT/GWI ...5629-5633 (1953).
[numerical error]

271 **9. Bibliography**
Incorrect 54MCC/FIN 2 ...J. Am. Chem. Soc. **78**,...
Correct 54MCC/FIN 2 ...J. Am. Chem. Soc. **76**,...
[numerical error]

272 **9. Bibliography**
Incorrect 56FIN/SCO...1,3,5-cyclo-oD heptatriene...
Correct 56FIN/SCO...1,3,5-cycloheptatriene...
[spelling error]

273 **9. Bibliography**
59SCO/DOU Scott, D.W., Douslin, D.R., etc.
[reference entered twice]

274 **9. Bibliography**
Incorrect 59WES ...in simmetrical molecules...
Correct 59WES ...in symmetrical molecules...
[spelling error]

275 **9. Bibliography**
Incorrect 62SCO/GOO...J. Chem. Phys. **26**, 406-412 (1962).
J. Chem. Phys. **36**, 406-412 (1962).
Correct 62SCO/GOO...J. Chem. Phys. **36**, 406-412 (1962).
[double citation of journal with errors]

275 **9. Bibliography**
Incorrect 62SCO/MES...4-Fluortoluene:...
...J. Chem. Physa. ...
Correct 62SCO/MES...4-Fluorotoluene:...
...J. Chem. Phys. ....
[typographical errors]

275 **9. Bibliography**
Incorrect 63HUT/COL...L-laucine...
Correct 63HUT/COL...L-leucine...
[typopgraphical error]

277 **9. Bibliography**
Incorrect 66GEL Geller, B.E., Some physicochemical properties of dimethylformamide,
Zhur. Fiz. Khim. **40**, 1956-1958 (1966).
Correct 61GEL Geller, B.E., Some physococochemical properties of dimethylformamide,
Zhur. Fiz. Khim. *35*, 2210-2216 (1961).
[reference error]

277 **9. Bibliography**
Incorrect 66ZAL/STR...Zalikin, and A.A., Strepikheev, Yu.A.,...
Correct 66ZAL/STR...Zalikin, A.A., and Strepikheev, Yu.A.,...
[typographical error]

278 **9. Bibliography**
Incorrect 68GEE/MEL...Makroknol. Chem. ...
Correct 68GEE/MEL...Makromol. Chem. ...
[typographical error]

278 **9. Bibliography**
Incorrect 68WES/WUL Westrum, E.F., Jr., and Wulff, C.A.,...
Correct 68GIR/WES Girdhar, H.L., Westrum, E.F., Jr., and Wulff, C.A.,...
[author citation error]

278 **9. Bibliography**
Incorrect 69HUT/COL...bovine chymotripsinogen...
Correct 69HUT/COL...bovine chymotrypsinogen...
[typographical error]

279 **9. Bibliography**
Incorrect 70TAK/WFS Takahashi, Y., and Westrum, E.F., Jr.,...
Correct 70TAK/WES Takahashi, Y., and Westrum, E.F., Jr.,...
[typorgaphical error]

280 **9. Bibliography**
Incorrect 73AND/MAR...Part II. ...
Correct 73AND/MAR...Part 11. ...
[eleven, not Roman II]

281 **9. Bibliography**
Incorrect 73KUS/SUU...and Wadso, Thermochemistry of ...
Correct 73KUS/SUU...and Wadso, I., Thermochemistry of...
[first name initial omitted]

282 **9. Bibliography**
Incorrect [reference missing]
Correct 75LEB/TSV Lebedev, B.V., Tsvetkova, L. Ya., Kirparisova, E.G., and Lebedev, N.K., Thermodynamic properties of cycloocta-1,5-diene, Zhur. Fiz. Khim. **49**, 2152 (1975).
[reference omitted]

284 **9. Bibliography**
Incorrect 79LEB/LIT...264–265 (1979).
Correct 79LEB/LIT...364–365 (1979).
[numerical error]

284 **9. Bibliography**
Incorrect 79PUC/PEA Fuchs, R., and Peabody, L.A.,...
Correct 79FUC/PEA Fuchs, R., and Peabody, L.A.,...
[typographical error]

285 **9. Bibliography**
Incorrect [reference missing]
Correct 80WON/WES Wong, W.K., and Westrum, E.F., Jr., Thermodynamics of polynuclear aromatic molecules. II. Low temperature thermal properties of perylene, coronene, and naphthacene, Mol. Cryst. Liq. Cryst. **61**, 207-228 (1980).
[reference omitted]

285 **9. Bibliography**
Incorrect 81LEB/YEV 2 ...Kiparisova, Y.E.,...
Correct 81LEB/YEV 2 ...Kiparisova, Y.G.,...
[spelling error]

286 **9. Bibliography**
Incorrect 81TOM/CUR ...1,1'-dibenzolferrocene...
Correct 81TOM/CUR ...1,1'-dibenzoylferrocene...
[spelling error]

286 **9. Bibliography**
Incorrect 82MOR/MAT ...cryo-refigerator...
Correct 82MOR/MAT ...cryo-refrigerator...
[spelling error]

286 **9. Bibliography**
Incorrect 82SCH/MIL 2 ...II. Molar heat of seven...
Correct 82SCH/MIL 2 ...II. Molar heat capacities of seven...
[word omitted]

286 **9. Bibliography**
82WIL/ING
[out of place alphabetically].