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Heat Capacity of Liquids: Critical Review and Recommended Values. Supplement I

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A study was carried out in which new experimental data on heat capacities of pure liquid organic and some inorganic compounds were compiled, critically evaluated, and recommended values provided. Compounds included in the compilation have a melting point below 573 K. The bulk of the compiled data covers data published in the primary literature between 1993 and 1999 and some data of 2000. However, some data from older sources were also included. The data were taken from almost 1030 literature references. Parameters of correlating equations for temperature dependence of heat capacities of liquids were developed. This paper is an update of a two volume monograph entitled *Heat Capacity of Liquids: Critical Review and Recommended Values* (96ZAB/RUZ) that was published in 1996 in the Journal of Physical and Chemical Reference Data as Monograph No. 6 and was the product of the IUPAC Project No. 121/11/87. © *2002 by the U.S. Secretary of Commerce on behalf of the United States. All rights reserved.*

Key words: bibliography; correlating equations; critically evaluated data; heat capacity; liquids.

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In the tabular part of the paper, a review of all primary sources of data, and results of correlation are summarized for each compound separately in one to four tables. Each table is coded with three numbers. More information is given in Sec. 4.2. The tabular information starts on page 104.

1. Introduction

Heat capacities belong among the basic thermophysical and thermodynamic properties which characterize a liquid. They are directly linked with temperature derivatives of basic thermodynamic functions and are therefore indispensable for the calculation of differences in these functions between different temperatures. This information is widely used in chemical engineering for establishing energy balances, in thermodynamics for obtaining entropy and enthalpy values, and in thermochemistry for calculating changes in reaction enthalpies with temperature. A knowledge of heat capacities

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is also required for evaluating the effect of temperature on phase and reaction equilibria. Variations in heat capacities serve as a sensitive indicator of phase transitions and are an important tool for understanding changes in the structure of liquid solutions.

Since 1993 when compilation of data published in Monograph No. 6 (96ZAB/RUZ) was ended a considerable amount of new data appeared in literature. In addition, some data published before 1993 that were omitted from Monograph No. 6 were found. First the new data entail heat capacities for about 350 compounds not included in Monograph No. 6. Second, new data that either extend the temperature range of recommended data for compounds already presented in Monograph No. 6 or improve the overall uncertainty of the recommended data by supplying new data that have a lower error of measurement were added for more than 320 compounds. Third, references to new data for about 50 compounds are presented in the form of a review of primary sources only as the data for such compounds do not extend or improve the previously developed recommended data.

The objectives of the present study were as follows:

(1) To provide an exhaustive survey of the literature for all isobaric and saturation heat capacities for pure organic and inorganic compounds in the liquid state which were published in the primary literature mainly between 1993 and 1999 and some data of 2000. The starting date, 1993, denotes the year when the compilation of data presented in Monograph No. 6 was ended.

(2) To compile newly published heat capacities supplemented by data omitted in the previous stage of a project that ended in 1993 and appeared in Monograph No. 6. To extend a computer readable database of raw experimental data established in the previous project. Only data for well-defined compounds in the isotropic liquid state, obtained by calorimetric measurements were considered. The criterion for inclusion of a compound in the compilation required the compound to have a melting point below 573 K. A large number of organic compounds exhibit signs of decomposition at temperatures above 573 K. This choice of limiting a compound to having a melting point below 573 K offers the assurance that almost all stable organic compounds are covered. In addition, it also excluded almost all metals and a large number of inorganic compounds [and has kept the focus of this work primarily on organic compounds].

(3) To critically evaluate heat capacity data and prepare sets of selected data.

(4) To correlate selected data and provide recommended values for the heat capacities of liquid compounds as a function of temperature. The recommended data are presented in terms of parameters of suitable correlating equations accompanied with an assessment of the data uncertainty.

An annotated bibliography is given in Sec. 4 of Monograph No. 6 (96ZAB/RUZ) which lists compilations containing reported values for the heat capacities of organic and some inorganic compounds from 1897 through 1991. Over the period from 1991 through 2000, only one large compilation by Palczewska-Tuliňska *et al.* (97PAL/WYR) was published which contains data on the heat capacity of organic compounds in the condensed phase. Palczewska-Tulinska *et al.* selected 610 sets of experimental data for 480 compounds which were obtained from 350 literature sources. From this selection, the authors usually chose one or two sets of experimental data which they considered the most reliable. Their compilation did not reveal any further critical assessment of the data.

In this paper we utilized some paragraphs from the textual part of Monograph No. 6 (96ZAB/RUZ) which are necessary for describing the compilation, critical assessment, and correlation of data as well as for understanding the tables. The text was updated where needed and/or new information was added.

1.1. Definitions, Basic Relationships

Heat capacity C is defined by the differential equation

$$C=(\partial Q/\partial T)_x, \tag{1}$$

where Q indicates the amount of heat exchanged between the system studied and the surroundings when the temperature T changes under conditions specified by x. These conditions have to be specified as the heat, Q, is not a state function or quantity, and C varies according to different paths along which Q is exchanged. The corresponding intensive quantities are related to the unit amount of mass—*specific* heat capacity c, or to one mole—*molar* heat capacity C_m. Sometimes, heat capacities are also denoted as *thermal coefficients*.

Several different temperature gradients of thermodynamic functions are encountered in the literature:

the *isochoric heat capacity* or *heat capacity at constant volume*

$$C_V=T(\partial S/\partial T)_V=(\partial U/\partial T)_V=-T(\partial^2 A/\partial T^2)_V \tag{2}$$

the *isobaric heat capacity* or *heat capacity at constant pressure*

$$C_p=T(\partial S/\partial T)_p=(\partial H/\partial T)_p=-T(\partial^2 G/\partial T^2)_p \tag{3}$$

the *saturation heat capacity*

$$C_{\mathrm{sat}}=T(\partial S/\partial T)_{\mathrm{sat}}. \tag{4}$$

The thermodynamic functions U, H, S, A, and G are internal energy, enthalpy, entropy, Helmholtz function, and Gibbs function, respectively. The subscript, sat, denotes derivatives along the *saturation (orthobaric) curve*. For simplification of the notation, we use throughout this paper the symbols C_p, C_V, and C_{sat}; they are also used for denoting molar heat capacities (omitting subscript m).

Using well known thermodynamic relationships, one can derive conversion equations between the individual heat ca-

pacities. Among them, the most important for the present study is the relationship between the isobaric and saturation heat capacity

$$C_p - C_{\mathrm{sat}} = T \frac{(\partial V/\partial T)_p}{(\partial p/\partial T)_{\mathrm{sat}}}. \tag{5}$$

For liquids, it is not necessary to make any clear distinction [between C_p at the saturation curve and C_{sat}] below about 0.9 T_{b}, where T_{b} is the normal boiling temperature, as the differences are less than the uncertainty obtainable in high precision measurements.

There are two principal methods for the determination of the heat capacities of liquids. The first method is an *indirect* approach and consists in the calculation from the other properties which are available experimentally. The second method consists of *direct* determination by a calorimetric measurement. In most calorimetric measurements, a sample under investigation is heated or cooled and the quantity measured is the amount of exchanged heat corresponding to a finite temperature change. The *true* heat capacity is, however, a differential quantity and the experimental value obtained as the ratio of heat and temperature increment cannot be automatically considered as C in Eq. (1). It is rather the *average* heat capacity, C_{avg}, defined as the amount of heat necessary to change the temperature of a system by 1 K. The average heat capacity is expressed by:

$$C_{\mathrm{avg}} = \frac{Q}{T_2 - T_1} \tag{6}$$

in an interval defined by the temperatures T_1 and T_2. This value is related to the average temperature, $T_{\mathrm{avg}} = (T_1 + T_2)/2$. The relationship between C and C_{avg} is obtained by introduction of the integrated Eq. (1) into Eq. (6):

$$C_{\mathrm{avg}} = \frac{1}{T_2 - T_1} \int_{T_1}^{T_2} C \, \mathrm{d}T. \tag{7}$$

The heat capacity of a liquid always changes with temperature and C and C_{avg} are identical at T_{avg} only when heat capacity is a linear function of temperature. The two quantities approach each other when the temperature interval over which the average heat capacity is determined converges and they are equal to each other in the limit:

$$C = \lim_{T_1 \to T_2} C_{\mathrm{avg}}. \tag{8}$$

We find that the heat capacity of most liquids changes moderately with temperature without a strong curvature (except in the region of high vapor pressures) and the true heat capacity agrees in most cases with the experimental value within the error of measurement provided the temperature interval is not too large (intervals up to 10 K are usually acceptable). Sometimes it is preferable to proceed with a wider temperature increment in order to reduce the time of experiments.

When the $C = C(T)$ function is nonlinear and the temperature steps are too large, it is possible to apply a *curvature correction*. Three methods have been described by McCullough and Scott (68MCC/SCO) and were briefly summarized in Zábranský *et al.* (96ZAB/RUZ).

2. Calorimetric Techniques for Determining Heat Capacities of Liquids

Calorimetry is the most frequently used method for determining heat capacities of compounds in the condensed state. Several publications describe heat capacity calorimeters and attempt to introduce some system of classification. A concise description of some selected publications was given in Zábranský *et al.* (96ZAB/RUZ). There are three recent publications dealing with calorimetry:

(1) Hemminger and Höhne presented in their first textbook (84HEM/HOH) an outline of fundamentals of calorimetry, an overview of calorimeters and a treatment of measured data. They also suggested and used in their book a classification of calorimeters.

(2) The textbook by Höhne *et al.* (96HOH/HEM) is devoted solely to a single technique, differential scanning calorimetry. Both textbooks (84HEM/HOH, 96HOH/HEM) deal with measurement of several quantities which include heat capacity.

(3) Marsh and O'Hare (94MAR/OHA) edited a book providing a comprehensive summary of the technique of solution calorimetry. A chapter in the book reviews experimental techniques for measurement of heat capacities of liquids with emphasis on modern techniques developed after 1950. Experimental techniques are divided into two main groups, static and dynamic, and a representative survey of calorimeters is presented.

2.1. Terminology and Criteria for Classification of Calorimeters

There is no officially established nomenclature for describing different types of calorimeters. An attempt was made by Rouquerol and Zielenkiewicz (86ROU/ZIE) to introduce a classification of calorimeters based on heat exchange considerations, paying special attention to the dynamic behavior of calorimeters. Another approach was suggested by Hemminger and Höhne (84HEM/HOH) based on three criteria: measuring principle, mode of operation, and construction principle.

A somewhat different terminology was proposed by Zábranský *et al.* (96ZAB/RUZ) and is used here for classifying calorimeters. Some basic ideas of this classification are described in this section.

Heat capacity calorimeters can be classified according to four criteria:

(1) *motion of the sample inside the instrument* (batch, flow, and drop calorimeters);
(2) *mode of measurement* (stationary or dynamic conditions);
(3) *temperature relationship between the calorimeter vessel and its surroundings—mode of heat transfer* (adiabatic, isoperibol, isothermal, and conduction calorimeters); and
(4) *number of calorimeter vessels* (single vessel and twin vessel calorimeters).

Table 1. Criteria codes used for classification of calorimeters

Motion of sample 1		Mode of measurement 2		Temperature relation of vessel to surroundings 3		Number of vessels 4	
batch	B	stationary	S	adiabatic	A	one vessel	O
flow	F	dynamic	D	isoperibol	I	two vessels	T
drop	D			isothermal	T		
				conduction	H		
				thermopile conduction	C		

Table 1 lists individual criteria with the codes used for characterizing calorimeters in Tables 2 and 3 and in tables with experimental values. It should be kept in mind that the codes serve as a concise categorization of instruments. The adopted system of classification does not pretend to be exhaustive.

Table 2. Types of calorimeters used for determining heat capacities of pure liquids

	Classification			
Type of calorimeter	1	2	3	4
Adiabatic batch calorimeters with intermittent heating	B	S	A	O
Adiabatic batch calorimeters with continuous heating	B	D	A	O
Isoperibol batch calorimeters	B	S	I	O/T
Isoperibol flow calorimeters	F	S	I	O/T
Isoperibol drop calorimeters	D	S	I	O
Adiabatic drop calorimeters	D	S	A	O
Isothermal drop (phase change) calorimeters	D	S	T	O
Thermopile conduction drop calorimeters	D	D	C	T
Measurement of heating and/or cooling curves	B	D	H	O
Differential heat conduction calorimeters (TA,DTA,DSC)	B	D	H	T
Differential thermopile conduction calorimeters	B	D	C	T
Special dynamic methods using pulse technique	B	D	H	O

Two types of calorimeters, ''adiabatic drop calorimeters'' and ''special dynamic methods using pulse technique'' are not listed in Table 3 as none of the authors cited in this work used them. Nevertheless, they were included in order to make the list of types of calorimeters complete.

TABLE 3. Survey of calorimeters for determining heat capacity of liquids referred to in this work

Reference	Temp. range	Meas. error	Note
Adiabatic batch calorimeters with intermittent heating			
20COH/MOE	room	medium	
24WIL/DAN	300–360 K	medium	
30SOU/AND	low	0.5%	
33SOU/BRI	low	high	
35AOY/KAN	low	medium	
38EUC/SCH	low	medium	
39AST/EID1	low	high	
39SAG/EVA	300–370 K	2.0%	high pressure, also for heat of vaporization
41YOS/GAR	low	0.2%	
43RUE/HUF	low	0.1%	
44BAI/TOD	80–340 K	1.0%	
45SCO/MEY	low	0.1%	
47HUF	low	0.1%	detailed description of improvements in calorimeter, 43RUE/HUF
47OSB/GIN	medium	0.1%	also for heat of vaporization
47SKU	room	0.3%	
49STA/GUP	low	medium	
50SAG/HOU	medium and high	1.0%	high pressure (up to 6.9 MPa)
51EUC/EIG	medium	medium	
53WES/HAT	250–550 K	0.15%	
54STR/ICK	low	0.3%	
55PAC/PIE	low	0.1%	also for heat of adsorption
55STA/TUP	283–373 K	1.0%	
56COO/BAL	room	high	also for heat of solution
56POP/KOL	60–300 K	0.5%	
58HIL/KRA	low	0.3%	
58JAR/FRI	226–360 K	medium	high pressure (up to 6 MPa)
58WES/GIN	303–773 K	0.1%	
59ONK	293–373 K	high	
61GOO	low	high	high pressure
61ROU	283–323 K	medium	
62KOL/SER	12–340 K	0.5%	
63AND/COU1	low	high	
64ARN1	293–453 K	0.3%	
64GRE/WHI	low	medium	
65STE/BLA	10–360 K	0.1%	
65SUG/SEK	15–310 K	0.3%	
66DWO/GUI	low	2.0%	
66KLE	293–343 K	high	
66NIK/LEB	60–300 K	0.3%	
66SHI/ATA	low	high	
67RAS/GAN	298–473 K	0.5%	
68BAG/KUC	2–300 K	1.0%	measurement error: 4% at 2.6 K, 2% at 4 K, 1% at higher temperatures
68CLE/MEL	80–320 K	high	
68LEA	298–773 K	high	measurement error 0.1% and 0.2% below and above 673 K, respectively
68REC1	room	medium	
68WES/FUR	low	high	
68WES/WES	300–800 K	high	
69PAU/LAV2	low	high	
71GOP/GAM	303–343 K	1.0%	
72VAN	123–373 K	high	
74ATA/CHI	2–300 K	high	
74DIA/REN	medium	0.3%	
74MOS/MOU	273–346 K	low	
75VYU/ZVE	medium	high	
76DWO/FIG	low	medium	
76LEB/LIT	5–340 K	0.3%	measurement error: 3–5% below 20 K, 0.5%–1% between 20 and 60 K, 0.15%–0.3% above 60 K
76MOU/WEI	12–300 K	1.0%	
77KU/COM	low	1.0%	
77NAZ/MUS	293–620 K	1.5%	high pressure (up to 50 MPa)
77VOR/PRI	room	high	

TABLE 3. Survey of calorimeters for determining heat capacity of liquids referred to in this work—Continued

Reference	Temp. range	Meas. error	Note
78ZHU/ATR	medium	medium	commercial instrument made by VNIIFTRI (Khabarovsk)
79SCH/OFF	90–350 K	high	
79VES/ZAB	293–318 K	0.5%	
80GUR/GAV	5–300 K	0.2%	measurement error: 1.5% below 12 K, 0.5% between 12 and 30 K and 0.2% above 30 K
80KAL/JED	90–300 K	0.1%	
80SHA/LYU	15–330 K	0.5%	
80VAS/TRE	313–623 K	low	
82KAR/IGA	medium	0.5%	
82MOR/MAT	14–350 K	high	
83KUK/KOR	263–353 K	0.2%	
83TAN/ZHO	medium	high	
83YOS/SOR1	15–390 K	0.2%	
84OGA/KOB	13–300 K	high	microcalorimeter; measurement error: 1% at 20 K, 0.1% at 70 K and 0.3% above 70 K
84POD/RAC	medium	medium	
85BOU/DEL	medium and high	medium	
85RAB/SHE	low	0.3%	measurement error: 1.8% below 10 K, 0.8% between 10 and 25 K, 0.3% above 30 K
87VAN/VAN	10–350 K	0.2%	
87VAN/WHI	30–380 K	0.5%	
87YAM/OGU	12–370 K	0.3%	high pressure (up to 250 MPa)
87ZAB/HYN	290–373 K	0.5%	
88STE/ARC	low and medium	0.1%	modification of the calorimeter originally described by 43RUE/HUF and 47HUF
90MAY/RAC	low and medium	medium	
91KIS/PIN	5–300 K	medium	calorimeter with simultaneously measurement of electric polarization
91SVO/ZAB1	293–353 K	0.3%	also for heat of vaporization
93DIK/KAB	5–305 K	0.4%	commercial instrument TAU-1 made by VNIFTRI (Moscow); the error at helium temperature is 2% at decreased to 0.4% at 40 K
93FUJ/OGU1	2–400 K	0.2%	inaccuracy to be within 0.3% and 0.2% below and above 35 K, respectively
94TEL/SHE	7–300 K	0.3%	measurement error 3% below 20 K, 0.8% between 20 and 30 K and 0.3% at higher temperatures
95TAN/SUN	60–350 K	0.5%	
97VAR/DRU1	5–350 K	0.2%	instrument made by VNIIFTRI (Mendeleevo)
98VAN/VAN	5–400 K	0.2%	
Adiabatic batch calorimeters with continuous heating			
31DEE	low	medium	
51POP/GAL	300–1000 K	medium	
64VAS2	203–423 K	0.5%	
65FIN/GRU	room	0.4%	
71MUS	293–773 K	2.5%	high pressure (up to 50 MPa)
75RAS/GRI	medium and high	1.0%	high pressure
87OKH/RAZ	medium	0.3%	
Isoperibol batch calorimeters			
07BAT	low	low	
07MCI	low and medium	low	
09SCH	medium	low	
12SCH1	medium	low	
13CAM	medium	low	
18OSB/VAN	233–313 K	0.4%	aneroid calorimeter
19DEJ	medium	low	
20GIB/LAT	low and medium	low	
23SIM/LAN	low	medium	
24EUC/KAR	low	0.6%	
25DRU/WEI	room	low	
25PAR	low	0.5%	
26DAN/JEN	low	2.0%	
28EUC/HAU	low	low	
28GIA/WIE1	low	0.2%	
28LAT/GRE	low	medium	

TABLE 3. Survey of calorimeters for determining heat capacity of liquids referred to in this work—Continued

Reference	Temp. range	Meas. error	Note
29KEL1	low	medium	
29MIT/HAR1	low	medium	
30WIE/HUB	low	medium	
31BLA/LEI	medium and high	3.0%	
31FIO/GIN	medium and high	high	also for heat of vaporization
31FOR/BRU	medium and high	low	
32NEU	medium	medium	
33LEB/MOE	room	medium	
33POH/MEH	medium	low	
34KOL/UDO	room	low	
34LON/REY	300–560 K	low	
36AST/MES	low	medium	
36CLU/GOL	low	medium	
36PEA/BAK	low	medium	
37ELL	medium	medium	
37GIA/EGA	low	high	measurement error: 3% at 15 K, 1% at 20 K, 0.2% above 35 K
37VOL	room	low	
38HIC	low	0.3%	
39BYK	298–305 K	low	
39MAZ3	low and medium	low	
39RIE3	low	1.0%	
40BEN/MCH	medium	low	
48TSC1	room	low	also for heat of mixing
49TSC/RIC1	room	medium	also for heat of mixing
49WEI	room	low	
52STA/AMI	medium	low	also for heat of vaporization
55HUT/MAN	297–299 K	medium	
55RUI1	room	medium	also for heat of mixing
55TAY/JOH	low	0.3%	
57CRU/JOS	medium	2.0%	
57HAR/MOE	medium	0.5%	
57KEN	medium	1.0%	also for heat of mixing
58MUR/VAN	room	2.35%	
61EGA/LUF	room	medium	
62KAT	medium	medium	
64MOE/THO	293–313 K	low	
64RAS/BAS	medium	1.5%	
66DRA/LAN	room	medium	
67GRA	303–338 K	1.0%	
69TOM/LIN	room	low	
70LKB/COM	278–333 K	medium	
70REC	room	medium	
75PED/KAY	medium	1.0%	
76BON/CER	room	medium	
78RYB/EME	medium	low	
79CZA	room	low	high pressure (up to 1000 MPa)
80FUC	293–300 K	0.5%	
83MEY/MEY	medium	medium	
88ROD/MAR	room	medium	commercial instrument Tronac model 458
93NAN/BHA	medium	low	
99ZIJ/WIT	room	low	
Isoperibol flow calorimeters			
59HAN/HUG	273–495 K	medium	heat exchanger (cooling water); high pressure (up to 4 MPa)
59RIB/EGO	293–573 K	medium	high pressure (up to 25 MPa)
65KAU/BIT	293–350 K	1.0%	
71PIC/LED	room	medium	
75SAF/GER	medium and high	0.6%	high pressure (up to 50 MPa)
75SAN	293–573 K	0.6%	high pressure (up to 5 MPa)
83GOR/SIM	medium	medium	
85OGA/MUR	room	0.1%	
87LAN/CRI	high	medium	high pressure (up to 20 MPa)
88CON/GIA	medium	medium	constructed according to Picker instrument (71PIC/LED)

TABLE 3. Survey of calorimeters for determining heat capacity of liquids referred to in this work—Continued

Reference	Temp. range	Meas. error	Note
99BUR/ZOC	258–373 K	2.0%	multipurpose apparatus for excess enthalpy, heat capacity, density, kinematic viscosity and thermal conductivity
Isoperibol drop calorimeters			
*79BER	medium	low	
*81VON	medium	medium	
*86LUD	medium	low	
*86SCH	medium	medium	
*94BRU	293–370 K	low	
*98LOU	medium	medium	
01KAH	medium	low	
03CON/WHI	medium	low	
07WAL	room	low	pure solid metal dropped into liquid sample
08BOG/WIN	medium	low	
11LEW/RAN	293–663 K	low	
12LUS	medium	low	
18NAR	medium	low	
20MAA/HAT	90–298 K	2.0%	
22HER/SCH	room	low	
24GAR/RAN	medium	low	
26AND/LYN	low and medium	low	
33ROT/MEY2	273–628 K	medium	
36KUR/VOS	room	low	
45DAV/WIE	medium	low	
47KUR	medium	low	estimated measurement error about 5%
47PUS/FED	room	low	
56WAL/GRA	high	medium	
58SWI/ZIE1	medium	low	
64CAM/NAG	medium and high	medium	
71MAR/CIO	300–1300 K	low	
Isothermal drop (phase change) calorimeters			
16BRA	medium	0.4%	Bunsen ice calorimeter
50GIN/DOU	273–1173 K	0.35%	Bunsen ice calorimeter
Thermopile conduction drop calorimeters			
71KON/SUU	273–343 K	0.1%	
74SUU/WAD	273–343 K	high	
Measurement of heating and/or cooling curve			
*90PIC	medium	low	
31THO/PAR	293–773 K	low	
33FER/MIL	293–323 K	1.0%	
33STR/MAL	medium	low	
37STU	90–320 K	1.0%	
49WUY/JUN	medium	medium	
50KUS/CRO	medium	1.5%	dielectric constant measured simultaneously
58LUT/PAN	323–380 K	0.7%	
59ABA/MUS	room	low	
81ATA/ELS	room	low	
82CHE/GE	medium	3.0%	thermal conductivity and heat of fusion measured simultaneously
84FIL/LAU	medium	2.0%	
86NAZ/BAS1	303–523 K	2.0%	high pressure (up to 50 MPa)
Differential heat conduction calorimeters (TA,DTA,DSC)			
31SWI/RYB2	room	0.5%	
59BEN/THO	room	low	
63GUD/CAM	medium	low	
66PER/COM	340–510 K	1.0%	
69PER/COM	medium and high	low	commercial calorimeter DSC-2; measurement error 1% above 200 K
69YAG	200–670 K	2.5%	commercial instrument denoted as ADKTTM; triple-heat bridge method
71DU/COM	room	low	
73PER/COM	medium and high	low	
76MET/COM	medium and high	5.0%	
79DU/COM	medium and high	low	

TABLE 3. Survey of calorimeters for determining heat capacity of liquids referred to in this work—Continued

Reference	Temp. range	Meas. error	Note
81ARU	medium and high	1.5%	high pressure (up to 60 MPa)
84GUS/MIR	303–523 K	2.0%	high pressure
87PER/COM	medium and high	1.5%	commercial instrument Shimadzu model DSC-50
89KNI/ARC	high	1.0%	commercial instrument Perkin-Elmer DSC-2
89PRA/RAJ	318–333 K	3.0%	
90JIN/WUN	180–750 K	1.0%	commercial instrument TA 2100 system; error between 180–370 K is 3%
92BAO/CAC	medium and high	low	commercial instrument TA 4000 Mettler
92HWA/DES	medium and high	low	commercial instrument Perkin-Elmer DSC-4
92KAB/KOZ	340–520 K	1.5%	triple-heat bridge method
93CON/GIR1	298–498 K	low	commercial instrument TA 2000 Mettler; used high pressure crucibles with a teflon membrane
93GIM/AUD	233–373 K	low	commercial instrument Mettler DSC30
93NGE/ABH	high	low	commercial instrument Perkin-Elmer with Du Pont TADS
94CHE/FER	medium and high	3.0%	commercial instrument Perkin-Elmer DSC-2C
94NAK/TAK	medium and high	low	commercial instrument Rigaku DSC 8240B
95DIO/MAN	medium and high	low	commercial instrument Perkin-Elmer DSC-7
95MOR/IDR1	medium and high	1.0%	commercial instrument Seiko heat-flux DSC 220 system
96KAB/BLO	310–660 K	2.0%	commercial instrument Du Pont TA 2000, model 910
98MUT/WIL	273–373 K	low	commercial instrument TA Instrument Modulated DSC-2910
98SAL/FER	medium	medium	modulated scaning calorimeter
99CHI/LIU	medium	low	commercial instrument TA instrument DSC-2010 and TA controller
99MO/YAN	medium	low	commercial instrument Perkin-Elmer PYRIS I
Differential thermopile conduction calorimeters			
68WAD	medium	medium	commercial instrument LKB-8700; for heat of mixing
70PAZ/PAZ	medium	medium	modified commercial SETARAM microcalorimeter
74PET/TER	298–475 K	1.0%	
76CON/GIA	medium	medium	
78BYV/JAS	medium	2.0%	
82ZAR	medium	medium	
83ROU/ROU	278–368 K	high	modified commercial SETARAM microcalorimeter DSC
86MER/BEN	150–1100 K	medium	commercial instrument SETARAM DSC 111
89BRE/LIC	170–370 K	2.0%	commercial SETARAM microcalorimeter DSC 111G
91BAN/GAR	298–573 K	medium	commercial instrument SETARAM model C-80
92FIL/AFA	283–353 K	medium	
00BEC/AUF	77–473 K	0.3%	commercial SETARAM calorimeter (model BT2.15)

3. Methodology of Data Treatment; Establishment of Recommended Data

3.1. Data Base of Raw Values

The experimental values extracted from the literature together with auxiliary data were stored in the database of raw experimental values. The database is a merged entity containing both the data compiled in a previous project leading to Monograph No. 6 (96ZAB/RUZ) and the newly compiled data covers 1984 compounds and consists of 4244 data sets (set of experimental values from one calorimeter reported by an author for one compound in one original source). Only the parameters for smoothing equations are available for 310 data sets (no discrete data points were reported in these sources). The data sets of discrete values contain 34 583 raw data points. The auxiliary data comprise information on the quality of experimental values, sample purity, and its determination, the nature of the experimental procedure (calorimetric technique and type of resulting heat capacity), and units used in the original source. This information was used later as a guide in the selection of data sets for the final correlation. Most auxiliary data are summarized for individual compounds in tables of experimental heat capacities.

According to the information in the literature sources, we distinguished three types of heat capacities in the data base of raw values: *isobaric heat capacity* C_p, *saturation heat capacity* C_{sat}, and the *average heat capacity* C_{avg}. These three quantities are defined by Eqs. (3), (4), and (6), respectively.

Below the normal boiling temperature, T_b, the measured isobaric heat capacity usually relates to atmospheric pressure though this is not frequently specified in the original source. C_p has limited dependence on pressure at low and moderate vapor pressures, and its effect can be neglected unless the pressure change is large. Below the normal boiling temperature no distinction was made between the literature C_p data relating to the saturation line, to atmospheric conditions, or to 101.325 kPa; these were considered as identical. Above the normal boiling temperature, the saturation heat capacities C_{sat} rather than C_p data are reported in the original literature.

3.2. Evaluation and Selection Process

All available sources were critically assessed. The important part of the selection process was the simultaneous correlation of all experimental data which served to test the consistency and helped to reveal systematic errors. The correlation was performed by the weighted least-squares method; the *minimized objective function S* had the form:

$$S=\sum_{i=1}^{n}\frac{(C_{\mathrm{sm}}-C_{\mathrm{exp}})^2}{\sigma^2 C_i}, \tag{9}$$

where the summation is over all the values included in the correlation and the subscripts "exp" and "sm" relate to experimental and smoothed values, respectively. The reciprocal of the *variance*, $\sigma^2 C$, is the *weighting factor*. It was estimated for each value on the basis of the assumed experimental error of the data set used in the correlation. The input information was the percentage error of the experimental data, $\sigma_{\mathrm{r}}C$, as given by the author for the whole data set or estimated by the evaluator in cases where no information was available in the literature. Thus the variance of the *i*th data point was expressed as:

$$\sigma^2 C_i=\left(\frac{C_i\sigma_{\mathrm{r}}C_i}{100}\right)^2. \tag{10}$$

The following criteria were observed in the selection process:

(1) accuracy of the experimental technique claimed by the author,
(2) performance history of the laboratory,
(3) consistency of the data with the values from other sources (if available),
(4) purity of the compound,
(5) type of the calorimeter,
(6) time of data origin (year of publication), and
(7) scatter of the data.

Selection and correlation of data for each compound was carried out simultaneously and involved the following steps:

(a) All available heat capacity data sets along with the information on their accuracies were read in and a preliminary joint correlation was performed. If necessary, experimental data were converted to the same type of heat capacity—C_p or C_{sat}. Prior to the correlation, data sets considered *a priori* as unreliable were discarded if more accurate data were available for the same temperature range. However, deviations of the discarded data from the final values were always determined within the temperature range of the recommended values. For those sources where only parameters of a smoothing equation were available, pseudodiscrete data were generated in the temperature range of the parameters' validity. When the number of the experimental data points was not indicated in the original source, a temperature step of 5–10 K was used according to the length of the temperature interval and density of data points from other sources.

(b) In the next steps it was possible to make the following tentative changes: to discard individual values, to reject parts of or whole data sets that showed little consistency with the other data, to change weights of whole data sets by altering the expected percent error of measurement, to modify the number of generated pseudodiscrete data points, and to change the temperature limits within which the data sets are considered.

(c) The correlation was repeated several times until the final fit with the selected data was obtained where differences between experimental and smoothed values were roughly equal to or smaller than expected experimental errors. The final correlation of the selected experimental data was assigned a level of accuracy (I–VI, for the definition of levels of accuracy see the Sec. 4.2.3) according to the quality of the correlated data.

The main criterion for judging the quality of the correlation was the *standard weighted deviation*, s_{w}:

$$s_{\mathrm{w}}=\left(\frac{S_{\min}}{n-m}\right)^{1/2}, \tag{11}$$

where $S_{\min}$ is the value of the objective function at its minimum, n is the overall number of the fitted data points, and m is number of independent adjustable parameters in a correlation equation. When experimental data are consistent within the expected error limits, s_{w} should be close to unity. In addition, use of the following statistical criteria was made:
the *standard deviation*

$$s=\left(\frac{\Sigma_{i=1}^{n}(C_{\mathrm{sm}}-C_{\mathrm{exp}})_i^2}{n-m}\right)^{1/2}, \tag{12}$$

the *percentage standard deviation*

$$s_{\mathrm{r}}=\left(\frac{\Sigma_{i=1}^{n}[(C_{\mathrm{sm}}-C_{\mathrm{exp}})/C_{\mathrm{exp}}]_i^2}{n-m}\right)^{1/2}100, \tag{13}$$

the *bias*

$$s_{\mathrm{b}}=\frac{\Sigma_{i=1}^{n}(C_{\mathrm{sm}}-C_{\mathrm{exp}})_i}{n}, \tag{14}$$

and the difference between the number of experimental points with positive and negative deviation from the smoothed values (denoted in tables as $\pm$).

In order to get information on how data from individual sources compare with the final correlation, the deviations d_{w}, d, d_{r}, and d_{b} defined analogously to s_{w}, s, s_{r}, and s_{b} were calculated for both included and rejected data sets.

The definitions are as follows:
the *average weighted deviation*

$$d_{\mathrm{w}}=\left(\frac{\Sigma_{i=1}^{n_1}[(C_{\mathrm{sm}}-C_{\mathrm{exp}})^2/\sigma^2 C]_i}{n_1}\right)^{1/2}, \tag{15}$$

the *average deviation*

$$d=\left(\frac{\Sigma_{i=1}^{n_1}(C_{\mathrm{sm}}-C_{\mathrm{exp}})_i^2}{n_1}\right)^{1/2}, \tag{16}$$

the *average percentage deviation*

$$d_{\mathrm{r}}=\left(\frac{\Sigma_{i=1}^{n_1}[(C_{\mathrm{sm}}-C_{\mathrm{exp}})/C_{\mathrm{exp}}]_i^2}{n_1}\right)^{1/2}100, \tag{17}$$

the *bias* of a data set

$$d_{\mathrm{b}}=\frac{\Sigma_{i=1}^{n_1}(C_{\mathrm{sm}}-C_{\mathrm{exp}})_i}{n_1}, \tag{18}$$

where n_1 denotes the number of data points in one data set.

When heat capacity was measured at one temperature only and several literature sources were available, simple selection of the best value or averaging of several measurements was performed.

3.3. Temperature Correlation and Establishment of Recommended Values

Two different approaches were adopted for correlating heat capacities as a function of temperature. *Polynomials* or *cubic spline polynomials* were used for accurately fitting heat capacity inside the temperature limits of experimental values. A *quasipolynomial equation* was also used when it was appropriate (see below); this equation enabled one to describe the temperature dependence by one set of parameters which, unlike polynomial equations, allows a meaningful extrapolation above the upper temperature limit of the experimental data.

3.3.1. Representation of Data by Polynomial(s)

When data are available only in a limited temperature range, one polynomial of a third or lower degree may be sufficient for fitting the data successfully. In all cases, when such a condition was probable, the correlation with one polynomial was tried first. Its degree was gradually increased to 3, and the statistical F test was used to determine when the addition of higher terms was no longer significant.

Fitting with cubic splines was used only when the F test indicated need for a higher than third degree polynomial. We used the correlation algorithm developed at the Technical University of Budapest (79KOL) in which the two boundary conditions are considered during minimization as two additional adjustable parameters. Usually three and sometimes four knots were necessary for the satisfactory fit of the data within the expected experimental error limits. For exceptional cases, five knots had to be used for the description of data covering a wide temperature range; in situations where the data sets reached the vicinity of the critical point, the heat capacity increased dramatically.

The results of spline correlation are usually reported in terms of the knot values and two boundary conditions; the spline routine is then necessary for generating the recommended data. Since such a routine is not available to all users of the data, we preferred to tabulate the parameters of the cubic polynomials directly which are easier to use. This presentation is also consistent with the tabulation when only one polynomial is used to represent the entire temperature range. The tabulated adjustable parameters, A_j, relate to the equation expressing the dimensionless quantity $C/\mathbf{R}$ as a function of the scaled temperature $T/100$:

$$\frac{C}{\mathbf{R}}=\sum_{j=0}^{n} A_{j+1}\left(\frac{T}{100}\right)^j, \tag{19}$$

where $\mathbf{R}$ is the gas constant ($\mathbf{R}$=8.314 51 $\mathrm{J\cdot K^{-1}\cdot mol^{-1}}$, 88COH/TAY); scaling was made to improve the numerical stability of the fitting procedure. The upper limit of the summation m is equal to 3 in all cases where the overall temperature range is subdivided (cubic splines fitting) or can be lower when only one polynomial is used to describe the data.

3.3.2. Representation of Data by a Quasipolynomial Equation

The quasipolynomial equation was used in the form derived by Zábranský *et al.* (96ZAB/RUZ):

$$\frac{C}{\mathbf{R}}=A_1\ln(1-T_{\mathrm{r}})+\frac{A_2}{1-T_{\mathrm{r}}}+\sum_{j=0}^{m} A_{j+3}T_{\mathrm{r}}^j, \tag{20}$$

where $T_{\mathrm{r}}=T/T_{\mathrm{c}}$ and m equals 3 for about 50% of compounds. The derivation of a quasipolynomial equation was based on the assumption that the heat capacity is always an increasing function of temperature and is unbounded at the critical point. The quasipolynomial equation was not used when fewer then seven experimental data points were available and the temperature range of experimental data was below 50 K, or when there was no possibility of obtaining the critical temperature.

The variation of heat capacity in the high-temperature range differs considerably from one compound to another. It should be kept in mind that the quasipolynomial equation is mainly empirical and extrapolation above the upper temperature limit of experimental data is correct only in a qualitative manner. No guarantee can be given that the extrapolation will describe quantitatively the real heat capacity in this region except for the value at the critical point which is always correct and corresponds to plus infinity.

For organic compounds, the critical temperatures from the TRC tables (#00MAR) or from the data bank of the Institute of Chemical Technology, Prague (#00CDA) containing assessed values taken from the literature, were used; for compounds where T_{c} values were not found, estimates were performed according to Lydersen (55LYD). The compilation by Morachevskii and Sladkov (87MOR/SLA) was used as the main source of critical temperatures for inorganic compounds.

3.3.3. Types of Heat Capacities Presented

When establishing the recommended values no distinction was made between the saturation heat capacity C_{sat} and the isobaric heat capacity C_p when their difference was smaller than the expected error of experimental data over the whole temperature range of their validity. This was the case for practically all compounds where data did not reach above the normal boiling temperature. Then only one set of parameters for the entire temperature range was presented for each of the correlation equations.

For the compounds where experimental values of reasonable accuracy are available above the normal boiling temperature, distinct recommended data sets are presented for C_p and C_{sat}. In this case, all raw data were first converted to one type of heat capacity which was used in the evaluation and selection process. After the experimental values for the final correlation had been set, they were expressed as C_p and C_{sat} and both sets were correlated separately under identical conditions using the polynomial or cubic spline representation. Only isobaric heat capacity C_p was correlated by the quasipolynomial equation.

Recommended C_{sat} data relate by definition to the saturation line. Recommended C_p data relate above the normal boiling temperature to the saturation pressure. Below T_b, they represent both the heat capacity at standard pressure 101.325 kPa and the saturation pressure as their difference is smaller than the accuracy of the best literature data.

When necessary, conversion between C_p and C_{sat} was performed using Eq. (5). As there are not enough data on expansivities, the term $(\partial V/\partial T)_p$ was approximated by $(\partial V/\partial T)_{sat}$; the difference between them becomes important only far above the normal boiling temperature. The latter term was calculated from the temperature correlation of densities along the saturation line using a modified Rackett equation (85CAM/THO) or the Francis equation (86SMI/SRI). The derivative, $(dp/dT)_{sat}$, was calculated from one of the following vapor pressure equations: Wagner, Frost-Kalkwarf, Cox or Antoine using parameters from the references 79DYK/REP, 83MCG, 84DYK/REP, 90CHI/GAM, respectively.

4. Guide to Tables

4.1. Division of Compounds into Groups

To make the data presentation logical and easy to follow, the compounds are divided into *sections* according to the kinds of atoms they contain. These are further divided into *groups* according to their chemical structure. This arrangement makes it possible to illustrate specific features of individual families of compounds, and to show the connection between the magnitude of the quantities listed and the chemical structure of individual compounds. The adopted ordering system can be seen in the Table 4. Each group is assigned a designated double digit.

Table 4. Division of compounds into groups

Main group No.	Subgroup No.	Group name
0		**Inorganic Compounds**
	01	Elements
	02	Inorganic compounds
1		**Compounds of Carbon and Hydrogen**
	11	Saturated aliphatic hydrocarbons
	12	Saturated cyclic hydrocarbons
	13	Unsaturated aliphatic hydrocarbons
	14	Aromatic and unsaturated cyclic hydrocarbons
2		**Compounds of Carbon, Hydrogen and Halogen**
	21	Fluorine derivatives
	22	Chlorine derivatives
	23	Bromine derivatives
	24	Iodine derivatives
	25	Mixed halogen derivatives
3		**Compounds of Carbon, Hydrogen and Nitrogen**
	31	Amines
	32	Nitriles
	33	Heterocyclic nitrogen compounds
	34	Miscellaneous nitrogen compounds
4		**Compounds of Carbon, Hydrogen and Oxygen**
	41	Ethers
	42	Alcohols and phenols
	43	Carbonyl compounds
	44	Acids and anhydrides
	45	Esters
	46	Heterocyclic oxygen compounds
	47	Miscellaneous oxygen compounds
5		**Compounds of Carbon, Hydrogen and Sulfur**
	51	Sulfides
	52	Thiols
	53	Heterocyclic sulfur compounds
6		**Other Organic Compounds Containing Halogens, Nitrogen, Oxygen and Sulfur**
	61	Compounds of carbon, hydrogen, halogen and oxygen
	62	Compounds of carbon, hydrogen, nitrogen and oxygen
	63	Compounds of carbon, hydrogen, oxygen and sulfur
	64	Miscellaneous compounds
7		**Organic Compounds Containing Other Elements than Halogens, Nitrogen, Oxygen and Sulfur**
	71	Organosilicon compounds
	72	Organic compounds containing phosphorus and boron
	73	Organometallic compounds
	74	Salts of organic acids

The compounds of section 0 (elements and inorganic compounds) are ordered according to their formulas in alphabetical order. Organic compounds (sections 1–7) are ordered within each group according to the usual convention (Hill system), i.e., in order of increasing number of carbon and hydrogen atoms. Other elements are placed in alphabetical order. The compounds having the same molecular formula are arranged in alphabetical order according to their names. Two numbers separated by a dash, the so-called *group-member number*, code each compound. The first two-digit number indicates the group (family of compounds), and the second three-digit number denotes the serial number of a compound inside the group. In naming the compounds, we adopted the Chemical Abstracts rules for the names under

which the compound was presented with exception of simple esters where we used shorter names, e.g., methyl acetate instead of methyl ester acetic acid. Codes for individual compounds permitting their location inside the tables and the corresponding CAS registry numbers can be found in the formula index at the end of the paper.

New compounds not included in Monograph No. 6 were put in the appropriate group after the last compound covered by Monograph No. 6 and then listed according to the Hill system. This retains the numbering of all compounds from Monograph No. 6 and makes it possible to find a particular compound from the knowledge of its group-member number.

Several specific tags were appended to the group-member number to distinguish between compounds located in this work only, in the Monograph No. 6 only, and in both works. The specific tags are described in more detail in Sec. 7.

4.2. Tables and Deviation Plot

Most of information on the data and their processing is given for each compound in tables which are described in detail below. Methodology and procedure which led to this presentation of data are described in Sec. 3. The tables for each compound are preceded with name of the compound, its formula, code, and CAS registry number.

The characterization of raw data, their consistency, results of correlation and recommended data are summarized for each compound separately in one to four tables and a deviation plot.

Table type number 1—*Experimental heat capacities*

Reviews all primary sources and characterizes briefly experimental conditions and the quality of data. For those compounds where new experimental data published after 1993 do not improve the uncertainty of recommended data and/or do not extend the temperature range only this table is presented in this paper.

Table type number 2—*Correlated heat capacities*

The upper half of the table lists sources selected for establishing the recommended values. The statistical criteria defined by Eqs. (11)–(18) indicate for both selected and discarded sources, if they fall within the temperature interval of the correlation equation parameters, how the individual data sets compare with values generated from the correlation equation. The consistency of raw data is graphically demonstrated in the *deviation plot*. The table of correlated heat capacities is not present when the data are available at only one temperature or when there is only one literature source.

Table type number 3—*Parameters of polynomial(s)*

The table obtained by fitting the selected data lists parameters of polynomial(s) and also gives information on the quality of the overall fit and reliability of the recommended data.

Table type number 4—*Parameters of quasipolynomial equation*

This table is presented for compounds where correlation of data by Eq. (20) is meaningful.

Each table is coded with three numbers separated by periods. The first two numbers are identical with the compound code (see Sec. 4.1.) and the third relates to the type of table (1–4). Even when some tables are missing, the numbering related to the type of table is retained.

The symbol C without a subscript specification or the term heat capacity are used in tables whenever we refer both to C_p and C_{sat} at temperatures where the difference between their values is negligible compared with the expected experimental error.

Certain statistics and parameters are listed in the modified E notation. The first part of the number denotes the fractional part which is followed by the exponent to the base 10. The exponent is separated from the fractional part by a plus or a minus sign (e.g., -1.53–5 means -1.53×10^{-5}).

4.2.1. Experimental Heat Capacities

Each line of the table contains information on one literature source of experimental data. When several distinct data sets were given for the same compound in one publication (for example, parameters of smoothing equations relating to different temperature subintervals or the data obtained from two different calorimeters) there are several lines for one data source, each relating to one data set.

First column: the abbreviated reference in the form YYAAA/BBBM where YY is the last two digits of the year of publication (for a year before 1900 the reference code is preceded by an asterisk, *, for the year 2000 the reference code is preceded by a pound sign, #), AAA and BBB are the first three letters of the last name of the first and second author (if present), respectively. M is a digit from 1 to 9 distinguishing papers published by the same author(s) within the same year. If the same data set appeared in two or more different publications the reference to the earliest or more readily available source is given; an appropriate note is given below the table.

For some sources, a footnote is added below the table. In these cases, there is a capital N between the first and second column.

Second column: temperature range of the data set in kelvin.

Third column: number of experimental data points; symbol ''eqn'' is used in those cases where only parameters of a smoothing equation were presented in the original literature; symbol ''S'' denotes that the discrete values given in the original literature source were generated from a smoothing equation.

Fourth column: error of measurement, $\sigma_{\mathrm{r}}C_{\mathrm{exp}}$, in percent claimed by the author(s); abbreviation ''nosp'' is used when no specification is given in the original literature.

Fifth column: purity of the compound in percent (given with the same number of significant digits as in the original source) and analytical method used for its determination; the meaning of the abbreviations used is as follows: ''anal''—analytical (used when the analytical method was not specified), ''chrom''—gas or liquid chromatography, ''estim''—

the purity was estimated by the author(s), "melpt"—determination of impurities from the melting point depression.

Sixth column: type of heat capacity reported in the original literature; *p*—isobaric heat capacity, sat—saturation heat capacity, avg—average heat capacity determined over a temperature range usually greater than 10 K.

Seventh column: type of calorimetric method used for determining the data and reference to the publication where the instrument is described. The coding used for classification of experimental techniques is introduced in Table 1 and the individual types of calorimeters are summarized in Table 2. The criteria for classifying heat capacity calorimeters are discussed in Sec. 2.1. All references to calorimeters listed in tables of experimental heat capacities are summarized in Table 3.

4.2.2. Correlated Heat Capacities

This table contains information on the results of the correlation presented for the individual data sets. The statistics for the selected and rejected data sets are listed in the upper and lower half of the table, respectively. The meaning of the columns in the *upper part* of the table is as follows.

First column: the abbreviated reference (the same as in the table of experimental heat capacities).

Second column: temperature range (in kelvin) in which the data from a particular source were included in the correlation.

Third column: number of values used in the final determination of the correlation parameters.

The entries in the second and third columns are identical to those in the table of experimental heat capacities when the whole data set was included in the correlation; they differ if part of the data was discarded.

Fourth column: percentage error, $\sigma_r C$, used in Eq. (10) to estimate the variance of individual data points. This value is either $\sigma_r C_{exp}$ (column 4 in the table of experimental heat capacities) or is assigned by the evaluator in cases when no error is specified in the original source or the author's estimate does not seem to be realistic. When $\sigma_r C$ was assigned or modified by the evaluator, the value is followed by the sign #.

Fifth column: average weighted deviation d_w defined by Eq. (15).

Sixth column: average deviation d, defined by Eq. (16), divided by **R** (dimensionless).

Seventh column: average percentage deviation d_r defined by Eq. (17).

Eighth column: bias of the data set d_b, defined by Eq. (18), divided by **R** (dimensionless).

Ninth column: the difference between the number of experimental points with positive and negative deviation from the recommended values (denoted by $\pm$).

In the *lower part* of the table, the quantities $d/\mathbf{R}$, d_r, $d_b/\mathbf{R}$, and $\pm$ are presented in parenthesis for each reference rejected from the final correlation. Information is not given for rejected data sets when they fall outside of the selected temperature range.

In some cases, the correlations for isobaric and saturation heat capacities were performed separately. We give, however, only one table of correlated heat capacities for these compounds as the selection of data sources did not differ and statistical values were practically identical in both correlations.

4.2.3. Parameters of Polynomials

This table contains parameters for both isobaric and saturation heat capacities when these two quantities can be distinguished or it contains parameters referring to the type of heat capacity given in the table of Experimental Heat Capacities. The symbol C is used when referring to both C_p and C_{sat}.

The table gives characteristics of the final correlation of the selected data in the upper part and, the corresponding parameters of the polynomial(s) in the lower part.

The *upper part* consists of two lines when both isobaric and saturation heat capacities are tabulated and of only one line when no distinction is made between the two heat capacities. The following items are listed.

First column: type of heat capacity listed—*p* and sat denote isobaric and saturation heat capacities, respectively. The C is used when no distinction was made between the two types of heat capacities.

Second column: the total number of all experimental data points available.

Third column: the total number of experimental data points used in the correlation.

Fourth column: the standard weighted deviation s_w defined by Eqs. (9) and (11).

Fifth column: standard deviation s, defined by Eq. (12), divided by **R** (dimensionless).

Sixth column: standard percentage deviation s_r defined by Eq. (13).

Seventh column: bias s_b, defined by Eq. (14), divided by **R** (dimensionless).

Eighth column: the overall difference between the numbers of experimental points with positive and negative deviations from the recommended values (denoted by $\pm$).

The parameters of the cubic spline polynomials describing individual subintervals of the temperature range of the selected data are listed in the *lower part* of the table. When the isobaric and saturation heat capacities are distinguished, two sets of parameters are listed separately, the first set relating to the temperature correlation of C_p and the second to that of C_{sat}. When the whole temperature range of experimental data is described by only one equation the parameters were obtained by simple unconstrained fitting using a polynomial of third or lower degree. The meaning of the individual columns is as follows:

First column: temperature subinterval in kelvin to which the listed parameters relate.

Second to fifth columns: parameters of the polynomial defined by Eq. (19) valid in the given subinterval. Dimension of the parameters is T^j.

Sixth column: level of uncertainty assigned by the evaluators to the data generated from the polynomial in the given temperature subinterval. This characteristic expresses the expected overall uncertainty of the recommended data and reflects both the uncertainty in the experimental values and possible error due to the fitting procedure. The following levels of uncertainty were assigned:

I excellent data (uncertainty below 0.1%)
II highly reliable data (uncertainty below 0.3%)
III reliable data (uncertainty below 0.5%)
IV medium quality data (uncertainty below 1%)
V data of low reliability (uncertainty below 3%)
VI very unreliable data with a possibility of gross systematic errors (uncertainty above 3%).

The level of uncertainty assigned to individual subintervals for cubic splines often differs due to the unequal reliability of experimental data in different parts of the temperature range. On the other hand in certain cases one set of parameters was used for describing two (or exceptionally three) experimental data sets of different accuracy, which related to different temperature ranges. Then the level of uncertainty assigned to recommended data always relates to the data set of lower quality; in reality the recommended data are more reliable than indicated at temperatures where the experimental data set of higher quality was available. The reader can obtain information regarding changes of reliability within the temperature interval of recommended data from the table of Correlated Heat Capacities.

4.2.4. Parameters of the Quasipolynomial Equation

The quasipolynomial Eq. (20) is useful as a simple expression permitting extrapolations to higher temperatures. The quasipolynomial fit was performed only for isobaric heat capacity as the application of this quantity is wider compared to C_{sat}. In all other cases where C_p and C_{sat} heat capacities are identical within error of measurement parameters of the quasipolynomial equation are presented for a single type of the heat capacity presented in the table.

The table is organized analogously to the table presenting parameters of polynomials; the *upper part* of the table is identical. The items tabulated in the *lower part* have the following meaning.

First column: temperature interval in kelvin to which the listed parameters relate. This interval is not necessarily identical with the temperature range of the representation by polynomials.

Second column: critical temperature in kelvin.

Third to eighth columns: four or six parameters of the quasipolynomial equation ($m=1$ or 3). The parameters are dimensionless.

Ninth column: level of uncertainty assigned by the evaluators to the data generated from the quasipolynomial equation within the temperature range of the experimental data. When using the equation outside this range, the uncertainty decreases with the length of the extrapolation.

4.2.5. Deviation Plots

An overview of the deviations from the recommended values for all experimental data (both included in and rejected from the final correlation) measured by various authors is presented in graphical form in the deviation plots. The temperature is plotted along the x axis and the relative percentage deviation for individual data points along the y axis. Data from different sources are distinguished by different symbols. Points that lie outside the range of the ordinate in the plot are accompanied by the numerical value of the deviation. Some points that overlap each other or the accompanying figures are omitted. When too many data points were available some less important sets and values exhibiting large deviations from the recommended data were not included.

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6. References

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The paper by Čenský *et al.* (#00CEN/LIP) and the Ph.D. thesis by Roháč (#00ROH) were published only after completion of the tabular part of this work in November 2000. For this reason, the digit in the abbreviated reference is incorrect and should be (#01CEN/LIP) and (#01ROH), respectively.

7. Formula Index of Compounds

The formula index of compounds lists both compounds for which data were compiled and presented in Monograph No. 6 (96ZAB/RUZ) and newly compiled data. This enables the reader to find out where the data for a particular compound are to be sought.

Compounds are sorted in the order of empirical formulas. The empirical formula is listed on the first line. The second line introduced by the sign • gives the name of a compound and the Chemical Abstracts Service Registry Number (CAS RN) enclosed in brackets. The next line(s), if present, gives synonyms, common names or commercial names. The last line for each compound lists the group-member number. The system of dividing compounds into groups is described in detail in Sec. 4.1. The first two digit-number indicates the group, and the second three-digit number denotes the serial number of a compound inside the group. Tables in the compilation are coded with three numbers separated by full stops. The first two numbers are identical with the compound group and member number.

If there are more compounds of the same empirical formula, they are listed under a common formula and each compound is introduced by the sign •.

For geometric isomers which are common among alkenes the symbols (*Z*) and (*E*) are used to identify similar groups either on the same side of the double bond or across from the double bond. For simple systems (*Z*) and (*E*) are equivalent to *cis* and *trans*.

Several specific tags were appended to the group-member number to distinguish between compounds located in this work only, in Monograph No. 6 only, and in both works. The tag is separated from the group-member number by a slash. No tag means the compound is present in the Monograph No. 6 only. /**S1** denotes compounds present in this work, only /**B**+**S1** compounds are present both in Monograph No. 6 and in this work with a new set of correlation equation parameters given in this work, and /**B**+**S1**$^{\mathbf{E}}$ compounds are present both in Monograph No. 6 and in this work but with no new correlation equation parameters. For the last group of compounds this work presents a table of experimental data only, as new experimental data do not extend or improve previously developed recommended data.

$AgNO_3$
• Silver(1+) salt nitric acid [7761-88-8]
Silver nitrate
Group-member nr.: 02-001

$AlBr_3$
• Aluminium bromide [7727-15-3]
Group-member nr.: 02-002

$AlCl_3$
• Aluminium chloride [7446-70-0]
Group-member nr.: 02-003

AlI_3
• Aluminium iodide [7784-23-8]
Group-member nr.: 02-004

Ar
• Argon [7440-37-1]
Group-member nr.: 01-001

$AsCl_3$
• Arsenous trichloride [7784-34-1]
Arsenic trichloride
Arsenic chloride
Group-member nr.: 02-005

AsF_3
• Arsenous trifluoride [7784-35-2]
Arsenic trifluoride
Group-member nr.: 02-006

AsH_3
• Arsine [7784-42-1]
Group-member nr.: 02-007

BF_3
• Trifluoroborane [7637-07-2]
Boron fluoride (BF_3)
Boron trifluoride
Group-member nr.: 02-008/B+S1

B_2Cl_4
• Boron chloride (B_2Cl_4) [13701-67-2]
Diboron tetrachloride
Group-member nr.: 02-009

B_2H_6
• Diborane (6) [19287-45-7]
Group-member nr.: 02-010

$B_3H_6N_3$
• Borazine [6569-51-3]
Borazole
Group-member nr.: 02-011

B_5H_9
• Pentaborane (9) [19624-22-7]
Group-member nr.: 02-012

$B_{10}H_{14}$
• Decaborane (14) [17702-41-9]
Group-member nr.: 02-013

Bi
• Bismuth [7440-69-9]
Group-member nr.: 01-002

BrD
• Hydrobromic acid-*d* [13536-59-9]
Deuterium bromide
Group-member nr.: 02-014

BrF_3
- Bromine fluoride (BrF_3) [7787-71-5]
  Bromine trifluoride
  Group-member nr.: 02-015

BrH
- Hydrobromic acid [10035-10-6]
  Hydrogen bromide
  Group-member nr.: 02-016

BrIn
- Indium bromide (InBr) [14280-53-6]
  Group-member nr.: 02-017

Br_2
- Bromine [7726-95-6]
  Group-member nr.: 01-003

Br_2Sn
- Tin bromide ($SnBr_2$) [10031-24-0]
  Group-member nr.: 02-018

Br_4Sn
- Tetrabromostannane [7789-67-5]
  Tin(IV) bromide
  Tin tetrabromide
  Group-member nr.: 02-019

$CBrCl_3$
- Bromotrichloromethane [75-62-7]
  Group-member nr.: 25-001

$CBrF_3$
- Bromotrifluoromethane [75-63-8]
  R13B1
  Group-member nr.: 25-002

CBr_4
- Tetrabromomethane [558-13-4]
  Carbon tetrabromide
  Perbromomethane
  Group-member nr.: 23-001

$CClF_3$
- Chlorotrifluoromethane [75-72-9]
  R13
  Group-member nr.: 25-003

$CClN_3O_6$
- Chlorotrinitromethane [1943-16-4]
  Group-member nr.: 64-001

CCl_2F_2
- Dichlorodifluoromethane [75-71-8]
  R12
  Group-member nr.: 25-004/B+S1

CCl_2O
- Carbonic dichloride [75-44-5]
  Phosgene
  Group-member nr.: 02-020

CCl_3F
- Trichlorofluoromethane [75-69-4]
  R11
  Group-member nr.: 25-005

CCl_4
- Tetrachloromethane [56-23-5]
  Carbon tetrachloride
  Perchloromethane
  Group-member nr.: 22-001/B+S1^E

CD_4
- Methane-d_4 [558-20-3]
  Deuteromethane
  Group-member nr.: 11-001

CD_4O
- Methanol-d_4 [811-98-3]
  Methyl-d_3 alcohol-d
  Group-member nr.: 42-106/S1

CF_2O
- Carbonic difluoride [353-50-4]
  Carbonyl fluoride
  Group-member nr.: 02-021

CF_4
- Tetrafluoromethane [75-73-0]
  Carbon tetrafluoride
  Perfluoromethane
  R 14
  Group-member nr.: 21-001/B+S1

$CHBr_3$
- Tribromomethane [75-25-2]
  Bromoform
  Methenyl tribromide
  Group-member nr.: 23-002

$CHClF_2$
- Chlorodifluoromethane [75-45-6]
  R22
  Group-member nr.: 25-006

$CHCl_2F$
- Dichlorofluoromethane [75-43-4]
  R21
  Group-member nr.: 25-007

$CHCl_3$
- Trichloromethane [67-66-3]
  Chloroform
  Methenyl trichloride
  Group-member nr.: 22-002/B+S1^E

CHD_3O
- Methan-d_3-ol [1849-29-2]
  Methyl-d_3 alcohol
  Group-member nr.: 42-107/S1

CHF_3
- Trifluoromethane [75-46-7]
  Fluoroform
  R23
  Group-member nr.: 21-002

CHF_3S
- Trifluoromethanethiol [1493-15-8]

Group-member nr.: 64-002

$CHLiO_2$
- Lithium salt formic acid [556-63-8]
  Lithium formate
  Lithium methanoate
  Group-member nr.: 74-023/S1

CHN
- Hydrocyanic acid [74-90-8]
  Hydrogen cyanide
  Group-member nr.: 02-022

$CHNaO_2$
- Sodium salt formic acid [141-53-7]
  Sodium formate
  Natrium formate
  Group-member nr.: 74-001

CH_2Br_2
- Dibromomethane [74-95-3]
  Methylene bromide
  Group-member nr.: 23-003/B+S1

CH_2Cl_2
- Dichloromethane [75-09-2]
  Methylene chloride
  Group-member nr.: 22-003

CH_2F_2
- Difluoromethane [75-10-5]
  Methylene difluoride
  R32
  Group-member nr.: 21-034/S1

CH_2I_2
- Diiodomethane [75-11-6]
  Methylene iodide
  Group-member nr.: 24-001/B+S1

CH_2N_2
- Cyanamide [420-04-2]
  Group-member nr.: 34-001

CH_2O_2
- Formic acid [64-18-6]
  Methanoic acid
  Hydrogen carboxylic acid
  Group-member nr.: 44-001/B+S1^E

CH_2S_3
- Trithiocarbonic acid [594-08-1]
  Dihydrosulfide carbon sulfide
  Group-member nr.: 02-023

CH_3Br
- Bromomethane [74-83-9]
  Methyl bromide
  Group-member nr.: 23-004

CH_3Cl
- Chloromethane [74-87-3]
  Methyl chloride
  Group-member nr.: 22-004

CH_3ClFOP
- Methylphosphonic chloride fluoride [753-71-9]
  Methylphosphonic chlorofluoride
  Group-member nr.: 72-001

CH_3Cl_2OP
- Methylphosphonic dichloride [676-97-1]
  Group-member nr.: 72-002

CH_3Cl_3Si
- Trichloromethylsilane [75-79-6]
  Group-member nr.: 71-057/S1

CH_3D
- Methane-*d* [676-49-3]
  Monodeuteromethane
  Group-member nr.: 11-002

CH_3DO
- Methanol-*d* [1455-13-6]
  Monodeuteromethanol
  Group-member nr.: 42-001/B+S1

CH_3F_2OP
- Methylphosphonic difluoride [676-99-3]
  Group-member nr.: 72-003

CH_3I
- Iodomethane [74-88-4]
  Methyl iodide
  Group-member nr.: 24-002/B+S1

CH_3NO
- Formamide [75-12-7]
  Methanamide
  Group-member nr.: 62-001/B+S1

CH_3NO_2
- Nitromethane [75-52-5]
  Group-member nr.: 62-002/B+S1

CH_3NO_3
- Methyl ester nitric acid [598-58-3]
  Methyl nitrate
  Group-member nr.: 62-003

CH_4
- Methane [74-82-8]
  Group-member nr.: 11-003

CH_4N_2O
- Urea [57-13-6]
  Carbamide
  Group-member nr.: 62-004

CH_4O
- Methanol [67-56-1]
  Methyl alcohol
  Carbinol
  Group-member nr.: 42-002/B+S1^E

CH_4S
- Methanethiol [74-93-1]
  Methyl mercaptan
  Group-member nr.: 52-001

CH_5N
- Methanamine [74-89-5]
  Methylamine
  Aminomethane
  Group-member nr.: 31-001

CH_6N_2
- Methylhydrazine [60-34-4]
  Monomethylhydrazine
  Group-member nr.: 34-002

CO
- Carbon monoxide [630-08-0]
  Group-member nr.: 02-024

COS
- Carbon oxide sulfide [463-58-1]
  Carbonyl sulfide
  Group-member nr.: 02-025

CO_2
- Carbon dioxide [124-38-9]
  Group-member nr.: 02-026/B+S1

CS_2
- Carbon disulfide [75-15-0]
  Group-member nr.: 02-027

CSe_2
- Carbon selenide (CSe_2) [506-80-9]
  Group-member nr.: 02-028

$C_2Br_2D_4$
- 1,2-Dibromoethane-1,1,2,2-d_4 [22581-63-1]
  1,2-Dibromodeuteroethane
  Group-member nr.: 23-005

$C_2Br_2F_4$
- 1,2-Dibromo-1,1,2,2-tetrafluoroethane [124-73-2]
  R114
  Group-member nr.: 25-008

$C_2Br_3D_3$
- 1,1,2-Tribromoethane-1,2,2-d_3 [unknown]
  Group-member nr.: 23-006

C_2ClF_3
- Chlorotrifluoroethene [79-38-9]
  Chlorotrifluoroethylene
  Group-member nr.: 25-009

C_2ClF_5
- Chloropentafluoroethane [76-15-3]
  R115
  Group-member nr.: 25-010

$C_2Cl_2F_4$
- Dichlorotetrafluoroethane (unspecified isomer) [1320-37-2]
  Group-member nr.: 25-011
- 1,2-Dichloro-1,1,2,2-tetrafluoroethane [76-14-2]
  sym-Dichlorotetrafluoroethane
  Fluorocarbon-114
  R114
  Group-member nr.: 25-012/B+S1^E

$C_2Cl_3F_3$
- 1,1,1-Trichloro-2,2,2-trifluoroethane [354-58-5]
  Group-member nr.: 25-013
- 1,1,2-Trichloro-1,2,2-trifluoroethane [76-13-1]
  R113
  Group-member nr.: 25-014/B+S1^E

C_2Cl_4
- Tetrachloroethene [127-18-4]
  Perchloroethylene
  Group-member nr.: 22-005

$C_2Cl_4F_2$
- 1,1,2,2-Tetrachloro-1,2-difluoroethane [76-12-0]
  sym-Tetrachlorodifluoroethane
  R112
  Group-member nr.: 25-015

$C_2F_2O_2$
- Ethanedioyl difluoride [359-40-0]
  Oxalyl fluoride
  Group-member nr.: 61-001

C_2F_3N
- Trifluoroacetonitrile [353-85-5]
  Trifluoroethanenitrile
  Trifluoromethyl cyanide
  Group-member nr.: 64-003

C_2F_4
- Tetrafluoroethene [116-14-3]
  Perfluoroethylene
  Group-member nr.: 21-003

C_2F_4O
- Trifluoroacetyl fluoride [354-34-7]
  Group-member nr.: 61-002

C_2F_6
- Hexafluoroethane [76-16-4]
  Perfluoroethane
  Group-member nr.: 21-004

$C_2HBrClF_3$
- 1-Bromo-2-chloro-1,1,2-trifluoroethane [354-06-3]
  Group-member nr.: 25-016
- 2-Bromo-2-chloro-1,1,1-trifluoroethane [151-67-7]
  Halothane
  Group-member nr.: 25-017/B+S1^E

$C_2HBr_2D_3$
- 1,2-Dibromoethane-1,1,2-d_3 [117164-17-7]
  Group-member nr.: 23-007

$C_2HBr_3D_2$
- 1,1,2-Tribromoethane-2,2-d_2 [unknown]
  Group-member nr.: 23-008

C_2HClF_4
- 2-Chloro-1,1,1,2-tetrafluoroethane [2837-89-0]
  Monochlor-1,1,1,2-tetrafluoroethane
  R124
  Group-member nr.: 25-036/S1

$C_2HCl_2F_3$
- 1,2-Dichloro-1,1,2-trifluoroethane [354-23-4]
  R123a
  Group-member nr.: 25-037/S1
- 2,2-Dichloro-1,1,1-trifluoroethane [306-83-2]
  R123
  Group-member nr.: 25-038/S1

C_2HCl_3
- Trichloroethene [79-01-6]
  Trichloroethylene
  Group-member nr.: 22-006

$C_2HCl_3F_2$
- 1,1,2-Trichloro-1,2-difluoroethane [354-15-4]
  R122
  Group-member nr.: 25-018/B+S1[a]
- 1,2,2-Trichloro-1,1-difluoroethane [354-21-2]
  R122a
  Group-member nr.: 25-039/S1

C_2HCl_3O
- Trichloroacetaldehyde [75-87-6]
  Trichloroethanal
  Chloral
  Group-member nr.: 61-003

$C_2HCl_3O_2$
- Trichloroacetic acid [76-03-9]
  Trichloroethanoic acid
  Group-member nr.: 61-004

C_2HCl_5
- Pentachloroethane [76-01-7]
  Pentalin
  Group-member nr.: 22-007

C_2HF_4O
- (Difluoromethoxy)trifluoromethane [3822-68-2]
  Difluoromethyl trifluoromethyl ether
  Group-member nr.: 61-047/S1

C_2HF_5
- Pentafluoroethane [354-33-6]
  R125
  Group-member nr.: 21-035/S1

C_2H_2
- Ethyne [74-86-2]
  Acetylene
  Group-member nr.: 13-039/S1

$C_2H_2AsCl_3$
- (*E*)-(2-Chloroethenyl)arsonous dichloride [50361-05-2]
  trans-Chlorovinyldichlorarsine
  β-Chlorovinyldichlorarsine
  β-Lewisite
  Group-member nr.: 73-033/S1

$C_2H_2Br_2D_2$
- 1,2-Dibromoethane-1,1-d_2 [unknown]
  Group-member nr.: 23-009
- 1,2-Dibromoethane-1,2-d_2 [unknown]
  Group-member nr.: 23-010

$C_2H_2Br_3D$
- 1,1,2-Tribromoethane-1-*d* [unknown]
  Group-member nr.: 23-011
- 1,1,2-Tribromoethane-2-*d* [unknown]
  Group-member nr.: 23-012

$C_2H_2Br_4$
- 1,1,2,2-Tetrabromoethane [79-27-6]
  sym-Tetrabromoethane
  Acetylene tetrabromide
  Group-member nr.: 23-013

$C_2H_2Cl_2$
- 1,1-Dichloroethene [75-35-4]
  1,1-Dichloroethylene
  Vinylidene chloride
  Group-member nr.: 22-008
- 1,2-Dichloroethene [540-59-0]
  1,2-Dichloroethylene (unspecified stereoisomer)
  Group-member nr.: 22-009
- (*E*)-1,2-Dichloroethene [156-60-5]
  trans-1,2-Dichloroethene
  trans-1,2-Dichloroethylene
  Group-member nr.: 22-010
- (*Z*)-1,2-Dichloroethene [156-59-2]
  cis-1,2-Dichloroethene
  cis-1,2-Dichloroethylene
  Group-member nr.: 22-011

$C_2H_2Cl_2F_2$
- 1,1-Dichloro-1,2-difluoroethane [1842-05-3]
  R132
  Group-member nr.: 25-019/B+S1[a]

$C_2H_2Cl_2O_2$
- Dichloroacetic acid [79-43-6]
  Dichloroethanoic acid
  Group-member nr.: 61-005

$C_2H_2Cl_4$
- 1,1,1,2-Tetrachloroethane [630-20-6]
  Group-member nr.: 22-012
- 1,1,2,2-Tetrachloroethane [79-34-5]
  sym-Tetrachloroethane
  Acetylene tetrachloride
  Group-member nr.: 22-013

$C_2H_2F_3NO$
- 2,2,2-Trifluoroacetamide [354-38-1]
  Group-member nr.: 64-031/S1

$C_2H_2F_4$
- 1,1,1,2-Tetrafluoroethane [811-97-2]
  R134a
  Group-member nr.: 21-036/S1

[a]Incorrect correlating equation parameters were presented in Monograph No. 6 (96ZAB/RUZ).

C_2H_3Br
- Bromoethene [593-60-2]
  Bromoethylene
  Vinyl bromide
  Group-member nr.: 23-014

$C_2H_3Br_2D$
- 1,2-Dibromoethane-*d* [unknown]
  Group-member nr.: 23-015

$C_2H_3Br_3$
- 1,1,2-Tribromoethane [78-74-0]
  Group-member nr.: 23-016

C_2H_3Cl
- Chloroethene [75-01-4]
  Vinyl chloride
  Group-member nr.: 22-014

$C_2H_3ClF_2$
- 1-Chloro-1,1-difluoroethane [75-68-3]
  R142
  Group-member nr.: 25-020

C_2H_3ClO
- Acetyl chloride [75-36-5]
  Ethanoyl chloride
  Group-member nr.: 61-006

$C_2H_3ClO_2$
- Chloroacetic acid [79-11-8]
  Chloroethanoic acid
  Group-member nr.: 61-007

$C_2H_3Cl_2F$
- 1,1-Dichloro-1-fluoroethane [1717-00-6]
  R141b
  Group-member nr.: 25-040/S1

$C_2H_3Cl_3$
- 1,1,1-Trichloroethane [71-55-6]
  Methylchloroform
  Group-member nr.: 22-015
- 1,1,2-Trichloroethane [79-00-5]
  Vinyl trichloride
  β-Trichloroethane
  Group-member nr.: 22-016

$C_2H_3Cl_3Si$
- Trichloroethenylsilane [75-94-5]
  Trichlorovinylsilane
  Group-member nr.: 71-001

$C_2H_3F_3$
- 1,1,1-Trifluoroethane [420-46-2]
  Group-member nr.: 21-005/B+S1

$C_2H_3F_3O$
- 2,2,2-Trifluoroethanol [75-89-8]
  Group-member nr.: 61-008/B+S1

$C_2H_3LiO_2$
- Lithium salt acetic acid [546-89-4]
  Lithium acetate
  Lithium ethanoate
  Group-member nr.: 74-024/S1

C_2H_3N
- Acetonitrile [75-05-8]
  Ethanenitrile
  Group-member nr.: 32-002/B+S1

C_2H_4
- Ethene [74-85-1]
  Ethylene
  Group-member nr.: 13-001

C_2H_4BrCl
- 1-Bromo-2-chloroethane [107-04-0]
  Ethylene chlorobromide
  Group-member nr.: 25-021

$C_2H_4Br_2$
- 1,2-Dibromoethane [106-93-4]
  Ethylene dibromide
  Group-member nr.: 23-017/B+S1^E

$C_2H_4Cl_2$
- 1,1-Dichloroethane [75-34-3]
  Ethylidene chloride
  Group-member nr.: 22-017
- 1,2-Dichloroethane [107-06-2]
  Ethylene dichloride
  Group-member nr.: 22-018/B+S1^E

$C_2H_4D_2O_2$
- 1,2-Ethanediol-d_2 [2219-52-5]
  Dideutero-1,2-ethanediol
  Dideuteroethylene glycol
  Group-member nr.: 42-003

$C_2H_4F_2$
- 1,1-Difluoroethane [75-37-6]
  R152a
  Group-member nr.: 21-037/S1

$C_2H_4N_4$
- Cyanoguanidine [461-58-5]
  Dicyandiamide
  Group-member nr.: 34-014/S1

C_2H_4O
- Acetaldehyde [75-07-0]
  Ethanal
  Group-member nr.: 43-001
- Oxirane [75-21-8]
  Epoxyethane
  Ethylene oxide
  Group-member nr.: 46-001

$C_2H_4O_2$
- Acetic acid [64-19-7]
  Ethanoic acid
  Methane carboxylic acid
  Group-member nr.: 44-002/B+S1^E
- Methyl formate [107-31-3]
  Methyl methanoate
  Group-member nr.: 45-001

C_2H_5Br
- Bromoethane [74-96-4]
  Ethyl bromide
  Group-member nr.: 23-018/B+S1^E

C_2H_5Cl
- Chloroethane [75-00-3]
  Ethyl chloride
  Group-member nr.: 22-019

$C_2H_5Cl_3Si$
- Trichloroethylsilane [115-21-9]
  Group-member nr.: 71-002

C_2H_5DO
- Ethanol-*d* [925-93-9]
  Monodeuteroethanol
  Group-member nr.: 42-004

C_2H_5I
- Iodoethane [75-03-6]
  Ethyl iodide
  Group-member nr.: 24-003/B+S1

C_2H_5N
- Aziridine [151-56-4]
  Ethyleneimine
  Group-member nr.: 33-001

C_2H_5NO
- Acetamide [60-35-5]
  Ethanamide
  Group-member nr.: 62-005
- *N*-Methylformamide [123-39-7]
  Group-member nr.: 62-006/B+S1

$C_2H_5NO_2$
- Nitroethane [79-24-3]
  Group-member nr.: 62-007

$C_2H_5NO_3$
- Ethyl nitrate [625-58-1]
  Ethyl ester nitric acid
  Group-member nr.: 62-008

C_2H_6
- Ethane [74-84-0]
  Group-member nr.: 11-004/B+S1

C_2H_6Cd
- Dimethylcadmium [506-82-1]
  Group-member nr.: 73-001

$C_2H_6Cl_2Si$
- Dichlorodimethylsilane [75-78-5]
  Group-member nr.: 71-058/S1
- Dichloroethylsilane [1789-58-8]
  Group-member nr.: 71-003

C_2H_6O
- Ethanol [64-17-5]
  Ethyl alcohol
  Group-member nr.: 42-005/B+S1^E
- Oxybismethane [115-10-6]
  Dimethyl ether
  Methyl ether
  Methyl oxide
  Group-member nr.: 41-001

C_2H_6OS
- Sulfinylbismethane [67-68-5]
  Dimethyl sulfoxide
  DMSO
  Group-member nr.: 63-001/B+S1

$C_2H_6O_2$
- 1,2-Ethanediol [107-21-1]
  Ethylene glycol
  Glycol
  Group-member nr.: 42-006/B+S1

$C_2H_6O_2S$
- Sulfonylbismethane [67-71-0]
  Dimethyl sulfone
  Group-member nr.: 63-002

C_2H_6S
- Ethanethiol [75-08-1]
  Ethyl mercaptan
  Group-member nr.: 52-002
- Thiobismethane [75-18-3]
  Dimethyl sulfide
  Group-member nr.: 51-001

$C_2H_6S_2$
- 2,3-Dithiabutane [624-92-0]
  Dimethyl disulfide
  Methyl disulfide
  Group-member nr.: 51-002

C_2H_6Se
- Selenobismethane [593-79-3]
  Dimethyl selenide
  Methyl selenide
  Group-member nr.: 73-002

$C_2H_6Se_2$
- Dimethyl diselenide [7101-31-7]
  Methyl diselenide
  Group-member nr.: 73-003

C_2H_6Te
- Tellurobismethane [593-80-6]
  Dimethyltellurium
  Group-member nr.: 73-034/S1

C_2H_6Zn
- Dimethylzinc [544-97-8]
  Group-member nr.: 73-004

C_2H_7N
- Ethanamine [75-04-7]
  Ethylamine
  Group-member nr.: 31-002/B+S1
- *N*-Methylmethanamine [124-40-3]
  Dimethylamine
  Group-member nr.: 31-003

C_2H_7NO
- 2-Aminoethanol [141-43-5]
  Ethanolamine
  Group-member nr.: 62-128/S1

$C_2H_8N_2$
- 1,1-Dimethylhydrazine [57-14-7]
  unsym-Dimethylhydrazine
  Group-member nr.: 34-003
- 1,2-Dimethylhydrazine [540-73-8]
  sym-Dimethylhydrazine
  Group-member nr.: 34-004
- 1,2-Ethanediamine [107-15-3]
  Ethylenediamine
  1,2-Diaminoethane
  Group-member nr.: 31-004

$C_2H_8N_2O_3$
- Nitrate ethylamine [22113-86-6]
  Ethylammonium nitrate
  Group-member nr.: 62-009

$C_2H_{11}B_2N$
- (Dimethylamino)diborane (6) [22580-01-4]
  Group-member nr.: 72-004

C_2N_2
- Ethanedinitrile [460-19-5]
  Cyanogen
  Group-member nr.: 32-001

C_3Cl_6
- 1,1,2,3,3,3-Hexachloro-1-propene [1888-71-7]
  Hexachloropropene
  Hexachloropropylene
  Group-member nr.: 22-050/S1

C_3F_6O
- 1,1,1,3,3,3-Hexafluoro-2-propanone [684-16-2]
  Hexafluoroacetone
  Perfluoroacetone
  Group-member nr.: 61-009

C_3F_8
- Octafluoropropane [76-19-7]
  Perfluoropropane
  Group-member nr.: 21-006

C_3HClF_6
- 1-Chloro-1,1,2,3,3,3-hexafluoropropane [359-58-0]
  R226ea
  Group-member nr.: 25-041/S1
- 2-Chloro-1,1,1,3,3,3-hexafluoropropane [431-87-8]
  R226da
  Group-member nr.: 25-042/S1

$C_3HCl_2F_5$
- 1,2-Dichloro-1,1,3,3,3-pentafluoropropane [431-86-7]
  R225da
  Group-member nr.: 25-043/S1
- 2,3-Dichloro-1,1,1,2,3-pentafluoropropane [422-48-0]
  R225ba
  Group-member nr.: 25-044/S1

C_3HF_7
- 1,1,1,2,2,3,3-Heptafluoropropane [2252-84-8]
  R227ca
  Group-member nr.: 21-038/S1
- 1,1,1,2,3,3,3-Heptafluoropropane [431-89-0]
  R227ea
  Group-member nr.: 21-039/S1

$C_3H_2ClF_5$
- 1-Chloro-1,1,3,3,3-pentafluoropropane [460-92-4]
  Group-member nr.: 25-022
- 3-Chloro-1,1,1,2,2-pentafluoropropane [422-02-6]
  R235ca
  Group-member nr.: 25-045/S1

$C_3H_2Cl_2F_4$
- 2,3-Dichloro-1,1,1,3-tetrafluoropropane [146916-90-7]
  R234da
  Group-member nr.: 25-046/S1

$C_3H_2Cl_2O_3$
- 4,5-Dichloro-1,3-dioxolan-2-one [3967-55-3]
  Group-member nr.: 61-048/S1

$C_3H_2Cl_3F_3$
- 1,1,1-Trichloro-3,3,3-trifluoropropane [7125-84-0]
  Group-member nr.: 25-023

$C_3H_2F_6$
- 1,1,1,2,2,3-Hexafluoropropane [677-56-5]
  R236cb
  Group-member nr.: 21-040/S1
- 1,1,1,2,3,3-Hexafluoropropane [431-63-0]
  R236ea
  Group-member nr.: 21-041/S1
- 1,1,1,3,3,3-Hexafluoropropane [690-39-1]
  R236fa
  Group-member nr.: 21-042/S1

$C_3H_2N_2$
- Propanedinitrile [109-77-3]
  Malononitrile
  Dicyanomethane
  Group-member nr.: 32-003

$C_3H_3ClO_3$
- 4-Chloro-1,3-dioxolan-2-one [3967-54-2]
  Group-member nr.: 61-049/S1

$C_3H_3Cl_2F_3$
- 2,3-Dichloro-1,1,1-trifluoropropane [338-75-0]
  R243da
  Group-member nr.: 25-047/S1
- 3,3-Dichloro-1,1,1-trifluoropropane [460-69-5]
  Group-member nr.: 25-024

$C_3H_3Cl_3O_2$
- Methyl trichloroacetate [598-99-2]
  Methyl ester trichloroacetic acid
  Group-member nr.: 61-010

$C_3H_3F_5$
- 1,1,1,2,2-Pentafluoropropane [1814-88-6]
  R245cb
  Group-member nr.: 21-043/S1
- 1,1,1,3,3-Pentafluoropropane [460-73-1]
  R245fa
  Group-member nr.: 21-044/S1
- 1,1,2,2,3-Pentafluoropropane [679-86-7]
  R245ca
  Group-member nr.: 21-045/S1

C_3H_3N
- 2-Propenenitrile [107-13-1]
  Acrylonitrile
  Vinyl cyanide
  Group-member nr.: 32-004/B+S1^E

C_3H_3NO
- Isoxazole [288-14-2]
  Group-member nr.: 62-010/B+S1
- Oxazole [288-42-6]
  Group-member nr.: 62-011

C_3H_3NS
- Thiazole [288-47-1]
  Group-member nr.: 64-004

$C_3H_3N_3$
- 1,3,5-Triazine [290-87-9]
  sym-Triazine
  Group-member nr.: 33-002

$C_3H_4ClF_3$
- 3-Chloro-1,1,1-trifluoropropane [460-35-5]
  Group-member nr.: 25-025

$C_3H_4Cl_2O_2$
- Methyl dichloroacetate [116-54-1]
  Methyl ester dichloroacetic acid
  Group-member nr.: 61-011

$C_3H_4Cl_3NSi$
- 3-Trichlorosilylpropanenitrile [1071-22-3]
  Group-member nr.: 71-004

$C_3H_4Cl_4$
- 1,1,1,3-Tetrachloropropane [1070-78-6]
  Group-member nr.: 22-020

$C_3H_4F_4$
- 1,1,2,2-Tetrafluoropropane [40723-63-5]
  R254cb
  Group-member nr.: 21-046/S1

$C_3H_4N_2$
- 1*H*-Imidazole [288-32-4]
  1,3-Diazole
  Glyoxaline
  Group-member nr.: 33-003
- 1*H*-Pyrazole [288-13-1]
  1,2-Diazole
  Group-member nr.: 33-004

$C_3H_4N_2O$
- 2-Cyanoacetamide [107-91-5]
  Group-member nr.: 62-012

$C_3H_4O_2$
- 2-Oxetanone [57-57-8]
  β-Propiolactone
  Hydracrylolactone
  USAN
  Group-member nr.: 47-001
- 2-Propenoic acid [79-10-7]
  Acrylic acid
  Acroleic acid
  Group-member nr.: 44-003/B+S1

$C_3H_4O_3$
- 1,3-Dioxolan-2-one [96-49-1]
  Cyclic ethylene ester carbonic acid
  Ethylene carbonate
  Group-member nr.: 47-002

C_3H_5Br
- 3-Bromo-1-propene [106-95-6]
  Allyl bromide
  Group-member nr.: 23-019

$C_3H_5Br_3$
- 1,2,3-Tribromopropane [96-11-7]
  Group-member nr.: 23-020

C_3H_5Cl
- 3-Chloro-1-propene [107-05-1]
  3-Chloropropene
  Allyl chloride
  Group-member nr.: 22-021

C_3H_5ClO
- Propanoyl chloride [79-03-8]
  Propionyl chloride
  Group-member nr.: 61-012

$C_3H_5ClO_2$
- Methyl chloroacetate [96-34-4]
  Methyl ester chloroacetic acid
  Group-member nr.: 61-013

$C_3H_5Cl_3$
- 1,2,3-Trichloropropane [96-18-4]
  Group-member nr.: 22-022

$C_3H_5D_3O_3$
- 1,2,3-Propanetriol-*O*,*O*,*O*-d_3 [7325-16-8]
  Glycerol-*O*,*O*,*O*-d_3
  Trideuteroglycerol
  Group-member nr.: 42-007

C_3H_5N
- Propanenitrile [107-12-0]
  Propionitrile
  Ethyl cyanide
  Group-member nr.: 32-005/B+S1^E

C_3H_5NO
- Methoxyacetonitrile [1738-36-9]

Group-member nr.: 62-129/S1
- 2-Propenamide [79-06-1]
  Acrylamide
  Group-member nr.: 62-013

$C_3H_5NO_4$
- Methyl ester nitroacetic acid [2483-57-0]
  Methyl nitroacetate
  Group-member nr.: 62-014

C_3H_5NS
- Isothiocyanatoethane [542-85-8]
  Ethyl isothiocyanate
  Group-member nr.: 64-005

$C_3H_5NaO_2$
- Sodium salt propanoic acid [137-40-6]
  Sodium propanoate
  Natrium propionate
  Group-member nr.: 74-002

C_3H_6
- Cyclopropane [75-19-4]
  Trimethylene
  Group-member nr.: 12-001
- 1-Propene [115-07-1]
  Propylene
  Group-member nr.: 13-002

$C_3H_6Br_2$
- 1,2-Dibromopropane [78-75-1]
  Propylene bromide
  Group-member nr.: 23-021
- 1,3-Dibromopropane [109-64-8]
  Trimethylene bromide
  Group-member nr.: 23-022/B+S1

$C_3H_6Cl_2$
- 1,2-Dichloropropane [78-87-5]
  Propylene chloride
  Group-member nr.: 22-023/B+S1
- 1,3-Dichloropropane [142-28-9]
  Trimethylene dichloride
  Group-member nr.: 22-024/B+S1
- 2,2-Dichloropropane [594-20-7]
  Isopropylidene chloride
  Group-member nr.: 22-025

$C_3H_6Cl_2Si$
- Dichloroethenylmethylsilane [124-70-9]
  Dichloromethylvinylsilane
  Group-member nr.: 71-059/S1

$C_3H_6F_4N_2$
- N,N,N',N'-Tetrafluoro-1,2-propanediamine [15403-25-5]
  Group-member nr.: 64-006

$C_3H_6I_2$
- 1,3-Diiodopropane [627-31-6]
  Group-member nr.: 24-010/S1

$C_3H_6N_2O_4$
- 2,2-Dinitropropane [595-49-3]
  Group-member nr.: 62-015

C_3H_6O
- Methyloxirane [75-56-9]
  1,2-Epoxypropane
  1,2-Propylene oxide
  Group-member nr.: 46-002
- Oxetane [503-30-0]
  Trimethylene oxide
  Group-member nr.: 46-003
- Propanal [123-38-6]
  Propionaldehyde
  Group-member nr.: 43-003
- 2-Propanone [67-64-1]
  Dimethyl ketone
  Acetone
  Group-member nr.: 43-004/B+S1^E
- 2-Propen-1-ol [107-18-6]
  Allyl alcohol
  Group-member nr.: 42-008

$C_3H_6O_2$
- 1,3-Dioxolane [646-06-0]
  Group-member nr.: 46-004/B+S1^E
- Ethyl formate [109-94-4]
  Ethyl methanoate
  Group-member nr.: 45-002/B+S1
- Methyl acetate [79-20-9]
  Methyl ethanoate
  Group-member nr.: 45-003/B+S1
- Propanoic acid [79-09-4]
  Propionic acid
  Methylacetic acid
  Group-member nr.: 44-004/B+S1^E

$C_3H_6O_2S$
- 3-Mercaptopropanoic acid [107-96-0]
  3-Thiolpropionic acid
  β-Thiolacetic acid
  Group-member nr.: 63-003

$C_3H_6O_3$
- Dimethyl carbonate [616-38-6]
  Methyl carbonate
  Group-member nr.: 45-004/B+S1
- (R,S)-2-Hydroxypropanoic acid [598-82-3]
  Lactic acid (racemic)
  Group-member nr.: 47-003
- Methyl ester hydroxyacetic acid [96-35-5]
  Methyl glycolate
  Group-member nr.: 47-052/S1
- 1,3,5-Trioxane [110-88-3]
  sym-Trioxane
  Group-member nr.: 46-005

C_3H_6S
- Thietane [287-27-4]
  Thiacyclobutane
  Trimethylene sulfide
  Group-member nr.: 53-001

C_3H_7Br
- 1-Bromopropane [106-94-5]
  Propyl bromide
  Group-member nr.: 23-023/B+S1
- 2-Bromopropane [75-26-3]
  Isopropyl bromide
  Group-member nr.: 23-024/B+S1^E

C_3H_7Cl
- 1-Chloropropane [540-54-5]
  Propyl chloride
  Group-member nr.: 22-026

C_3H_7I
- 1-Iodopropane [107-08-4]
  Propyl iodide
  Group-member nr.: 24-004/B+S1
- 2-Iodopropane [75-30-9]
  Isopropyl iodide
  Group-member nr.: 24-011/S1

C_3H_7N
- Cyclopropanamine [765-30-0]
  Cyclopropylamine
  Group-member nr.: 31-005

C_3H_7NO
- *N*,*N*-Dimethylformamide [68-12-2]
  N,*N*-Dimethylmethanamide
  Group-member nr.: 62-016/B+S1

$C_3H_7NO_2$
- Ethyl ester carbamic acid [51-79-6]
  Ethyl carbamate
  Ethyl urethane
  Group-member nr.: 62-017
- 1-Nitropropane [108-03-2]
  Group-member nr.: 62-130/S1

$C_3H_7NO_3$
- 1-Methylethyl ester nitric acid [1712-64-7]
  Isopropyl nitrate
  Group-member nr.: 62-018

C_3H_8
- Propane [74-98-6]
  Group-member nr.: 11-005

C_3H_8O
- 1-Propanol [71-23-8]
  Propyl alcohol
  Group-member nr.: 42-009/B+S1
- 2-Propanol [67-63-0]
  Isopropyl alcohol
  Group-member nr.: 42-010/B+S1^E

$C_3H_8O_2$
- Dimethoxymethane [109-87-5]
  2,4-Dioxapentane
  Formaldehyde dimethyl acetal
  Methylal
  Group-member nr.: 41-002/B+S1^E
- 2-Methoxyethanol [109-86-4]
  Methyl cellosolve
  Glycol monomethyl ether
  Group-member nr.: 47-004
- 1,2-Propanediol [57-55-6]
  Propylene glycol
  Group-member nr.: 42-011/B+S1

$C_3H_8O_3$
- 1,2,3-Propanetriol [56-81-5]
  Glycerol
  Glycyl alcohol
  Glycerine
  Group-member nr.: 42-012/B+S1

C_3H_8S
- (Methylthio)ethane [624-89-5]
  Ethyl methyl sulfide
  Group-member nr.: 51-003
- 1-Propanethiol [107-03-9]
  1-Propyl mercaptan
  Group-member nr.: 52-003
- 2-Propanethiol [75-33-2]
  Isopropyl mercaptan
  Group-member nr.: 52-004

C_3H_9Al
- Trimethylaluminium [75-24-1]
  Group-member nr.: 73-005

C_3H_9As
- Trimethylarsine [593-88-4]
  Group-member nr.: 73-006

C_3H_9B
- Trimethylborane [593-90-8]
  Group-member nr.: 72-005

$C_3H_9BO_3$
- Trimethyl ester boric acid(H_3BO_3) [121-43-7]
  Trimethyl borate
  Methyl borate
  Group-member nr.: 72-016/S1

C_3H_9ClSi
- Chlorotrimethylsilane [75-77-4]
  Group-member nr.: 71-060/S1

C_3H_9Ga
- Trimethylgallium [1445-79-0]
  Group-member nr.: 73-007

C_3H_9N
- *N*,*N*-Dimethylmethanamine [75-50-3]
  Trimethylamine
  Group-member nr.: 31-006
- 1-Propanamine [107-10-8]
  n-Propylamine
  Group-member nr.: 31-007
- 2-Propanamine [75-31-0]
  Isopropylamine
  Group-member nr.: 31-008

C_3H_9NO
- 2-(Methylamino)ethanol [109-83-1]

N-Methylethanolamine
Group-member nr.: 62-131/S1

$C_3H_{10}N_2$
• (*R*,*S*)-1,2-Propanediamine [10424-38-1]
1,2-Diaminopropane (racemic)
Group-member nr.: 31-009
• Trimethylhydrazine [1741-01-1]
Group-member nr.: 34-005

$C_3H_{12}BN$
• Trimethylamineborane [75-22-9]
N,*N*-Dimethylmethanamine compd. with borane (1:1)
Group-member nr.: 72-006

C_3O_2
• 1,2-Propadiene-1,3-dione [504-64-3]
Carbon suboxide
Group-member nr.: 43-002

$C_4Br_2Cl_2F_6$
• 1,4-Dibromo-2,3-dichloro-1,1,2,3,4,4-hexafluorobutane [375-42-8]
Group-member nr.: 25-026

C_4D_8O
• Tetrahydro-*d*4-furan-*d*4 [1693-74-9]
Tetradeuterofuran
Group-member nr.: 46-027/S1

C_4F_8
• Octafluorocyclobutane [115-25-3]
Perfluorocyclobutane
Group-member nr.: 21-007

C_4HClF_6
• 4-Chloro-1,1,2,2,3,3-hexafluorocyclobutane [132186-30-2]
Rc-326d
Group-member nr.: 25-048/S1

C_4HF_9
• 1,1,1,2,2,3,3,4,4-Nonafluorobutane [375-17-7]
R329cca
Group-member nr.: 21-047/S1

$C_4H_2F_8$
• 1,1,1,2,2,3,3,4-Octafluorobutane [662-35-1]
R338ccb
Group-member nr.: 21-048/S1
• 1,1,2,2,3,3,4,4-Octafluorobutane [377-36-6]
R338cca
Group-member nr.: 21-049/S1

$C_4H_2O_3$
• 2,5-Furandione [108-31-6]
(*Z*)-Butenedioic acid anhydride
Maleic anhydride
Group-member nr.: 44-005/B+S1[E]

C_4H_3BrS
• 2-Bromothiophene [1003-09-4]
Group-member nr.: 64-032/S1

C_4H_3ClS
• 2-Chlorothiophene [96-43-5]
Group-member nr.: 64-033/S1

$C_4H_3Cl_3OS$
• *O*-Methyl ester 2,3,3-trichloro-2-propenethioic acid [76619-91-5]
O-Methyl ester trichlorothioacrylic acid
Methyl trichlorothioacrylate
Group-member nr.: 64-007

$C_4H_3F_7$
• 1,1,1,2,2,3,3-Heptafluorobutane [662-00-0]
R347ccd
Group-member nr.: 21-050/S1

$C_4H_4N_2$
• Butanedinitrile [110-61-2]
Succinonitrile
Ethylene dicyanide
Group-member nr.: 32-006

C_4H_4O
• Furan [110-00-9]
Furfuran
Tetrol
Group-member nr.: 46-006

$C_4H_4O_4$
• 1,4-Dioxane-2,5-dione [502-97-6]
p-Dioxane-2,5-dione
Glycolide
Diglycolide
Group-member nr.: 47-005

C_4H_4S
• Thiophene [110-02-1]
Thiofuran
Group-member nr.: 53-002

C_4H_5Cl
• 2-Chloro-1,3-butadiene [126-99-8]
Chloroprene
Group-member nr.: 22-027

$C_4H_5ClO_3$
• 4-(Chloromethyl)-1,3-dioxolan-2-one [2463-45-8]
4-Chloromethyl carbonate
Group-member nr.: 61-050/S1

$C_4H_5ClO_2$
• (*E*)-3-Chloro-2-butenoic acid [6214-28-4]
trans-3-Chloro-2-butenoic acid
3-Chlorocrotonic acid
Group-member nr.: 61-014
• (*Z*)-3-Chloro-2-butenoic acid [6213-90-7]
cis-3-Chloro-2-butenoic acid
3-Chloroisocrotonic acid
Group-member nr.: 61-015

$C_4H_5Cl_3O$
• 2,2,3-Trichlorobutanal [76-36-8]
2,2,3-Trichlorobutyraldehyde
Butylchloral
Group-member nr.: 61-016

$C_4H_5Cl_3O_2$
- Ethyl trichloroacetate [515-84-4]
  Ethyl ester trichloroacetic acid
  Group-member nr.: 61-017

C_4H_5N
- Cyclopropanecarbonitrile [5500-21-0]
  Cyclopropyl cyanide
  Cyanocyclopropane
  Group-member nr.: 32-007
- 2-Methyl-2-propenenitrile [126-98-7]
  Methacrylonitrile
  Group-member nr.: 32-008
- 1*H*-Pyrrole [109-97-7]
  Azole
  Group-member nr.: 33-005

C_4H_5NO
- 4-Oxobutanenitrile [3515-93-3]
  β-Cyanopropionaldehyde
  Group-member nr.: 62-019

$C_4H_5NO_2$
- Methyl ester cyanoacetic acid [105-34-0]
  Methyl cyanoacetate
  Group-member nr.: 62-132/S1
- 2,5-Pyrrolidinedione [123-56-8]
  Succinimide
  Group-member nr.: 62-020

C_4H_5NS
- 3-Isothiocyanato-1-propene [57-06-7]
  Allyl isothiocyanate
  Group-member nr.: 64-008
- 2-Methylthiazole [3581-87-1]
  Group-member nr.: 64-009

C_4H_6
- 1,2-Butadiene [590-19-2]
  Group-member nr.: 13-003
- 1,3-Butadiene [106-99-0]
  Vinylethylene
  Divinyl
  Erythrene
  Group-member nr.: 13-004
- 1-Butyne [107-00-6]
  Ethylacetylene
  Group-member nr.: 13-005
- 2-Butyne [503-17-3]
  Dimethylacetylene
  Crotonylene
  Group-member nr.: 13-006

$C_4H_6Cl_2O_2$
- Ethyl dichloroacetate [535-15-9]
  Ethyl ester dichloroacetic acid
  Group-member nr.: 61-018

$C_4H_6N_2$
- 1-Methyl-1*H*-imidazole [616-47-7]
  Group-member nr.: 33-047/S1
- 1-Methyl-1*H*-pyrazole [930-36-9]
  Group-member nr.: 33-048/S1

C_4H_6O
- 2-Butenal [4170-30-3]
  Crotonoaldehyde
  Group-member nr.: 43-005
- 2,3-Dihydrofuran [1191-99-7]
  Group-member nr.: 46-007

$C_4H_6O_2$
- (*E*)-2-Butenoic acid [107-93-7]
  trans-2-Butenoic acid
  Crotonic acid
  Group-member nr.: 44-006/B+S1
- 2(3*H*)-Dihydrofuranone [96-48-0]
  γ-Butyrolactone
  4-Butanolide
  Group-member nr.: 47-006/B+S1
- Ethenyl acetate [108-05-4]
  Vinyl acetate
  Ethenyl ethanoate
  Group-member nr.: 45-005/B+S1
- Methyl propenoate [96-33-3]
  Methyl acrylate
  Group-member nr.: 45-006
- 2-Methyl-2-propenoic acid [79-41-4]
  Methacrylic acid
  α-Methacrylic acid
  Group-member nr.: 44-007

$C_4H_6O_3$
- Acetic acid anhydride [108-24-7]
  Acetic anhydride
  Ethanoic acid anhydride
  Group-member nr.: 44-008
- 4-Methyl-1,3-dioxolan-2-one [108-32-7]
  Cyclic propylene ester carbonic acid
  Propylene carbonate
  Group-member nr.: 47-007/B+S1

$C_4H_6O_4$
- Dimethyl ester ethanedioic acid [553-90-2]
  Dimethyl ethanedioate
  Dimethyl oxalate
  Group-member nr.: 45-131/S1

C_4H_6Te
- 1,1′-Tellurobisethene [63000-06-6]
  Divinyltellurium
  Group-member nr.: 73-035/S1

C_4H_7ClO
- Butanoyl chloride [141-75-3]
  Butyryl chloride
  Group-member nr.: 61-019
- 2-Methylpropanoyl chloride [79-30-1]
  2-Methylpropionyl chloride
  Isobutyryl chloride
  Group-member nr.: 61-020

$C_4H_7ClO_2$
- Ethyl chloroacetate [105-39-5]
  Ethyl ester chloroacetic acid
  Group-member nr.: 61-021

$C_4H_7Cl_2NSi$
- 3-(Dichloromethylsilyl)propanenitrile [1071-21-2]
  3-(Dichloromethylsilyl)propionitrile
  Dichloro-(2-cyanethyl)methylsilane
  Group-member nr.: 71-005

$C_4H_7LiO_2$
- Lithium salt 2-methylpropanoic acid [25179-23-1]
  Lithium isobutyrate
  Group-member nr.: 74-025/S1

C_4H_7N
- Butanenitrile [109-74-0]
  Butyronitrile
  Propyl cyanide
  Group-member nr.: 32-009
- 2-Methylpropanenitrile [78-82-0]
  2-Methylpropionitrile
  Isobutyronitrile
  Isopropyl cyanide
  Group-member nr.: 32-010

C_4H_7NO
- Ethoxyacetonitrile [62957-60-2]
  Group-member nr.: 62-133/S1
- 3-Methoxypropionitrile [110-67-8]
  Group-member nr.: 62-021
- 2-Pyrrolidinone [616-45-5]
  2-Pyrrolidone
  γ-Butyrolactam
  Group-member nr.: 62-022

$C_4H_7NO_2$
- Tetrahydro-2*H*-1,3-oxazin-2-one [5259-97-2]
  Group-member nr.: 62-134/S1

$C_4H_7NaO_2$
- Sodium salt butanoic acid [156-54-7]
  Sodium butanoate
  Natrium butyrate
  Group-member nr.: 74-003

$C_4H_7O_2Tl$
- Thallium(1+) salt butanoic acid [63424-49-7]
  Thallium(I) butyrate
  Group-member nr.: 74-026/S1

C_4H_8
- 1-Butene [106-98-9]
  Group-member nr.: 13-007/B+S1
- (*E*)-2-Butene [624-64-6]
  trans-2-Butene
  trans-Dimethylethylene
  Group-member nr.: 13-008
- (*Z*)-2-Butene [590-18-1]
  cis-2-Butene
  cis-Dimethylethylene
  Group-member nr.: 13-009
- Cyclobutane [287-23-0]
  Tetramethylene
  Group-member nr.: 12-002
- 2-Methyl-1-propene [115-11-7]
  Isobutene
  Group-member nr.: 13-010

$C_4H_8Br_2$
- 1,4-Dibromobutane [110-52-1]
  Group-member nr.: 23-041/S1

$C_4H_8Cl_2$
- 1,2-Dichlorobutane [616-21-7]
  Group-member nr.: 22-051/S1
- 1,4-Dichlorobutane [110-56-5]
  Tetramethylene dichloride
  Group-member nr.: 22-028/B+S1

$C_4H_8Cl_2O$
- 1,1′-Oxybis(2-chloroethane) [111-44-4]
  Bis(2-chloroethyl) ether
  β,β'-Dichlorodiethyl ether
  Chlorex
  Group-member nr.: 61-022

$C_4H_8N_2$
- 1,4,5,6-Tetrahydropyrimidine [1606-49-1]
  Group-member nr.: 33-049/S1

C_4H_8O
- Butanal [123-72-8]
  Butyraldehyde
  Group-member nr.: 43-006
- 2-Butanone [78-93-3]
  Ethyl methyl ketone
  Group-member nr.: 43-007/B+S1^E
- Ethyloxirane [106-88-7]
  1,2-Epoxybutane
  1,2-Butylene oxide
  Group-member nr.: 46-008/B+S1^E
- 2-Methoxy-1-propene [116-11-0]
  Isopropenyl methyl ether
  Group-member nr.: 41-003
- Tetrahydrofuran [109-99-9]
  Oxolane
  Tetramethylene oxide
  Group-member nr.: 46-009/B+S1^E

$C_4H_8O_2$
- Butanoic acid [107-92-6]
  Butyric acid
  Ethylacetic acid
  Propylformic acid
  Group-member nr.: 44-009
- 1,3-Dioxane [505-22-6]
  m-Dioxane
  Group-member nr.: 46-010
- 1,4-Dioxane [123-91-1]
  p-Dioxane
  1,4-Diethylene dioxide

Dioxyethylene ether
Diethylene ether
Group-member nr.: 46-011/B+S1[E]
- Ethyl acetate [141-78-6]
Ethyl ethanoate
Group-member nr.: 45-007/B+S1
- Methyl propanoate [554-12-1]
Methyl propionate
Group-member nr.: 45-008/B+S1[E]
- 2-Methylpropanoic acid [79-31-2]
Isobutyric acid
Group-member nr.: 44-010/B+S1
- Propyl formate [110-74-7]
Propyl methanoate
Group-member nr.: 45-009/B+S1[E]

$C_4H_8O_2S$
- Tetrahydrothiophene 1,1-dioxide [126-33-0]
Tetramethylene sulfone
Sulfolane
Group-member nr.: 63-004/B+S1

$C_4H_8O_3$
- 1,2-Ethanediol monoacetate [542-59-6]
Ethylene glycol monoacetate
2-Hydroxyethyl acetate
Group-member nr.: 47-053/S1[E]
- Methyl ester methoxyacetic acid [6290-49-9]
Methyl methoxyacetate
Group-member nr.: 47-054/S1

$C_4H_8O_4$
- 1,3,5,7-Tetroxocane [293-30-1]
1,3,5,7-Tetraoxacyclooctane
Group-member nr.: 46-012

C_4H_8S
- Tetrahydrothiophene [110-01-0]
Thiolane
Tetramethylenesulfide
Group-member nr.: 53-003

$C_4H_8S_2$
- 1,3-Dithiane [505-23-7]
m-Dithiane
Group-member nr.: 53-004
- 1,4-Dithiane [505-29-3]
p-Dithiane
Group-member nr.: 53-005

C_4H_9Br
- 1-Bromobutane [109-65-9]
n-Butyl bromide
Group-member nr.: 23-025/B+S1
- 1-Bromo-2-methylpropane [78-77-3]
Isobutyl bromide
Group-member nr.: 23-026/B+S1
- 2-Bromo-2-methylpropane [507-19-7]
tert-Butyl bromide
Group-member nr.: 23-027/B+S1

C_4H_9Cl
- 1-Chlorobutane [109-69-3]
n-Butyl chloride
Group-member nr.: 22-029/B+S1[E]
- 2-Chlorobutane [78-86-4]
sec-Butyl chloride
Group-member nr.: 22-052/S1
- 1-Chloro-2-methylpropane [513-36-0]
Isobutyl chloride
Group-member nr.: 22-030
- 2-Chloro-2-methylpropane [507-20-0]
tert-Butyl chloride
Group-member nr.: 22-031/B+S1

C_4H_9I
- 1-Iodobutane [542-69-8]
Butyl iodide
Group-member nr.: 24-012/S1
- 2-Iodobutane [513-48-4]
sec-Butyl iodide
Group-member nr.: 24-013/S1
- 1-Iodo-2-methylpropane [513-38-2]
Isobutyl iodide
Group-member nr.: 24-005/B+S1

C_4H_9N
- Pyrrolidine [123-75-1]
Tetrahydropyrrole
Azolidine
Group-member nr.: 33-006

C_4H_9NO
- 2-Butanone oxime [96-29-7]
Ethyl methyl ketoxime (unspecified stereoisomer)
Group-member nr.: 62-023
- *N*,*N*-Dimethylacetamide [127-19-5]
Group-member nr.: 62-024
- *N*-Ethylacetamide [625-50-3]
N-Ethylethanamide
Group-member nr.: 62-025
- *N*-Methylpropanamide [1187-58-2]
N-Methylpropionamide
Group-member nr.: 62-026
- Morpholine [110-91-8]
Tetrahydro-4*H*-1,4-oxazine
Diethylenimide oxide
Group-member nr.: 62-027

C_4H_{10}
- Butane [106-97-8]
Group-member nr.: 11-006
- 2-Methylpropane [75-28-5]
Isobutane
Trimethylmethane
Group-member nr.: 11-007

$C_4H_{10}Cl_2Si$
- Dichlordiethylsilane [1719-53-5]
Group-member nr.: 71-006

$C_4H_{10}Hg$
- Diethylmercury [627-44-1]
  Group-member nr.: 73-008

$C_4H_{10}N_2$
- Piperazine [110-85-0]
  Hexahydropyrazine
  Perhydro-1,4-diazine
  Diethylenediamine
  Group-member nr.: 33-007/B+S1

$C_4H_{10}O$
- 1-Butanol [71-36-3]
  Butyl alcohol
  Group-member nr.: 42-013/B+S1^E
- 2-Butanol [78-92-2]
  sec-Butyl alcohol
  Methyl ethyl carbinol (unspecified chirality)
  Group-member nr.: 42-014
- (*R*,*S*)-2-Butanol [15892-23-6]
  sec-Butyl alcohol
  Methyl ethyl carbinol (racemic)
  Group-member nr.: 42-015
- (*S*)-2-Butanol [4221-99-2]
  D-*sec*-Butyl alcohol
  D-Methylethylcarbinol
  Group-member nr.: 42-016
- 1-Methoxypropane [557-17-5]
  Methyl propyl ether
  Group-member nr.: 41-004
- 2-Methoxypropane [598-53-8]
  Methyl 1-methylethyl ether
  Isopropyl methyl ether
  Group-member nr.: 41-005
- 2-Methyl-1-propanol [78-83-1]
  Isobutyl alcohol
  Group-member nr.: 42-017/B+S1
- 2-Methyl-2-propanol [75-65-0]
  tert-Butyl alcohol
  Trimethyl carbinol
  Group-member nr.: 42-018
- 1,1′-Oxybisethane [60-29-7]
  Diethyl ether
  Ethyl ether
  Ethyl oxide
  Diethyl oxide
  Group-member nr.: 41-006

$C_4H_{10}O_2$
- (±)-1,2-Butanediol [26171-83-5]
  Group-member nr.: 42-108/S1
- 1,3-Butanediol [107-88-0]/B+S1
  1,3-Butylene glycol
  Group-member nr.: 42-019
- 1,4-Butanediol [110-63-4]
  1,4-Butylene glycol
  Tetramethylene glycol
  Group-member nr.: 42-020
- 2,3-Butanediol [513-85-9]
  2,3-Butylene glycol
  Group-member nr.: 42-021
- 1,2-Dimethoxyethane [110-71-4]
  2,5-Dioxahexane
  Ethylene glycol dimethyl ether
  Monoglyme
  GDME
  Group-member nr.: 41-007/B+S1
- 2-Ethoxyethanol [110-80-5]
  3-Oxa-1-pentanol
  Ethyl cellosolve
  Ethylene glycol monoethyl ether
  Group-member nr.: 47-008/B+S1

$C_4H_{10}O_2Se$
- 2,2′-Selenodiethanol [27974-49-8]
  β-Selenium diglycol
  Group-member nr.: 73-009

$C_4H_{10}O_3$
- 2,2′-Oxybisethanol [111-46-6]
  1,5-Dihydroxy-3-oxapentane
  2,2′-Dihydroxydiethyl ether
  Diethylene glycol
  Group-member nr.: 47-009/B+S1

$C_4H_{10}O_4$
- (*R**,*S**)-1,2,3,4-Butanetetrol [149-32-6]
  Erythro-1,2,3,4-butanetetrol
  Erythritol
  Group-member nr.: 42-022

$C_4H_{10}S$
- 1-Butanethiol [109-79-5]
  1-Butyl mercaptan
  Group-member nr.: 52-005
- 2-Butanethiol [513-53-1]
  2-Butyl mercaptan
  sec-Butyl mercaptan
  Group-member nr.: 52-006
- 2-Methyl-1-propanethiol [513-44-0]
  Isobutyl mercaptan
  Group-member nr.: 52-007
- 2-Methyl-2-propanethiol [75-66-1]
  tert-Butyl mercaptan
  Group-member nr.: 52-008
- 1-(Methylthio)propane [3877-15-4]
  Methyl propyl sulfide
  Group-member nr.: 51-004
- 2-(Methylthio)propane [1551-21-9]
  Methyl 1-methylethyl sulfide
  Isopropyl methyl sulfide
  Group-member nr.: 51-005
- 1,1′-Thiobisethane [352-93-2]
  Diethyl sulfide
  Group-member nr.: 51-006

$C_4H_{10}S_2$
- 3,4-Dithiahexane [110-81-6]
  Diethyl disulfide

Ethyl disulfide
Group-member nr.: 51-007

$C_4H_{10}Te$
• Diethyltelluride [627-54-3]
Group-member nr.: 73-036/S1

$C_4H_{10}Zn$
• Diethylzinc [557-20-0]
Group-member nr.: 73-010

$C_4H_{11}N$
• 1-Butanamine [109-73-9]
n-Butylamine
Group-member nr.: 31-010
• *N*-Ethylethanamine [109-89-7]
Diethylamine
Group-member nr.: 31-011/B+S1^E
• 2-Methyl-1-propanamine [78-81-9]
Isobutylamine
Group-member nr.: 31-012
• 2-Methyl-2-propanamine [75-64-9]
tert-Butylamine
Group-member nr.: 31-013

$C_4H_{11}NO$
• 2-Amino-2-methyl-1-propanol [124-68-5]
Isobutanolamine
Group-member nr.: 62-028/B+S1
• *N*,*N*-Diethylhydroxylamine [3710-84-7]
Group-member nr.: 62-029
• 2-(Dimethylamino)ethanol [108-01-0]
Dimethylethanolamine
Group-member nr.: 62-135/S1
• 2-(Ethylamino)ethanol [110-73-6]
Ethylethanolamine
Group-member nr.: 62-136/S1
• 3-Methoxy-1-propanamine [5332-73-0]
3-Methoxypropylamine
4-Oxapentanamine
Group-member nr.: 62-030

$C_4H_{11}NO_2$
• 2-(2-Aminoethoxy)ethanol [929-06-6]
Diglycolamine
Group-member nr.: 62-137/S1
• 2-Amino-2-methyl-1,3-propanediol [115-69-5]
Group-member nr.: 62-031
• 2,2′-Iminobisethanol [111-42-2]
Diethanolamine
2-(2-Hydroxyethylamino)ethanol
Group-member nr.: 62-138/S1

$C_4H_{11}NO_3$
• 2-Amino-2-(hydroxymethyl)-1,3-propanediol [77-86-1]
Trometamol
Group-member nr.: 62-032

$C_4H_{12}CdSe$
• Dimethyl[selenobis(methane)]cadmium [143481-65-6]
Group-member nr.: 73-011

$C_4H_{12}CdTe$
• Dimethyl[tellurobis(methane)]cadmium [143481-66-7]
Group-member nr.: 73-012

$C_4H_{12}Ge$
• Tetramethylgermane [865-52-1]
Group-member nr.: 73-013

$C_4H_{12}N_2$
• 2-Methyl-1,2-propanediamine [811-93-8]
1,2-Diamino-2-methylpropane
Group-member nr.: 31-014

$C_4H_{12}O_4Si$
• Tetramethyl ester silicic acid [681-84-5]
Tetramethyl orthosilicate
Tetramethoxysilane
Group-member nr.: 71-007

$C_4H_{12}Pb$
• Tetramethylplumbane [75-74-1]
Tetramethyllead
Group-member nr.: 73-014

$C_4H_{12}SZn$
• Dimethyl[thiobis[methane]]zinc [91071-61-3]
Group-member nr.: 73-037/S1

$C_4H_{12}SeZn$
• Dimethyl[selenobis(methane)]zinc [108430-95-1]
Complex dimethylzinc with dimethylselenium
Group-member nr.: 73-015

$C_4H_{12}Si$
• Tetramethylsilane [75-76-3]
Group-member nr.: 71-008

$C_4H_{12}Sn$
• Tetramethylstannane [594-27-4]
Tetramethyltin
Group-member nr.: 73-016

$C_4H_{12}TeZn$
• Dimethyl[tellurobis(methane)]zinc [127283-03-8]
Complex dimethylzinc with dimethyltellurium
Group-member nr.: 73-017

$C_4H_{13}N_3$
• *N*-(2-Aminoethyl)-1,2-ethanediamine [111-40-0]
Diethylenetriamine
Group-member nr.: 31-015/B+S1

C_4NiO_4
• Nickel carbonyl [13463-39-3]
Group-member nr.: 02-029

$C_5F_{11}N$
• Undecafluoropiperidine [836-77-1]
Perfluoropiperidine
Group-member nr.: 64-010

C_5F_{12}
• Dodecafluoropentane [678-26-2]
Perfluoropentane
Group-member nr.: 21-008

$C_5F_{13}N$
• 1,1,2,2,2-Pentafluoro-*N*-(pentafluoroethyl)-*N*-(trifluoromethyl)-ethanamine [758-48-5]
Group-member nr.: 64-011

$C_5H_3F_7O_2$
• Methyl heptafluorobutanoate [356-24-1]
Methyl ester heptafluorobutanoic acid
Methyl perfluorobutyrate
Group-member nr.: 61-023

$C_5H_4N_4$
• [1,2,4]Triazolo[1,5-*a*]pyrimidine [275-02-5]
Group-member nr.: 33-050/S1

$C_5H_4O_2$
• 2-Furancarboxaldehyde [98-01-1]
Furfural
Pyromucic aldehyde
Furfuraldehyde
Group-member nr.: 47-010/B+S1

$C_5H_5Cl_3OS$
• *O*-Ethyl ester 2,3,3-trichloro-2-propenethioic acid [76619-92-6]
O-Ethyl ester trichlorothioacrylate
Group-member nr.: 64-034/S1

$C_5H_5Cl_3O_2$
• 2-Propenyl trichloroacetate [6304-34-3]
2-Propenyl ester trichloroacetic acid
Allyl trichloroacetate
Group-member nr.: 61-024

C_5H_5N
• Bicyclo[1.1.0]butane-1-carbonitrile [16955-35-4]
1-Bicyclobutyl cyanide
1-Cyanobicyclobutane
Group-member nr.: 32-011
• Pyridine [110-86-1]
Azine
Group-member nr.: 33-008/B+S1

C_5H_6
• 1,3-Cyclopentadiene [542-92-7]
Group-member nr.: 14-098/S1

$C_5H_6Cl_2O_2$
• 2-Propenyl dichloroacetate [30895-77-3]
2-Propenyl ester dichloroacetic acid
Allyl dichloroacetate
Group-member nr.: 61-025

$C_5H_6N_2$
• Dimethylpropanedinitrile [7321-55-3]
2,2-Dicyanopropane
Dimethylmalononitrile
Group-member nr.: 32-012
• Pentanedinitrile [544-13-8]
1,3-Dicyanopropane
Glutaronitrile
Trimethylenedicyanide
Group-member nr.: 32-013

C_5H_6O
• 2-Methylfuran [534-22-5]
Sylvan
Group-member nr.: 46-013

$C_5H_6O_2$
• 2-Furanmethanol [98-00-0]
Furfuryl alcohol
Furyl carbinol
Group-member nr.: 47-011

C_5H_6S
• 2-Methylthiophene [554-14-3]
Group-member nr.: 53-006
• 3-Methylthiophene [616-44-4]
Group-member nr.: 53-007

$C_5H_7ClO_2$
• 2-Propenyl chloroacetate [2916-14-5]
2-Propenyl ester chloroacetic acid
Allyl chloroacetate
Group-member nr.: 61-026

$C_5H_7Cl_3O_2$
• Propyl trichloroacetate [13313-91-2]
Propyl ester trichloroacetic acid
Group-member nr.: 61-027

C_5H_7N
• Cyclobutanecarbonitrile [4426-11-3]
Cyclobutyl cyanide
Cyanocyclobutane
Group-member nr.: 32-014
• 1-Methyl-1*H*-pyrrole [96-54-8]
Group-member nr.: 33-009

$C_5H_7NO_2$
• Ethyl ester cyanoacetic acid [105-56-6]
Ethyl cyanoacetate
Group-member nr.: 62-033
• Methyl ester 2-cyanopropanoic acid [14618-77-0]
Methyl 2-cyanopropionate
Group-member nr.: 62-139/S1

C_5H_8
• Cyclopentene [142-29-0]
Group-member nr.: 14-001
• 2-Methyl-1,3-butadiene [78-79-5]
Isoprene
Group-member nr.: 13-011
• 3-Methyl-1,2-butadiene [598-25-4]
Group-member nr.: 13-012
• Methylenecyclobutane [1120-56-5]
Group-member nr.: 12-003
• 1,2-Pentadiene [591-95-7]
Group-member nr.: 13-013
• (*E*)-1,3-Pentadiene [2004-70-8]
trans-1,3-Pentadiene
Group-member nr.: 13-014
• (*Z*)-1,3-Pentadiene [1574-41-0]
cis-1,3-Pentadiene

Group-member nr.: 13-015
- 1,4-Pentadiene [591-93-5]
  Group-member nr.: 13-016
- 2,3-Pentadiene [591-96-8]
  Group-member nr.: 13-017
- Spiropentane [157-40-4]
  Spirocyclane
  Cyclopropanespirocyclopropane
  Group-member nr.: 12-004

$C_5H_8Br_4$
- 1,3-Dibromo-2,2-bis(bromomethyl)propane [3229-00-3]
  2,2-Bis(bromomethyl)-1,3-dibromopropane
  Pentaerythrityl tetrabromide
  Group-member nr.: 23-028

$C_5H_8Cl_2O$
- 3,3-Bis(chloromethyl)oxetane [78-71-7]
  3,3-Bis(chloromethyl)oxacyclobutane
  Group-member nr.: 61-028

$C_5H_8Cl_2O_2$
- Ethyl 2,3-dichloropropanoate [6628-21-3]
  Ethyl ester 2,3-dichloropropanoic acid
  Group-member nr.: 61-029
- Propyl dichloroacetate [37587-81-8]
  Propyl ester dichloroacetic acid
  Group-member nr.: 61-030

$C_5H_8Cl_4$
- 1,3-Dichloro-2,2-bis(chloromethyl)propane [3228-99-7]
  2,2-Bis(chloromethyl)-1,3-dichloropropane
  Pentaerythrityl tetrachloride
  Group-member nr.: 22-032

$C_5H_8F_4$
- 1,3-Difluoro-2,2-bis(fluoromethyl)propane [338-23-8]
  2,2-Bis(fluoromethyl)-1,3-difluoropropane
  Pentaerythrityl tetrafluoride
  Group-member nr.: 21-009

$C_5H_8N_2$
- 1-Ethyl-1*H*-imidazole [7098-07-9]
  Group-member nr.: 33-051/S1
- 1-Ethyl-1*H*-pyrazole [2817-71-2]
  Group-member nr.: 33-052/S1

C_5H_8O
- Cyclopentanone [120-92-3]
  Group-member nr.: 43-008/B+S1

$C_5H_8O_2$
- Methyl 2-methyl-2-propenoate [80-62-6]
  Methyl methacrylate
  Group-member nr.: 45-010
- 2,4-Pentanedione [123-54-6]
  Acetylacetone
  Diacetylmethane
  Group-member nr.: 43-009/B+S1
- 2-Propenyl acetate [591-87-7]
  2-Propenyl ethanoate
  Allyl acetate
  Group-member nr.: 45-011
- Tetrahydro-2*H*-pyran-2-one [542-28-9]
  δ-Valerolactone
  5-Pentanolide
  Group-member nr.: 47-012

$C_5H_8O_3$
- Methyl ester 3-oxobutanoic acid [105-45-3]
  Methyl acetoacetate
  Group-member nr.: 47-055/S1

$C_5H_8O_4$
- Dimethyl ester propanedioic acid [108-59-8]
  Dimethyl malonate
  Group-member nr.: 45-132/S1

C_5H_9Cl
- Chlorocyclopentane [930-28-9]
  Cyclopentyl chloride
  Group-member nr.: 22-053/S1

C_5H_9ClO
- Pentanoyl chloride [638-29-9]
  Valeryl chloride
  Group-member nr.: 61-031

$C_5H_9ClO_2$
- Ethyl 2-chloropropanoate [535-13-7]
  Ethyl ester 2-chloropropanoic acid
  Ethyl α-chloropropionate
  Group-member nr.: 61-032
- Propyl chloroacetate [5396-24-7]
  Propyl ester chloroacetic acid
  Group-member nr.: 61-033

C_5H_9N
- 2,2-Dimethylpropanenitrile [630-18-2]
  2-Cyano-2-methylpropane
  Pivalonitrile
  Trimethylacetonitrile
  Group-member nr.: 32-015
- Pentanenitrile [110-59-8]
  Valeronitrile
  Butyl cyanide
  Group-member nr.: 32-016

C_5H_9NO
- 2-Methoxy-2-methylpropanenitrile [76474-09-4]
  2-Methoxy-2-methylpropionitrile
  Group-member nr.: 62-140/S1
- 1-Methyl-2-pyrrolidinone [872-50-4]
  1-Methyl-2-pyrrolidone
  Group-member nr.: 62-034
- 2-Piperidinone [675-20-7]
  δ-Valerolactam
  2-Piperidone
  Group-member nr.: 62-035

$C_5H_9NO_2$
- 4-Methyl-3-morpholinone [20721-78-2]
  4-Methyl-3-oxomorpholine
  Group-member nr.: 62-141/S1

C_5H_{10}
- Cyclopentane [287-92-3]
  Pentamethylene
  Group-member nr.: 12-005
- 2-Methyl-1-butene [563-46-2]
  Group-member nr.: 13-018
- 3-Methyl-1-butene [563-45-1]
  Isopropylethylene
  α-Isoamylene
  Group-member nr.: 13-020
- 2-Methyl-2-butene [513-35-9]
  Trimethylethylene
  β-Isoamylene
  Group-member nr.: 13-019
- 1-Pentene [109-67-1]
  Group-member nr.: 13-021/B+S1
- 2-Pentene [109-68-2]
  β-Amylene
  Methylethylethylene (unspecified stereoisomer)
  Group-member nr.: 13-022
- (*E*)-2-Pentene [646-04-8]
  trans-2-Pentene
  trans-β-Amylene
  trans-Methylethylethylene
  Group-member nr.: 13-023
- (*Z*)-2-Pentene [627-20-3]
  cis-2-Pentene
  cis-β-Amylene
  cis-Methylethylethylene
  Group-member nr.: 13-024

$C_5H_{10}Cl_2$
- 1,5-Dichloropentane [628-76-2]
  Pentamethylene dichloride
  Group-member nr.: 22-033/B+S1

$C_5H_{10}N_2$
- 3-(Dimethylamino)-propanenitrile [1738-25-6]
  3-(Dimethylamino)-propionitrile
  Group-member nr.: 34-006

$C_5H_{10}O$
- Cyclopentanol [96-41-3]
  Cyclopentyl alcohol
  Group-member nr.: 42-023/B+S1
- 2,2-Dimethylpropanal [630-19-3]
  Pivalaldehyde
  Trimethylacetaldehyde
  Group-member nr.: 43-010/B+S1
- 3-Methyl-2-butanone [563-80-4]
  Isopropyl methyl ketone
  Group-member nr.: 43-011
- 2-Methyl-3-buten-2-ol [115-18-4]
  Group-member nr.: 42-024
- Pentanal [110-62-3]
  Valeraldehyde
  Pentyl aldehyde
  Amyl aldehyde
  Group-member nr.: 43-012
- 2-Pentanone [107-87-9]
  Methyl propyl ketone
  Group-member nr.: 43-013
- 3-Pentanone [96-22-0]
  Diethyl ketone
  Metacetone
  Ethyl propionyl
  Propione
  Group-member nr.: 43-014
- Tetrahydropyran [142-68-7]
  Oxane
  Pentamethylene oxide
  Group-member nr.: 46-014/B+S1^E

$C_5H_{10}O_2$
- Butyl formate [592-84-7]
  Butyl methanoate
  Group-member nr.: 45-012/B+S1
- 2,2-Dimethylpropanoic acid [75-98-9]
  Trimethylacetic acid
  Pivalic acid
  Group-member nr.: 44-037/S1
- 1,3-Dioxepane [505-65-7]
  m-Dioxepane
  Group-member nr.: 46-015
- Ethyl propanoate [105-37-3]
  Ethyl propionate
  Group-member nr.: 45-013/B+S1^E
- Methyl butanoate [623-42-7]
  Methyl butyrate
  Group-member nr.: 45-014
- 3-Methylbutanoic acid [503-74-2]
  Isovaleric acid
  Group-member nr.: 44-011
- 1-Methylethyl acetate [108-21-4]
  Isopropyl acetate
  1-Methylethyl ethanoate
  Group-member nr.: 45-016
- Methyl 2-methylpropanoate [547-63-7]
  Methyl isobutyrate
  Group-member nr.: 45-015
- 2-Methylpropyl formate [542-55-2]
  2-Methylpropyl methanoate
  Isobutyl formate
  Group-member nr.: 45-017
- Pentanoic acid [109-52-4]
  Valeric acid
  Group-member nr.: 44-012
- Propyl acetate [109-60-4]
  Propyl ethanoate
  Group-member nr.: 45-018/B+S1^E
- Tetrahydro-2-furanmethanol [97-99-4]
  Tetrahydrofurfuryl alcohol
  Group-member nr.: 47-013

$C_5H_{10}O_3$
- Diethyl carbonate [105-58-8]

Ethyl carbonate
Group-member nr.: 45-019/B+S1
• 2-Methoxyethanol acetate [110-49-6]
2-Methoxyethyl acetate
Group-member nr.: 47-014/B+S1

$C_5H_{10}O_5$
• 1,3,5,7,9-Pentoxecane [16528-92-0]
Pentoxane
Group-member nr.: 46-016

$C_5H_{10}S$
• Cyclopentanethiol [1679-07-8]
Cyclopentyl mercaptan
Group-member nr.: 52-009
• 2-Methyltetrahydrothiophene [1795-09-1]
2-Methylthiolane
2-Methylcyclothiapentane
Group-member nr.: 53-008
• 3-Methyltetrahydrothiophene [4740-00-5]
3-Methylthiolane
3-Methylcyclothiapentane
Group-member nr.: 53-009
• Tetrahydro-2*H*-thiopyran [1613-51-0]
Thiacyclohexane
Pentamethylene sulfide
Group-member nr.: 53-010

$C_5H_{11}Br$
• 1-Bromo-3-methylbutane [107-82-4]
Isoamyl bromide
Group-member nr.: 23-029
• 1-Bromopentane [110-53-2]
n-Amyl bromide
Group-member nr.: 23-030/B+S1

$C_5H_{11}Cl$
• 1-Chloro-3-methylbutane [107-84-6]
Isoamyl chloride
Group-member nr.: 22-034
• 1-Chloropentane [543-59-9]
Pentyl chloride
Amyl chloride
Group-member nr.: 22-054/S1

$C_5H_{11}I$
• 1-Iodo-3-methylbutane [541-28-6]
Isoamyl iodide
Group-member nr.: 24-006
• 1-Iodopentane [628-17-1]
Pentyl iodide
Amyl iodide
Group-member nr.: 24-014/S1

$C_5H_{11}N$
• Cyclopentanamine [1003-03-8]
Cyclopentylamine
Group-member nr.: 31-016
• 1-Methylpyrrolidine [120-94-5]
N-Methylpyrrolidine
Group-member nr.: 33-010
• 3-Methylpyrrolidine [34375-89-8]
Group-member nr.: 33-011
• Piperidine [110-89-4]
Pentamethylenimine
Hexahydropyridine
Perhydroazine
Group-member nr.: 33-012/B+S1

$C_5H_{11}NO$
• *N*,2-Dimethylpropanamide [2675-88-9]
N-Methylisobutyramide
Group-member nr.: 62-036
• *N*-Methylbutanamide [17794-44-4]
N-Methylbutyramide
Group-member nr.: 62-037
• *N*-(1-Methylethyl)acetamide [1118-69-0]
N-(1-Methylethyl)ethanamide
N-Isopropylacetamide
Group-member nr.: 62-038
• *N*-Propylacetamide [5331-48-6]
N-Propylethanamide
Group-member nr.: 62-039

$C_5H_{11}NO_2$
• Methyl ester *N*,*N*-dimethylglycine [7148-06-3]
Methyl ester *N*,*N*-dimethylaminoacetic acid
Group-member nr.: 62-142/S1

C_5H_{12}
• 2,2-Dimethylpropane [463-82-1]
Neopentane
Tetramethylmethane
Group-member nr.: 11-008
• 2-Methylbutane [78-78-4]
Isopentane
Group-member nr.: 11-009
• Pentane [109-66-0]
Group-member nr.: 11-010

$C_5H_{12}N_2O$
• *N*,*N*-Diethylurea [634-95-7]
1,1-Diethylurea
Group-member nr.: 62-143/S1
• Tetramethylurea [632-22-4]
Group-member nr.: 62-040

$C_5H_{12}O$
• 2,2-Dimethyl-1-propanol [75-84-3]
Neopentyl alcohol
Group-member nr.: 42-109/S1
• 1-Ethoxypropane [628-32-0]
Ethyl propyl ether
Group-member nr.: 41-008
• 2-Methoxy-2-methylpropane [1634-04-4]
1,1-Dimethylethyl methyl ether
tert-Butyl methyl ether
Group-member nr.: 41-010
• 1-Methoxybutane [628-28-4]
Butyl methyl ether

Group-member nr.: 41-009/B+S1[E]
- 2-Methyl-1-butanol [137-32-6]
  sec-Butyl carbinol
  Group-member nr.: 42-025/B+S1
- 2-Methyl-2-butanol [75-85-4]
  tert-Amyl alcohol
  tert-Pentyl alcohol
  Dimethyl ethyl carbinol
  Group-member nr.: 42-026/B+S1
- 3-Methyl-1-butanol [123-51-3]
  Isopentyl alcohol
  Isoamyl alcohol
  Group-member nr.: 42-027/B+S1
- 3-Methyl-2-butanol [598-75-4]
  sec-Isoamyl alcohol
  Group-member nr.: 42-028/B+S1
- 1-Pentanol [71-41-0]
  n-Amyl alcohol/B+S1[E]
  Group-member nr.: 42-029
- 2-Pentanol [6032-29-7]
  sec-Amyl alcohol
  Methyl propyl carbinol
  Group-member nr.: 42-030/B+S1
- 3-Pentanol [584-02-1]
  1-Ethyl-1-propanol
  Diethyl carbinol
  Group-member nr.: 42-031/B+S1

$C_5H_{12}O_2$
- 2,2-Dimethoxypropane [77-76-9]
  Acetone dimethyl acetal
  Group-member nr.: 41-011
- 2,2-Dimethyl-1,3-propanediol [126-30-7]
  Group-member nr.: 42-032
- 1-Ethoxy-2-methoxyethane [5137-45-1]
  2,5-Dioxaheptane
  Ethylene glycol ethyl ether methyl ether
  Group-member nr.: 41-012
- 1,5-Pentanediol [111-29-5]
  Group-member nr.: 42-033
- 1,1′-[Methylenebis(oxy)]bisethane [462-95-3]
  3,5-Dioxaheptane
  Diethoxymethane
  Formaldehyde diethyl acetal
  Group-member nr.: 41-049/S1
- 2-(1-Methylethoxy)ethanol [109-59-1]
  4-Methyl-3-oxa-1-pentanol
  2-Isopropoxyethanol
  Ethylene glycol monoisopropyl ether
  Group-member nr.: 47-015/B+S1
- 1,5-Pentanediol [111-29-5]
  Group-member nr.: 42-033
- 2-Propoxyethanol [2807-30-9]
  3-Oxa-1-hexanol
  Ethylene glycol monopropyl ether
  Propyl cellosolve
  Group-member nr.: 47-016/B+S1[E]

$C_5H_{12}O_3$
- 2-(2-Methoxyethoxy)ethanol [111-77-3]
  Diethylene glycol monomethyl ether
  Group-member nr.: 47-017

$C_5H_{12}S$
- 1-(Ethylthio)propane [4110-50-3]
  Ethyl propyl sulfide
  Group-member nr.: 51-008
- 2-Methyl-2-butanethiol [1679-09-0]
  2-Methyl-2-butyl mercaptan
  tert-Amyl mercaptan
  Group-member nr.: 52-010
- 3-Methyl-1-butanethiol [541-31-1]
  3-Methylbutyl mercaptan
  Isopentyl mercaptan
  Isoamyl mercaptan
  Group-member nr.: 52-011
- 3-Methyl-2-butanethiol [2084-18-6]
  3-Methyl-2-butyl mercaptan
  sec-Isoamyl mercaptan
  Group-member nr.: 52-012
- 2-Methyl-2-(methylthio)propane [6163-64-0]
  1,1-Dimethylethyl methyl sulfide
  tert-Butyl methyl sulfide
  Group-member nr.: 51-009
- 1-(Methylthio)butane [628-29-5]
  Butyl methyl sulfide
  Group-member nr.: 51-010
- 2-(Methylthio)butane [10359-64-5]
  3-Methyl-2-thiapentane
  Methyl 1-methylpropyl sulfide
  sec-Butyl methyl sulfide
  Group-member nr.: 51-011
- 1-Pentanethiol [110-66-7]
  1-Pentyl mercaptan
  Group-member nr.: 52-013
- Tetrakis(methylthia)methane [6156-25-8]
  Tetramethyl ester tetrathiacarbonic acid
  Group-member nr.: 51-012

$C_5H_{12}Si$
- 1,1-Dimethylsilacyclobutane [2295-12-7]
  Group-member nr.: 71-009
- Ethenyltrimethylsilane [754-05-2]
  Trimethylvinylsilane
  Group-member nr.: 71-010/B+S1

$C_5H_{13}N$
- *N*,*N*-Dimethyl-2-propanamine [996-35-0]
  Isopropyldimethylamine
  Group-member nr.: 31-046/S1
- *N*-Ethyl-*N*-methylethanamine [616-39-7]
  N-Methyldiethylamine
  N,*N*-Diethylmethylamine
  Group-member nr.: 31-017
- 1-Pentanamine [110-58-7]

Pentylamine
n-Amylamine
Group-member nr.: 31-018

$C_5H_{13}NO$
• 2-(Ethylmethylamino)ethanol [2893-43-8]
N,*N*-Ethylmethylethanolamine
Group-member nr.: 62-041
• 2-(Propylamino)ethanol [16369-21-4]
Propylethanolamine
Group-member nr.: 62-144/S1

$C_5H_{13}NO_2$
• 2,2′-(Methylimino)bisethanol [105-59-9]
Methyldiethanolamine
2-[(2-Hydroxyethyl)methylamino]ethanol
Group-member nr.: 62-145/S1

$C_5H_{13}NSi$
• 1-(Trimethylsilyl)aziridine [2116-90-7]
Trimethylsilylethyleneimine
Group-member nr.: 71-061/S1

$C_5H_{14}N_2$
• *N*,*N*-Dimethyl-1,3-propanediamine [109-55-7]
N,*N*-Dimethylpropylenediamine
Group-member nr.: 31-019

C_6BrF_5
• Bromopentafluorobenzene [344-04-7]
Group-member nr.: 25-027

$C_6Br_2Cl_3F_9$
• 1,6-Dibromo-2,3,5-trichloro-1,1,2,3,4,4,5,6,6-nonafluorohexane [85131-86-8]
Group-member nr.: 25-028

C_6ClF_5
• Chloropentafluorobenzene [344-07-0]
Group-member nr.: 25-029

$C_6Cl_3F_3$
• 1,3,5-Trichloro-2,4,6-trifluorobenzene [319-88-0]
Group-member nr.: 25-030

C_6D_6
• Benzene-*d*6 [1076-43-3]
Hexadeuterobenzene
Group-member nr.: 14-002

C_6D_{12}
• Cyclohexane-*d*12 [1735-17-7]
Dodecadeuterocyclohexane
Group-member nr.: 12-006

$C_6F_5NO_2$
• Pentafluoronitrobenzene [880-78-4]
Group-member nr.: 64-012

C_6F_6
• Hexafluorobenzene [392-56-3]
Perfluorobenzene
Group-member nr.: 21-010/B+S1[E]

C_6F_{12}
• 1,1,1,2,3,4,5,5,5-Nonafluoro-4-(trifluoromethyl)-2-pentene [2070-70-4]
Perfluoro-4-methyl-2-pentene
Group-member nr.: 21-051/S1

C_6F_{14}
• Tetradecafluorohexane [355-42-0]
Perfluorohexane
Group-member nr.: 21-011

$C_6F_{15}N$
• 1,1,2,2,2-Pentafluoro-*N*,*N*-bis(pentafluoroethyl)ethanamine [359-70-6]
Group-member nr.: 64-013

C_6HCl_5
• Pentachlorobenzene [608-93-5]
Group-member nr.: 22-055/S1

C_6HF_5
• Pentafluorobenzene [363-72-4]
Group-member nr.: 21-012

C_6HF_5O
• Pentafluorophenol [771-61-9]
Group-member nr.: 61-034/B+S1

$C_6H_2F_4$
• 1,2,3,4-Tetrafluorobenzene [551-62-2]
Group-member nr.: 21-013
• 1,2,3,5-Tetrafluorobenzene [2367-82-0]
Group-member nr.: 21-014
• 1,2,4,5-Tetrafluorobenzene [327-54-8]
Group-member nr.: 21-015

$C_6H_2F_5N$
• 2,3,4,5,6-Pentafluorobenzenamine [771-60-8]
Pentafluoroaniline
Group-member nr.: 64-014

$C_6H_3Cl_3$
• 1,2,3-Trichlorobenzene [87-61-6]
Group-member nr.: 22-056/S1
• 1,2,4-Trichlorobenzene [120-82-1]
Group-member nr.: 22-035/B+S1
• 1,3,5-Trichlorobenzene [108-70-3]
Group-member nr.: 22-057/S1

$C_6H_3Cl_4N$
• 2-Chloro-6-(trichloromethyl)pyridine [1929-82-4]
Group-member nr.: 64-015

C_6H_4BrCl
• 1-Bromo-2-chlorobenzene [694-80-4]
o-Bromochlorobenzene
Group-member nr.: 25-031
• 1-Bromo-3-chlorobenzene [108-37-2]
m-Bromochlorobenzene
Group-member nr.: 25-032
• 1-Bromo-4-chlorobenzene [106-39-8]
p-Bromochlorobenzene
Group-member nr.: 25-033/B+S1

C_6H_4BrI
- 1-Bromo-2-iodobenzene [583-55-1]
  o-Bromoiodobenzene
  Group-member nr.: 25-034
- 1-Bromo-3-iodobenzene [591-18-4]
  m-Bromoiodobenzene
  Group-member nr.: 25-035

$C_6H_4BrNO_2$
- 1-Bromo-3-nitrobenzene [585-79-5]
  m-Bromonitrobenzene
  Group-member nr.: 64-016

$C_6H_4Br_2$
- 1,2-Dibromobenzene [583-53-9]
  o-Dibromobenzene
  Group-member nr.: 23-031
- 1,3-Dibromobenzene [108-36-1]
  m-Dibromobenzene
  Group-member nr.: 23-032
- 1,4-Dibromobenzene [106-37-6]
  p-Dibromobenzene
  Group-member nr.: 23-042/S1

$C_6H_4Br_2O$
- 2,4-Dibromophenol [615-58-7]
  Group-member nr.: 61-035

C_6H_4ClI
- 1-Chloro-4-iodobenzene [637-87-6]
  p-Chloroiodobenzene
  Group-member nr.: 25-049/S1

$C_6H_4ClNO_2$
- 1-Chloro-3-nitrobenzene [121-73-3]
  m-Chloronitrobenzene
  Group-member nr.: 64-017/B+S1
- 1-Chloro-4-nitrobenzene [100-00-5]
  p-Chloronitrobenzene
  Group-member nr.: 64-018/B+S1

$C_6H_4Cl_2$
- 1,2-Dichlorobenzene [95-50-1]
  o-Dichlorobenzene
  Group-member nr.: 22-036/B+S1
- 1,3-Dichlorobenzene [541-73-1]
  m-Dichlorobenzene
  Group-member nr.: 22-037/B+S1
- 1,4-Dichlorobenzene [106-46-7]
  p-Dichlorobenzene
  Group-member nr.: 22-038/B+S1

$C_6H_4F_2$
- 1,2-Difluorobenzene [367-11-3]
  o-Difluorobenzene
  Group-member nr.: 21-016/B+S1^E
- 1,3-Difluorobenzene [372-18-9]
  m-Difluorobenzene
  Group-member nr.: 21-017/B+S1^E
- 1,4-Difluorobenzene [540-36-3]
  p-Difluorobenzene
  Group-member nr.: 21-018/B+S1

$C_6H_4I_2$
- 1,2-Diiodobenzene [615-42-9]
  o-Diiodobenzene
  Group-member nr.: 24-007
- 1,3-Diiodobenzene [626-00-6]
  m-Diiodobenzene
  Group-member nr.: 24-008

$C_6H_4N_2O_4$
- 1,2-Dinitrobenzene [528-29-0]
  o-Dinitrobenzene
  Group-member nr.: 62-042
- 1,3-Dinitrobenzene [99-65-0]
  m-Dinitrobenzene
  Group-member nr.: 62-043
- 1,4-Dinitrobenzene [100-25-4]
  p-Dinitrobenzene
  Group-member nr.: 62-044

$C_6H_4O_2$
- 2,5-Cyclohexadiene-1,4-dione [106-51-4]
  p-Benzoquinone
  p-Quinone
  Group-member nr.: 43-015

C_6H_5Br
- Bromobenzene [108-86-1]
  Phenyl bromide
  Group-member nr.: 23-033/B+S1^E

C_6H_5BrO
- 4-Bromophenol [106-41-2]
  p-Bromophenol
  Group-member nr.: 61-036

C_6H_5Cl
- Chlorobenzene [108-90-7]
  Phenyl chloride
  Group-member nr.: 22-039/B+S1

C_6H_5ClO
- 2-Chlorophenol [95-57-8]
  o-Chlorophenol
  Group-member nr.: 61-037/B+S1
- 3-Chlorophenol [108-43-0]
  m-Chlorophenol
  Group-member nr.: 61-051/S1
- 4-Chlorophenol [106-48-9]
  p-Chlorophenol
  Group-member nr.: 61-052/S1

$C_6H_5Cl_3Si$
- Trichlorophenylsilane [98-13-5]
  Group-member nr.: 71-011

C_6H_5F
- Fluorobenzene [462-06-6]
  Group-member nr.: 21-019

C_6H_5FO
- 2-Fluorophenol [367-12-4]
  o-Fluorophenol

Group-member nr.: 61-053/S1
- 3-Fluorophenol [372-20-3]
  m-Fluorophenol
  Group-member nr.: 61-054/S1
- 4-Fluorophenol [371-41-5]
  p-Fluorophenol
  Group-member nr.: 61-038

C_6H_5I
- Iodobenzene [591-50-4]
  Group-member nr.: 24-009/B+S1

$C_6H_5NO_2$
- Nitrobenzene [98-95-3]
  Group-member nr.: 62-045/B+S1^E

$C_6H_5NO_3$
- 2-Nitrophenol [88-75-5]
  o-Nitrophenol
  Group-member nr.: 62-046/B+S1^E
- 3-Nitrophenol [554-84-7]
  m-Nitrophenol
  Group-member nr.: 62-047
- 4-Nitrophenol [100-02-7]
  p-Nitrophenol
  Group-member nr.: 62-048

C_6H_6
- Benzene [71-43-2]
  Group-member nr.: 14-003/B+S1

C_6H_6ClN
- 3-Chlorobenzenamine [108-42-9]
  3-Chlorophenylamine
  m-Chloroaniline
  Group-member nr.: 64-019
- 4-Chlorobenzenamine [106-47-8]
  4-Chlorophenylamine
  p-Chloroaniline
  Group-member nr.: 64-035/S1

C_6H_6FN
- 2-Fluorobenzenamine [348-54-9]
  o-Fluoroaniline
  Group-member nr.: 64-036/S1
- 4-Fluorobenzenamine [371-40-4]
  p-Fluoroaniline
  Group-member nr.: 64-020

$C_6H_6N_2O_2$
- 2-Nitrobenzenamine [88-74-4]
  o-Nitroaniline
  Group-member nr.: 62-049
- 3-Nitrobenzenamine [99-09-2]
  m-Nitroaniline
  Group-member nr.: 62-050
- 4-Nitrobenzenamine [100-01-6]
  p-Nitroaniline
  Group-member nr.: 62-051

C_6H_6O
- Phenol [108-95-2]
  Group-member nr.: 42-034

$C_6H_6O_2$
- 1,2-Benzenediol [120-80-9]
  1,2-Dihydroxybenzene
  Pyrocatechol
  Catechol
  Group-member nr.: 42-035
- 1,3-Benzenediol [108-46-3]
  1,3-Dihydroxybenzene
  Resorcinol
  Group-member nr.: 42-036
- 1,4-Benzenediol [123-31-9]
  1,4-Dihydroxybenzene
  Hydroquinone
  Group-member nr.: 42-037

C_6H_6S
- Benzenethiol [108-98-5]
  Thiophenol
  Phenyl mercaptan
  Group-member nr.: 52-014

C_6H_7N
- Benzenamine [62-53-3]
  Aniline
  Aminobenzene
  Phenylamine
  Group-member nr.: 31-020
- Bicyclo[2.1.0]pentane-1-carbonitrile [31357-71-8]
  1-Bicyclo[2.1.0]pentyl cyanide
  1-Cyanobicyclo[2.1.0]pentane
  Group-member nr.: 32-017
- 3-Methylenecyclobutanecarbonitrile [15760-35-7]
  3-Methylenecyclobutyl cyanide
  1-Cyano-3-methylenecyclobutane
  Group-member nr.: 32-018
- 2-Methylpyridine [109-06-8]
  α-Picoline
  Group-member nr.: 33-013/B+S1
- 3-Methylpyridine [108-99-6]
  β-Picoline
  Group-member nr.: 33-014/B+S1
- 4-Methylpyridine [108-89-4]
  γ-Picoline
  Group-member nr.: 33-015/B+S1

C_6H_8
- 1,3-Cyclohexadiene [592-57-4]
  Group-member nr.: 14-004
- 1,4-Cyclohexadiene [628-41-1]
  Group-member nr.: 14-005

$C_6H_8N_2$
- 1,3-Benzenediamine [108-45-2]
  1,3-Phenylenediamine
  Group-member nr.: 31-021
- Phenylhydrazine [100-63-0]
  Group-member nr.: 34-007

C_6H_8O
- 2-Cyclohexen-1-one [930-68-7]
  Group-member nr.: 43-065/S1
- 2,5-Dimethylfuran [625-86-5]
  Group-member nr.: 46-028/S1

$C_6H_8O_2$
- 1,4-Cyclohexanedione [637-88-7]
  Tetrahydroquinone
  Group-member nr.: 43-016
- Methyl bicyclo[1.1.0]butane-1-carboxylate [4935-01-7]
  Methyl ester bicyclo[1.1.0]butane-1-carboxylic acid
  Group-member nr.: 45-020

$C_6H_8O_4$
- Dimethyl (*Z*)-2-butenedioate [624-48-6]
  Dimethyl ester (*Z*)-2-butenedioic acid
  Dimethyl *cis*-2-butenedioate
  Dimethyl maleate
  Group-member nr.: 45-021
- 3,6-Dimethyl-1,4-dioxane-2,5-dione [95-96-5]
  Group-member nr.: 47-018
- (3*S*,6*S*)-3,6-Dimethyl-1,4-dioxane-2,5-dione [4511-42-6]
  l-Lactide
  Group-member nr.: 47-056/S1

C_6H_8S
- 2,5-Dimethylthiophene [638-02-8]
  Group-member nr.: 53-011

C_6H_9N
- Cyclopentanecarbonitrile [4254-02-8]
  Cyclopentyl cyanide
  Cyanocyclopentane
  Group-member nr.: 32-019
- 2,4-Dimethyl-1*H*-pyrrole [625-82-1]
  Group-member nr.: 33-016/B+S1
- 2,5-Dimethyl-1*H*-pyrrole [625-84-3]
  Group-member nr.: 33-017

C_6H_9NO
- 1-Ethenyl-2-pyrrolidinone [88-12-0]
  N-Vinylpyrrolidone
  Group-member nr.: 62-146/S1

$C_6H_9NO_2$
- Ethyl ester 2-cyanopropanoic acid [1572-99-2]
  Ethyl ester cyanomethylacetic acid
  Group-member nr.: 62-147/S1

C_6H_{10}
- Cyclohexene [110-83-8]
  1,2,3,4-Tetrahydrobenzene
  Group-member nr.: 14-006/B+S1^E
- 1,5-Hexadiene [592-42-7]
  Diallyl
  Group-member nr.: 13-025
- 1-Methylcyclopentene [693-89-0]
  Group-member nr.: 14-007
- 3-Methylcyclopentene [1120-62-3]
  Group-member nr.: 14-008

$C_6H_{10}O$
- Cyclohexanone [108-94-1]
  Pimelic ketone
  Ketohexamethylene
  Group-member nr.: 43-017/B+S1^E
- 4-Methyl-3-penten-2-one [141-79-7]
  Mesityl oxide
  Group-member nr.: 43-018/B+S1
- 7-Oxabicyclo[4.1.0]heptane [286-20-4]
  1,2-Epoxycyclohexane
  Cyclohexene oxide
  Group-member nr.: 46-017

$C_6H_{10}O_2$
- Ethyl cyclopropanecarboxylate [4606-07-9]
  Ethyl ester cyclopropanecarboxylic acid
  Group-member nr.: 45-022
- Methyl cyclobutanecarboxylate [765-85-5]
  Methyl ester cyclobutanecarboxylic acid
  Group-member nr.: 45-023
- 2-Oxepanone [502-44-3]
  ϵ-Caprolactone
  6-Hexanolide
  Group-member nr.: 47-019
- 2-Propenyl propanoate [2408-20-0]
  Allyl propionate
  Group-member nr.: 45-024

$C_6H_{10}O_3$
- Ethyl ester 3-oxobutanoic acid [141-97-9]
  Ethyl 3-oxobutanoate
  Ethyl acetoacetate
  Ethyl ester acetoacetic acid
  Group-member nr.: 47-020/B+S1

$C_6H_{10}O_4$
- Diethyl ethanedioate [95-92-1]
  Diethyl ester ethanedioic acid
  Diethyl oxalate
  Group-member nr.: 45-025
- Dimethyl ester methylpropanedioic acid [609-02-9]
  Dimethyl methylmalonate
  Group-member nr.: 45-133/S1
- 1,2-Ethanediol diacetate [111-55-7]
  1,2-Ethanediyl ester acetic acid
  Ethylene glycol diacetate
  Group-member nr.: 45-026/B+S1^E
- Hexanedioic acid [124-04-9]
  Adipic acid
  1,4-Butanedicarboxylic acid
  Group-member nr.: 44-013

$C_6H_{11}BF_4N_2$
- 1-Ethyl-3-methyl-1*H*-imidazolium tetrafluoroborate [143314-16-3]
  Group-member nr.: 72-017/S1

$C_6H_{11}Br$
- Bromocyclohexane [108-85-0]
  Cyclohexyl bromide

Group-member nr.: 23-043/S1

$C_6H_{11}Cl$
- Chlorocyclohexane [542-18-7]
  Cyclohexyl chloride
  Group-member nr.: 22-058/S1
- 1-Chloro-1-methylcyclopentane [6196-85-6]
  Group-member nr.: 22-059/S1

$C_6H_{11}N$
- Hexanenitrile [628-73-9]
  Capronitrile
  Amyl cyanide
  Group-member nr.: 32-020

$C_6H_{11}NO$
- Cyclohexanone oxime [100-64-1]
  Group-member nr.: 62-052
- Hexahydro-2*H*-azepin-2-one [105-60-2]
  ϵ-Caprolactam
  6-Hexanelactam
  6-Aminohexanoic lactam
  Group-member nr.: 62-053

$C_6H_{11}NO_2$
- 4,4-Dimethoxybutanenitrile [14618-78-1]
  β-Cyanopropionaldehyde dimethyl acetal
  Group-member nr.: 62-054
- Tetrahydro-5,5-dimethyl-2*H*-1,3-oxazin-2-one [54953-79-6]
  5,5-Dimethylperhydro-1,3-oxazin-2-one
  Group-member nr.: 62-148/S1

C_6H_{12}
- Cyclohexane [110-82-7]
  Hexamethylene
  Group-member nr.: 12-007/B+S1^E
- 2,3-Dimethyl-2-butene [563-79-1]
  Tetramethylethylene
  Group-member nr.: 13-026
- 3,3-Dimethyl-1-butene [558-37-2]
  tert-Butylethylene
  Neohexene
  Group-member nr.: 13-027
- 1-Hexene [592-41-6]
  Hexylene
  Group-member nr.: 13-028
- (*Z*)-2-Hexene [7688-21-3]
  cis-2-Hexene
  Group-member nr.: 13-029
- Methylcyclopentane [96-37-7]
  Group-member nr.: 12-008
- 4-Methyl-1-pentene [691-37-2]
  Group-member nr.: 13-040/S1

$C_6H_{12}BNO_3$
- 2,8,9-Trioxa-5-aza-1-borabicyclo[3.3.3]undecane [283-56-7]
  2,2′,2″-Nitrilotriethanol cyclic ester with boric acid (1:1)
  Triethanolamine borate
  Group-member nr.: 72-007

$C_6H_{12}Cl_2$
- 1,6-Dichlorohexane [2163-00-0]
  Hexamethylene chloride
  Group-member nr.: 22-040

$C_6H_{12}Cl_3O_4P$
- 2-Chloroethanol phosphate (3:1) [115-96-8]
  Tri(2-chloroethyl)phosphate
  Group-member nr.: 72-008

$C_6H_{12}N_2$
- 1,4-Diazobicyclo[2.2.2]octane [280-57-9]
  Triethylenediamine
  Group-member nr.: 33-018
- (1-Methylethylidene)hydrazone 2-propanone [627-70-3]
  Acetone azine
  Dimethyl ketazine
  Group-member nr.: 34-008

$C_6H_{12}O$
- Cyclohexanol [108-93-0]
  Cyclohexyl alcohol
  Group-member nr.: 42-038/B+S1
- 3,3-Dimethyl-2-butanone [75-97-8]
  tert-Butyl methyl ketone
  Pinacolone
  Group-member nr.: 43-019
- 1-(Ethenyloxy)butane [111-34-2]
  Butyl vinyl ether
  Butoxyethylene
  Group-member nr.: 41-013/B+S1
- 1-(Ethenyloxy)-2-methylpropane [109-53-5]
  Isobutyl vinyl ether
  Isobutoxyethylene
  Group-member nr.: 41-014
- Hexanal [66-25-1]
  Hexaldehyde
  Caproaldehyde
  Group-member nr.: 43-020
- 2-Hexanone [591-78-6]
  Butyl methyl ketone
  Group-member nr.: 43-021
- 3-Hexanone [589-38-8]
  Ethyl propyl ketone
  Group-member nr.: 43-022
- 1-Methylcyclopentanol [1462-03-9]
  Group-member nr.: 42-110/S1
- 4-Methyl-2-pentanone [108-10-1]
  Isobutyl methyl ketone
  Group-member nr.: 43-023

$C_6H_{12}O_2$
- Butyl acetate [123-86-4]
  Butyl ethanoate
  Group-member nr.: 45-027/B+S1^E
- 1,1-Dimethylethyl acetate [540-88-5]
  1,1-Dimethylethyl ethanoate
  tert-Butyl acetate

Group-member nr.: 45-028
- Ethyl butanoate [105-54-4]
  Ethyl butyrate
  Group-member nr.: 45-029
- Ethyl 2-methylpropanoate [97-62-1]
  Ethyl isobutyrate
  Group-member nr.: 45-030
- Hexanoic acid [142-62-1]
  Caproic acid
  Group-member nr.: 44-014
- 3-Methylbutyl formate [110-45-2]
  3-Methylbutyl methanoate
  Isoamyl formate
  Isopentyl formate
  Group-member nr.: 45-033
- Methyl 2,2-dimethylpropanoate [598-98-1]
  Methyl ester 2,2-dimethylpropanoic acid
  Methyl pivalate
  Methyl trimethylacetate
  Group-member nr.: 45-031
- Methyl pentanoate [624-24-8]
  Methyl valerate
  Group-member nr.: 45-032
- 2-Methylpropyl acetate [110-19-0]
  2-Methylpropyl ethanoate
  Isobutyl acetate
  Group-member nr.: 45-034
- Propyl propanoate [106-36-5]
  Propyl propionate
  Group-member nr.: 45-035/B+S1[E]
- Tetrahydro-2*H*-pyran-2-methanol [100-72-1]
  Group-member nr.: 47-021

$C_6H_{12}O_3$
- 2-Ethoxyethanol acetate [111-15-9]
  2-Ethoxyethyl acetate
  Cellosolve acetate
  Group-member nr.: 47-022/B+S1
- 2,4,6-Trimethyl-1,3,5-trioxane [123-63-7]
  Paraldehyde
  Group-member nr.: 46-018

$C_6H_{12}S$
- Cyclohexanethiol [1569-69-3]
  Cyclohexyl mercaptan
  Group-member nr.: 52-015
- Methylthiocyclopentane [7133-36-0]
  Cyclopentyl methyl sulfide
  Group-member nr.: 51-013

$C_6H_{12}Si$
- Trimethyl-1-propynylsilane [6224-91-5]
  1-Trimethylsilyl-1-propyne
  Group-member nr.: 71-062/S1

$C_6H_{13}Br$
- 1-Bromohexane [111-25-1]
  n-Hexyl bromide
  Group-member nr.: 23-034/B+S1
- 3-Bromohexane [3377-87-5]
  Group-member nr.: 23-035

$C_6H_{13}Cl$
- 1-Chlorohexane [544-10-5]
  Hexyl chloride
  Group-member nr.: 22-060/S1

$C_6H_{13}I$
- 1-Iodohexane [638-45-9]
  Hexyl iodide
  Group-member nr.: 24-015/S1

$C_6H_{13}N$
- Cyclohexanamine [108-91-8]
  Cyclohexylamine
  Group-member nr.: 31-022
- Hexahydro-1*H*-azepine [111-49-9]
  Perhydroazepine
  Hexamethylenimine
  Azacycloheptane
  Group-member nr.: 33-019
- 1-Methylpiperidine [626-67-5]
  N-Methylpiperidine
  Group-member nr.: 33-020
- 2-Methylpiperidine [109-05-7]
  2-Pipecoline
  α-Pipecoline
  Group-member nr.: 33-021
- 4-Methylpiperidine [626-58-4]
  4-Pipecoline
  γ-Pipecoline
  Group-member nr.: 33-022

$C_6H_{13}NO$
- *N*-Butylacetamide [1119-49-9]
  N-Butylethanamide
  Group-member nr.: 62-055
- *N*,*N*-Diethylacetamide [685-91-6]
  N,*N*-Diethylethanamide
  Group-member nr.: 62-056
- *N*-Methylpentanamide [6225-10-1]
  N-Methylvaleramide
  Group-member nr.: 62-057

$C_6H_{13}NO_2$
- Ethyl ester *N*,*N*-dimethylglycine [33229-89-9]
  Ethyl ester *N*,*N*-dimethylaminoacetic acid
  Group-member nr.: 62-149/S1
- Methyl ester *N*,*N*-dimethyl-*L*-alanine [42293-86-7]
  Methyl ester 2-dimethylaminopropionic acid
  Group-member nr.: 62-150/S1

C_6H_{14}
- 2,2-Dimethylbutane [75-83-2]
  Neohexane
  Group-member nr.: 11-011
- 2,3-Dimethylbutane [79-29-8]
  Diisopropyl
  Group-member nr.: 11-012
- Hexane [110-54-3]

Group-member nr.: 11-013/B+S1^{E}
- 2-Methylpentane [107-83-5]
  Dimethylpropylmethane
  Group-member nr.: 11-014
- 3-Methylpentane [96-14-0]
  Diethylmethylmethane
  Group-member nr.: 11-015

$C_6H_{14}N_2O$
- Dipropyldiazene 1-oxide [17697-55-1]
  Group-member nr.: 62-058

$C_6H_{14}O$
- 3,3-Dimethyl-1-butanol [624-95-3]
  Group-member nr.: 42-039
- 2-Ethoxy-2-methylpropane [637-92-3]
  tert-Butyl ethyl ether
  Group-member nr.: 41-015
- 2-Ethyl-1-butanol [97-95-0]
  2-Ethylbutyl alcohol
  Group-member nr.: 42-040
- 1-Hexanol [111-27-3]
  Hexyl alcohol
  Group-member nr.: 42-041/B+S1
- 2-Hexanol [626-93-7]
  Group-member nr.: 42-042
- 3-Hexanol [623-37-0]
  Ethyl propyl carbinol
  Group-member nr.: 42-043
- 2-Methoxy-2-methylbutane [994-05-8]
  Methyl *tert*-pentyl ether
  3,3-Dimethyl-2-oxapentane
  tert-Amyl methyl ether
  Group-member nr.: 41-016
- 2-Methyl-1-pentanol [105-30-6]
  Group-member nr.: 42-044
- 2-Methyl-2-pentanol [590-36-3]
  Group-member nr.: 42-045
- 3-Methyl-2-pentanol [565-60-6]
  Group-member nr.: 42-046
- 3-Methyl-3-pentanol [77-74-7]
  Group-member nr.: 42-047
- 4-Methyl-2-pentanol [108-11-2]
  Group-member nr.: 42-048
- 1,1′-Oxybispropane [111-43-3]
  Dipropyl ether
  Group-member nr.: 41-017/B+S1^{E}
- 2,2′-Oxybispropane [108-20-3]
  1,1′-Bis(methylethyl) ether
  Diisopropyl ether
  Group-member nr.: 41-018/B+S1^{E}

$C_6H_{14}O_2$
- 2-Butoxyethanol [111-76-2]
  3-Oxa-1-heptanol
  Ethylene glycol monobutyl ether
  Butyl cellosolve
  Group-member nr.: 47-023/B+S1^{E}
- 1,1-Diethoxyethane [105-57-7]
  Acetaldehyde diethyl acetal
  Acetal
  Group-member nr.: 41-019
- 1,2-Diethoxyethane [629-14-1]
  3,6-Dioxaoctane
  Ethylene glycol diethyl ether
  Diethyl cellosolve
  Group-member nr.: 41-020
- 1,6-Hexanediol [629-11-8]
  Group-member nr.: 42-111/S1
- 1-Methoxy-2-propoxyethane [17081-22-0]
  2,5-Dioxaoctane
  Ethylene glycol methyl ether propyl ether
  Group-member nr.: 41-021
- 2-(2-Methylpropoxy)ethanol [4439-24-1]
  2-Isobutoxyethanol
  Group-member nr.: 47-057/S1

$C_6H_{14}O_3$
- 2-(2-Ethoxyethoxy)ethanol [111-90-0]
  Diethylene glycol monoethyl ether
  Group-member nr.: 47-024/B+S1
- 2-Ethyl-2-(hydroxymethyl)-1,3-propanediol [77-99-6]
  1,1,1-Tris(hydroxymethyl)propane
  Trimethylolpropane
  Group-member nr.: 42-049
- 2-(2-Hydroxypropoxy)-1-propanol [106-62-7]
  Di(propylene glycol)
  Group-member nr.: 47-058/S1
- 1,1′-Oxybis(2-methoxyethane) [111-96-6]
  2,5,8-Trioxanonane
  Diethylene glycol dimethyl ether
  Diglyme
  Group-member nr.: 41-022/B+S1^{E}

$C_6H_{14}O_4$
- 2,2′-[1,2-Ethanediylbis(oxy)]bisethanol [112-27-6]
  1,8-Dihydroxy-3,6-dioxaoctane
  Triethylene glycol
  Group-member nr.: 47-025/B+S1^{E}

$C_6H_{14}O_6$
- *D*-Mannitol [69-65-8]
  Group-member nr.: 42-050

$C_6H_{14}S$
- 1-Hexanethiol [111-31-9]
  1-Hexyl mercaptan
  Group-member nr.: 52-016/B+S1^{E}
- 2-(Methylthio)pentane [13286-91-4]
  3-Methyl-2-thiahexane
  Methyl 1-methylbutyl sulfide
  Group-member nr.: 51-014
- 1,1′-Thiobispropane [111-47-7]
  Dipropyl sulfide
  Group-member nr.: 51-015
- 2,2′-Thiobispropane [625-80-9]
  Bis(1-methylethyl) sulfide
  Diisopropyl sulfide
  Group-member nr.: 51-016

$C_6H_{14}S_2$
- Dipropyl disulfide [629-19-6]
  4,5-Dithiaoctane
  Group-member nr.: 51-017

$C_6H_{15}Al$
- Triethylaluminium [97-93-8]
  Group-member nr.: 73-018

$C_6H_{15}As$
- Triethylarsine [617-75-4]
  Group-member nr.: 73-019

$C_6H_{15}B$
- Triethylborane [97-94-9]
  Group-member nr.: 72-009

$C_6H_{15}Bi$
- Triethylbismuthine [617-77-6]
  Group-member nr.: 73-020

$C_6H_{15}ClSi$
- Chlorotriethylsilane [994-30-9]
  Group-member nr.: 71-012

$C_6H_{15}Ga$
- Triethylgallium [1115-99-7]
  Group-member nr.: 73-021

$C_6H_{15}In$
- Triethylindium [923-34-2]
  Group-member nr.: 73-022

$C_6H_{15}N$
- *N*,*N*-Diethylethanamine [121-44-8]
  Triethylamine
  Group-member nr.: 31-023/B+S1^E
- 1-Hexanamine [111-26-2]
  Hexylamine
  Group-member nr.: 31-024/B+S1^E
- *N*-(1-Methylethyl)-2-propanamine [108-18-9]
  Diisopropylamine
  Group-member nr.: 31-047/S1
- *N*-Propyl-1-propanamine [142-84-7]
  Dipropylamine
  Group-member nr.: 31-025/B+S1

$C_6H_{15}NO$
- 2-(Diethylamino)ethanol [100-37-8]
  Diethylethanolamine
  Group-member nr.: 62-151/S1

$C_6H_{15}NO_2$
- 2,2′-(Ethylimino)bisethanol [139-87-7]
  Ethyldiethanolamine
  2-[Ethyl(2-hydroxyethyl)amino]ethanol
  Group-member nr.: 62-152/S1
- 1,1′-Iminobis-2-propanol [110-97-4]
  Di-2-propanolamine
  Bis(2-hydroxypropyl)amine
  1,1′-Azanediylbis(propan-2-ol)
  Group-member nr.: 62-153/S1

$C_6H_{15}NO_3$
- 2,2′,2″-Nitrilotrisethanol [102-71-6]
  Tri(2-hydroxyethyl)amine
  Triethanolamine
  Group-member nr.: 62-059/B+S1

$C_6H_{15}N_2O_2$
- 2,2′-(1,2-Ethanediyldiimino)bisethanol [4439-20-7]
  2,2′-(Ethylenediimino)diethanol
  N,*N*′-Bis(2-hydroxyethyl)ethylenediamine
  Group-member nr.: 62-154/S1

$C_6H_{15}N_3$
- 1-Piperazineethanamine [140-31-8]
  1-(2-Aminoethyl)piperazine
  Group-member nr.: 33-023

$C_6H_{15}P$
- Triethylphosphine [554-70-1]
  Group-member nr.: 72-018/S1

$C_6H_{15}Sb$
- Triethylstibine [617-85-6]
  Triethylantimony
  Group-member nr.: 73-023

$C_6H_{16}Si_2$
- 1,1,3,3-Tetramethyl-1,3-disilacyclobutane [1627-98-1]
  Group-member nr.: 71-013

$C_6H_{18}BN$
- Triethylamineborane [1722-26-5]
  N,*N*-Dimethylethanamine compd. with borane (1:1)
  Group-member nr.: 72-010

$C_6H_{18}N_3OP$
- Hexamethyl phosphoric triamide [680-31-9]
  Hexamethylphosphoramide
  Group-member nr.: 72-011/B+S1

$C_6H_{18}N_4$
- *N*,*N*′-Bis(2-aminoethyl)-1,2-ethanediamine [112-24-3]
  Triethylenetetramine
  Group-member nr.: 31-026

$C_6H_{18}OSi_2$
- Hexamethyldisiloxane [107-46-0]
  Group-member nr.: 71-014

$C_6H_{18}O_3Si_3$
- Hexamethylcyclotrisiloxane [541-05-9]
  Group-member nr.: 71-015

$C_6H_{18}Si_2$
- Hexamethyldisilane [1450-14-2]
  Group-member nr.: 71-016

$C_6H_{21}N_3Si_3$
- 2,2,4,4,6,6-Hexamethylcyclotrisilazane [1009-93-4]
  Dimethylaminosilane trimer
  Group-member nr.: 71-017

C_7F_8
- Pentafluoro(trifluoromethyl)benzene [434-64-0]
  Octafluorotoluene

Perfluorotoluene
Group-member nr.: 21-020

C_7F_{14}
• (Trifluoromethyl)undecafluorocyclohexane [355-02-2]
Perfluoromethylcyclohexane
Group-member nr.: 21-021

C_7F_{16}
• Hexadecafluoroheptane [335-57-9]
Perfluoroheptane
Group-member nr.: 21-022/B+S1

$C_7H_3F_5$
• Pentafluoromethylbenzene [771-56-2]
2,3,4,5,6-Pentafluorotoluene
Group-member nr.: 21-023

C_7H_4ClNO
• 1-Chloro-3-isocyanatobenzene [2909-38-8]
m-Chlorophenylisocyanate
Group-member nr.: 64-021

$C_7H_4F_3NO_2$
• 1-Nitro-3-(trifluoromethyl)benzene [98-46-4]
m-Trifluoromethylnitrobenzene
Group-member nr.: 64-022

C_7H_5ClO
• Benzoyl chloride [98-88-4]
Group-member nr.: 61-039

$C_7H_5ClO_2$
• 2-Chlorobenzoic acid [118-91-2]
o-Chlorobenzoic acid
Group-member nr.: 61-040
• 3-Chlorobenzoic acid [535-80-8]
m-Chlorobenzoic acid
Group-member nr.: 61-041
• 4-Chlorobenzoic acid [74-11-3]
p-Chlorobenzoic acid
Group-member nr.: 61-042

$C_7H_5F_3$
• (Trifluoromethyl)benzene [98-08-8]
α,α,α-Trifluorotoluene
Group-member nr.: 21-024

$C_7H_5F_4NO_2$
• 2,2,3,3-Tetrafluoropropyl ester 2-cyano-2-propenic acid [27827-91-4]
1,1,2,2-Tetrafluoropro-3-yl 2-cyanoacrylate
1,1,3-Trihydrotetrafluoropropyl α-cyanoacrylate
Group-member nr.: 64-037/S1

C_7H_5N
• Benzonitrile [100-47-0]
Phenyl cyanide
Group-member nr.: 32-021/B+S1^E

C_7H_5NO
• Benzoxazole [273-53-0]
Group-member nr.: 62-060
• Isocyanatobenzene [103-71-9]
Phenyl isocyanate
Group-member nr.: 62-155/S1

$C_7H_5NO_4$
• 2-Nitrobenzoic acid [552-16-9]
o-Nitrobenzoic acid
o-Nitrodracylic acid
Group-member nr.: 62-061
• 3-Nitrobenzoic acid [121-92-6]
m-Nitrobenzoic acid
m-Nitrodracylic acid
Group-member nr.: 62-062
• 4-Nitrobenzoic acid [62-23-7]
p-Nitrobenzoic acid
p-Nitrodracylic acid
Group-member nr.: 62-063

C_7H_5NS
• Benzothiazole [95-16-9]
Group-member nr.: 64-023
• Isothiocyanatobenzene [103-72-0]
Phenyl ester isothiocyanic acid
Group-member nr.: 64-024

$C_7H_5N_3O_6$
• 2-Methyl-1,3,5-trinitrobenzene [118-96-7]
2,4,6-Trinitrotoluene
Tritol
TNT
Group-member nr.: 62-064

$C_7H_5N_5O_8$
• *N*-Methyl-*N*,2,4,6-tetranitrobenzeneamine [479-45-8]
Trinitrophenylmethylnitroamine
Tetryl
Group-member nr.: 62-065

$C_7H_6F_8O_3$
• Bis(2,2,3,3-tetrafluoropropyl) ester carbonic acid [1422-70-4]
Bis(2,2,3,3-tetrafluoropropyl) carbonate
Group-member nr.: 61-043

$C_7H_6N_2O_4$
• 2-Methyl-1,3-dinitrobenzene [606-20-2]
2,6-Dinitrotoluene
Group-member nr.: 62-066

C_7H_6O
• Benzaldehyde [100-52-7]
Benzoic aldehyde
Group-member nr.: 43-024

$C_7H_6O_2$
• Benzoic acid [65-85-0]
Benzenecarboxylic acid
Carboxybenzene
Phenylformic acid
Group-member nr.: 44-015
• 2-Hydroxybenzaldehyde [90-02-8]
Salicyl aldehyde
Group-member nr.: 47-026

$C_7H_6O_3$
- 2-Hydroxybenzoic acid [69-72-7]
  Salicylic acid
  Group-member nr.: 47-027

C_7H_7Cl
- (Chloromethyl)benzene [100-44-7]
  Benzyl chloride
  Group-member nr.: 22-041
- 1-Chloro-2-methylbenzene [95-49-8]
  2-Chlorotoluene
  o-Chlorotoluene
  o-Tolyl chloride
  Group-member nr.: 22-042

C_7H_7F
- 1-Fluoro-2-methylbenzene [95-52-3]
  2-Fluorotoluene
  o-Tolyl fluoride
  Group-member nr.: 21-025
- 1-Fluoro-3-methylbenzene [352-70-5]
  3-Fluorotoluene
  m-Tolyl fluoride
  Group-member nr.: 21-026
- 1-Fluoro-4-methylbenzene [352-32-9]
  4-Fluorotoluene
  p-Tolyl fluoride
  Group-member nr.: 21-027

C_7H_7NO
- Benzamide [55-21-0]
  Group-member nr.: 62-067

$C_7H_7NO_2$
- 1-Methyl-3-nitrobenzene [99-08-1]
  m-Nitrotoluene
  Group-member nr.: 62-068
- 1-Methyl-4-nitrobenzene [99-99-0]
  p-Nitrotoluene
  Group-member nr.: 62-069
- 2-Propenyl ester 2-cyano-2-propenoic acid [7324-02-9]
  Allyl α-cyanoacrylate
  Group-member nr.: 62-156/S1

$C_7H_7NO_3$
- 1-Methoxy-2-nitrobenzene [91-23-6]
  o-Nitroanisole
  Group-member nr.: 62-070
- 1-Methoxy-3-nitrobenzene [555-03-3]
  m-Nitroanisole
  Group-member nr.: 62-071
- 1-Methoxy-4-nitrobenzene [100-17-4]
  p-Nitroanisole
  Group-member nr.: 62-072

C_7H_8
- Bicyclo[2.2.1]hepta-2,5-diene [121-46-0]
  2,5-Norbornadiene
  Group-member nr.: 14-009/B+S1
- 1,3,5-Cycloheptatriene [544-25-2]
  Group-member nr.: 14-010
- Methylbenzene [108-88-3]
  Toluene
  Phenyl methane
  Group-member nr.: 14-011/B+S1
- Tetracyclo[3.2.0.0^{2,7}.0^{4,6}]heptane [278-06-8]
  Quadricyclane
  Group-member nr.: 12-009/B+S1

$C_7H_8Cl_2Si$
- Dichloromethylphenylsilane [149-74-6]
  Group-member nr.: 71-018

C_7H_8O
- Benzenemethanol [100-51-6]
  Benzyl alcohol
  Group-member nr.: 42-051
- Methoxybenzene [100-66-3]
  Methyl phenyl ether
  Anisole
  Group-member nr.: 41-023
- 2-Methylphenol [95-48-7]
  o-Hydroxytoluene
  o-Cresol
  Group-member nr.: 42-052
- 3-Methylphenol [108-39-4]
  m-Hydroxytoluene
  m-Cresol
  Group-member nr.: 42-053
- 4-Methylphenol [106-44-5]
  p-Hydroxytoluene
  p-Cresol
  Group-member nr.: 42-054

$C_7H_8O_2$
- 2,6-Dimethyl-4*H*-pyran-4-one [1004-36-0]
  2,6-Dimethyl-γ-pyrone
  Group-member nr.: 47-028

C_7H_8S
- Methylthiobenzene [100-68-5]
  Methyl phenyl sulfide
  Group-member nr.: 51-018

$C_7H_9Cl_3OS$
- *O*-Butyl ester 2,3,3-trichloro-2-propenethioic acid [79886-21-8]
  O-Butyl ester trichlorothioacrylic acid
  n-Butyl ester trichlorothioacrylate
  Group-member nr.: 64-038/S1

C_7H_9N
- Benzenemethanamine [100-46-9]
  Benzylamine
  Phenylmethylamine
  Aminotoluene
  Group-member nr.: 31-027
- Bicyclo[3.1.0]hexane-1-carbonitrile [31357-72-9]
  1-Bicyclo[3.1.0]hexyl cyanide
  1-Cyanobicyclo[3.1.0]hexane

Group-member nr.: 32-022
- 2,3-Dimethylpyridine [583-61-9]
  2,3-Lutidine
  Group-member nr.: 33-024/B+S1
- 2,4-Dimethylpyridine [108-47-4]
  2,4-Lutidine
  Group-member nr.: 33-025/B+S1
- 2,5-Dimethylpyridine [589-93-5]
  2,5-Lutidine
  Group-member nr.: 33-026/B+S1
- 2,6-Dimethylpyridine [108-48-5]
  2,6-Lutidine
  Group-member nr.: 33-027/B+S1
- 3,4-Dimethylpyridine [583-58-4]
  3,4-Lutidine
  Group-member nr.: 33-028/B+S1
- 3,5-Dimethylpyridine [591-22-0]
  3,5-Lutidine
  Group-member nr.: 33-029/B+S1
- *N*-Methylbenzenamine [100-61-8]
  N-Methylaniline
  Methylphenylamine
  Group-member nr.: 31-028
- 2-Methylbenzenamine [95-53-4]
  2-Methylaniline
  o-Toluidine
  Group-member nr.: 31-029/B+S1
- 3-Methylbenzenamine [108-44-1]
  3-Methylaniline
  m-Toluidine
  Group-member nr.: 31-030/B+S1
- 4-Methylbenzenamine [106-49-0]
  4-Methylaniline
  p-Toluidine
  Group-member nr.: 31-031/B+S1

C_7H_{10}
- Bicyclo[2.2.1]hept-2-ene [498-66-8]
  Norbornene
  Norbornylene
  Group-member nr.: 14-099/S1

$C_7H_{11}N$
- Cyclohexanecarbonitrile [766-05-2]
  Cyclohexyl cyanide
  Cyanocyclohexane
  Group-member nr.: 32-023
- Isocyanocyclohexane [931-53-3]
  Group-member nr.: 32-027/S1

C_7H_{12}
- Bicyclo[4.1.0]heptane [286-08-8]
  Norcarane
  Group-member nr.: 12-010
- (*Z*)-Cycloheptene [45510-00-7]
  cis-Cycloheptene
  Group-member nr.: 14-012
- 1-Ethylcyclopentene [2146-38-5]
  Group-member nr.: 14-013
- Ethylidenecyclopentane [2146-37-4]
  Group-member nr.: 12-011
- 4-Methylcyclohexene [591-47-9]
  Group-member nr.: 14-014
- Methylenecyclohexane [1192-37-6]
  Group-member nr.: 12-012

$C_7H_{12}O$
- Cycloheptanone [502-42-1]
  Suberone
  Group-member nr.: 43-025
- 2-Methylcyclohexanone [583-60-8]
  o-Methylcyclohexanone
  Group-member nr.: 43-026
- 3-Methylcyclohexanone [591-24-2]
  m-Methylcyclohexanone
  Group-member nr.: 43-027
- 4-Methylcyclohexanone [589-92-4]
  p-Methylcyclohexanone
  Group-member nr.: 43-028

$C_7H_{12}O_2$
- Butyl 2-propenoate [141-32-2]
  Butyl ester 2-propenoic acid
  Butyl acrylate
  Group-member nr.: 45-036/B+S1
- 2-Propenyl butanoate [2051-78-7]
  Allyl butyrate
  Group-member nr.: 45-037
- 2-Propenyl 2-methylpropanoate [15727-77-2]
  2-Propenyl ester 2-methylpropanoic acid
  Allyl isobutyrate
  Group-member nr.: 45-038

$C_7H_{12}O_4$
- Diethyl propanedioate [105-53-3]
  Diethyl ester propanedioic acid
  Diethyl malonate
  Group-member nr.: 45-039/B+S1
- Dimethyl ester dimethylpropanedioic acid [6065-54-9]
  Dimethyl dimethylmalonate
  Group-member nr.: 45-134/S1

$C_7H_{13}Cl$
- 1-Chloro-1-methylcyclohexane [931-78-2]
  Group-member nr.: 22-061/S1

$C_7H_{13}NO$
- Hexahydro-2(1*H*)-azocinone [673-66-5]
  ω-Enantholactam
  Group-member nr.: 62-073
- 2-Methoxy-3,3-dimethylbutanenitrile [162047-91-8]
  Group-member nr.: 62-157/S1
- 2-Methoxy-2-methylpentanenitrile [162047-90-7]
  Group-member nr.: 62-158/S1

C_7H_{14}
- Cycloheptane [291-64-5]
  Group-member nr.: 12-013
- 1,1-Dimethylcyclopentane [1638-26-2]

Group-member nr.: 12-014
- *cis*-1,2-Dimethylcyclopentane [1192-18-3]
  Group-member nr.: 12-015
- *trans*-1,2-Dimethylcyclopentane [822-50-4]
  Group-member nr.: 12-016
- *trans*-1,3-Dimethylcyclopentane [1759-58-6]
  Group-member nr.: 12-017
- Ethylcyclopentane [1640-89-7]
  Group-member nr.: 12-018
- 1-Heptene [592-76-7]
  1-Heptylene
  Group-member nr.: 13-030/B+S1
- Methylcyclohexane [108-87-2]
  Hexahydrotoluene
  Group-member nr.: 12-019/B+S1

$C_7H_{14}ClNO$
- Dipropylcarbamic chloride [27086-19-7]
  N,*N*-Dipropylcarbamoyl chloride
  Group-member nr.: 64-025

$C_7H_{14}O$
- Cycloheptanol [502-41-0]
  Group-member nr.: 42-055
- 3,4-Dimethylpentanal [19353-21-0]
  3,4-Dimethylvaleraldehyde
  Group-member nr.: 43-029
- 2,4-Dimethyl-3-pentanone [565-80-0]
  Diisopropyl ketone
  Group-member nr.: 43-030
- Heptanal [111-71-7]
  Heptyl aldehyde
  Enanthaldehyde
  Group-member nr.: 43-031
- 2-Heptanone [110-43-0]
  Methyl pentyl ketone
  Group-member nr.: 43-032
- 4-Heptanone [123-19-3]
  Dipropyl ketone
  Group-member nr.: 43-033
- 1-Methylcyclohexanol [590-67-0]
  Group-member nr.: 42-056/B+S1
- 2-Methylcyclohexanol [583-59-5]
  o-Methylcyclohexanol (unspecified stereoisomer and chirality)
  Group-member nr.: 42-057
- *cis*-2-Methylcyclohexanol [7443-70-1]
  Group-member nr.: 42-058
- *trans*-2-Methylcyclohexanol [7443-52-9]
  Group-member nr.: 42-059
- 3-Methylcyclohexanol [591-23-1]
  m-Methylcyclohexanol (unspecified stereoisomer and chirality)
  Group-member nr.: 42-060
- 4-Methylcyclohexanol [589-91-3]
  p-Methylcyclohexanol (unspecified stereoisomer)
  Group-member nr.: 42-061
- 3-Methylhexanal [19269-28-4]
  Group-member nr.: 43-034
- 2-Methyl-3-hexanone [7379-12-6]
  Group-member nr.: 43-035

$C_7H_{14}O_2$
- Ethyl 2,2-dimethylpropanoate [3938-95-2]
  Ethyl ester 2,2-dimethylpropanoic acid
  Ethyl pivalate
  Group-member nr.: 45-040/B+S1
- Ethyl ester 2-methylbutanoic acid [7452-79-1]
  Ethyl 2-methylbutyrate
  Group-member nr.: 45-135/S1
- Ethyl 3-methylbutanoate [108-64-5]
  Ethyl isovalerate
  Group-member nr.: 45-041
- Ethyl pentanoate [539-82-2]
  Ethyl valerate
  Group-member nr.: 45-042
- Heptanoic acid [111-14-8]
  Enanthic acid
  Group-member nr.: 44-016
- 3-Methylbutyl acetate [123-92-2]
  3-Methylbutyl ethanoate
  Isoamyl acetate
  Isopentyl acetate
  Group-member nr.: 45-043
- 2-Methylpropyl propanoate [540-42-1]
  Isobutyl propionate
  Group-member nr.: 45-044
- Pentyl acetate [628-63-7]
  Pentyl ethanoate
  Amyl acetate
  Group-member nr.: 45-045/B+S1
- Propyl butanoate [105-66-8]
  Propyl butyrate
  Group-member nr.: 45-046/B+S1
- Propyl 2-methylpropanoate [644-49-5]
  Propyl isobutyrate
  Group-member nr.: 45-047

$C_7H_{14}O_3$
- 2-Hydroxyethyl ester 2,2-dimethylpropanoic acid [20267-19-0]
  2-Hydroxyethyl pivalate
  Group-member nr.: 47-059/S1

$C_7H_{15}Br$
- 1-Bromoheptane [629-04-9]
  n-Heptyl bromide
  Group-member nr.: 23-036/B+S1

$C_7H_{15}Cl$
- 1-Chloroheptane [629-06-1]
  Heptyl chloride
  Group-member nr.: 22-062/S1
- 3-Chloroheptane [999-52-0]
  Group-member nr.: 22-043

$C_7H_{15}I$
- 1-Iodoheptane [4282-40-0]

Heptyl iodide
Group-member nr.: 24-016/S1

$C_7H_{15}N$
- Octahydroazocine [1121-92-2]
  Perhydroazocine
  Heptamethylenimine
  Group-member nr.: 33-030

$C_7H_{15}NO$
- 2-Piperidineethanol [1484-84-0]
  2-Piperidin-2-ylethanol
  Group-member nr.: 62-159/S1

$C_7H_{15}NO_2$
- Methyl ester *N*,*N*,2-trimethylalanine [140653-59-4]
  Methyl ester 2-dimethylamino-2-methylpropanoic acid
  Group-member nr.: 62-160/S1

C_7H_{16}
- 2,2-Dimethylpentane [590-35-2]
  Group-member nr.: 11-016
- 2,3-Dimethylpentane [565-59-3]
  Group-member nr.: 11-017
- 2,4-Dimethylpentane [108-08-7]
  Group-member nr.: 11-018
- 3,3-Dimethylpentane [562-49-2]
  Group-member nr.: 11-019
- 3-Ethylpentane [617-78-7]
  Triethylmethane
  Group-member nr.: 11-020
- Heptane [142-82-5]
  Group-member nr.: 11-021
- 2-Methylhexane [591-76-4]
  Isoheptane
  Ethylisobutylmethane
  Group-member nr.: 11-022
- 3-Methylhexane [589-34-4]
  Group-member nr.: 11-023
- 2,2,3-Trimethylbutane [464-06-2]
  Isopropyltrimethylmethane
  Triptane
  Group-member nr.: 11-024

$C_7H_{16}O$
- 2-Ethoxy-2-methylbutane [919-94-8]
  Ethyl *tert*-pentyl ether
  4,4-Dimethyl-3-oxahexane
  tert-Amyl ethyl ether
  Group-member nr.: 41-024
- 3-Ethyl-3-pentanol [597-49-9]
  Group-member nr.: 42-062
- 1-Heptanol [111-70-6]
  Heptyl alcohol
  Group-member nr.: 42-063/B+S1
- 2-Heptanol [543-49-7]
  Group-member nr.: 42-064
- 4-Heptanol [589-55-9]
  Dipropyl carbinol
  Group-member nr.: 42-065

$C_7H_{16}O_2$
- 1-Butoxy-2-methoxyethane [13343-98-1]
  2,5-Dioxanonane
  Ethylene glycol butyl ether methyl ether
  Group-member nr.: 41-025
- 1,3-Diethoxypropane [3459-83-4]
  3,7-Dioxanonane
  Propylene glycol diethyl ether
  Group-member nr.: 41-026
- 1,5-Dimethoxypentane [111-89-7]
  2,8-Dioxanonane
  Pentylene glycol dimethyl ether
  Group-member nr.: 41-027
- 1-Ethoxy-4-methoxybutane [36865-47-1]
  2,7-Dioxanonane
  Butylene glycol ethyl ether methyl ether
  Group-member nr.: 41-028
- 1-Ethoxy-2-propoxyethane [18854-31-4]
  3,6-Dioxanonane
  Ethylene glycol ethyl ether propyl ether
  Group-member nr.: 41-029
- 1-Methoxy-3-propoxypropane [89851-49-0]
  2,6-Dioxanonane
  Propylene glycol methyl ether propyl ether
  Group-member nr.: 41-030

$C_7H_{16}O_3$
- 1,1′,1″-[Methylidynetris(oxy)]trisethane [122-51-0]
  Triethoxymethane
  Triethyl ester orthoformic acid
  Triethyl orthoformate
  Group-member nr.: 41-031
- 2-(2-Propoxyethoxy)ethanol [6881-94-3]
  Diethylene glycol monopropyl ether
  Group-member nr.: 47-060/S1

$C_7H_{16}S$
- 1-Heptanethiol [1639-09-4]
  1-Heptyl mercaptan
  Group-member nr.: 52-017/B+S1^E
- 2-(Methylthio)hexane [76858-84-9]
  3-Methyl-2-thiaheptane
  Methyl 1-methylpentyl sulfide
  Group-member nr.: 51-019

$C_7H_{17}NSi$
- 1-[2-(Trimethylsilyl)ethyl]aziridine [18387-12-7]
  N-[(*β*-Trimethylsilyl)ethyl]ethylenimine
  Group-member nr.: 71-043/S1

$C_7H_{20}Si_2$
- Methylenebis[trimethylsilane] [2117-28-4]
  2,2,4,4-Tetramethyl-2,4-disilapentane
  Hexamethyldisilamethane
  Bis(trimethylsilyl)methane
  Group-member nr.: 71-019

C_8BrF_{17}
- 1-Bromo-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluorooctane [423-55-2]

1-Bromoperfluorooctane
Group-member nr.: 25-050/S1

C_8D_8
• Ethenyl-d_3-benzene-d_5 [19361-62-7]
Styrene-d_8
Group-member nr.: 14-100/S1

$C_8D_{14}O_2$
• Butyl-d_9 ester 2-(methyl-d_3)-2-propenoic-3,3-d_2 acid [158612-79-4]
Perdeuterobutyl methacrylate
Group-member nr.: 45-136/S1

C_8F_{16}
• Decafluorobis(trifluoromethyl)cyclohexane [26637-68-3]
Perfluorodimethylcyclohexane
Hexadecafluorodimethylcyclohexane (unspecified isomer)
Group-member nr.: 21-028

$C_8F_{16}O$
• 2,2,3,3,4,5,5-Heptafluorotetrahydro-4-(nonafluorobutyl)furan [646-85-5]
Perfluoro-3-butyltetrahydrofuran
Group-member nr.: 61-044

C_8F_{18}
• Octadecafluorooctane [307-34-6]
Perfluorooctane
Group-member nr.: 21-029

$C_8F_{18}O_2$
• 1-[1-[Difluoro(pentafluoroethoxy)methyl]-1,2,2,2-tetrafluoroethoxy]-1,1,2,2,3,3,3-heptafluoropropane [66804-94-2]
5-Trifluoromethylperfluoro-3,6-dioxanonane
Group-member nr.: 61-055/S1

$C_8H_4Cl_2O_2$
• 1,2-Benzenedicarbonyl dichloride [88-95-9]
Phthaloyl chloride
Phthaloyl dichloride
Group-member nr.: 61-045

$C_8H_4N_2$
• 1,2-Benzenedicarbonitrile [91-15-6]
1,2-Dicyanobenzene
Phthalonitrile
Group-member nr.: 32-024

C_8H_6
• Ethynylbenzene [536-74-3]
Phenylacetylene
Group-member nr.: 14-015

C_8H_6O
• Benzofuran [271-89-6]
Benzo[*b*]furan
Cumaron
Group-member nr.: 46-019

$C_8H_6O_3$
• α-Oxobenzeneacetic acid [611-73-4]
Benzoyl formic acid
Group-member nr.: 47-061/S1

C_8H_6S
• Benzo[*b*]thiophene [95-15-8]
Group-member nr.: 53-012

C_8H_7N
• Benzeneacetonitrile [140-29-4]
Phenylacetonitrile
Benzylcyanide
Group-member nr.: 32-028/S1

$C_8H_7N_5O_8$
• *N*-Ethyl-*N*,2,4,6-tetranitrobenzeneamine [6052-13-7]
Trinitrophenylethylnitroamine
Ethyltetryl
Group-member nr.: 62-074
• 3-Methyl-2,4,6-trinitro-*N*-(nitromethyl)benzenamine [43072-20-4]
2,4,6-Trinitro-*N*-(methylnitro)-*m*-toluidine
Methyltetryl
Group-member nr.: 62-075

C_8H_8
• 1,3,5,7-Cyclooctatetraene [629-20-9]
Group-member nr.: 14-016
• Ethenylbenzene [100-42-5]
Vinylbenzene
Styrene
Group-member nr.: 14-017

C_8H_8O
• 2,3-Dihydrobenzofuran [496-16-2]
Coumaran
Group-member nr.: 46-020
• 2,5-Dihydrobenzo-3,4-furan [496-14-0]
Phthalan
o-Xylylene oxide
Group-member nr.: 46-029/S1
• 1-Phenylethanone [98-86-2]
Methyl phenyl ketone
Acetophenone
Acetyl benzene
Hypnone
Group-member nr.: 43-036/B+S1

$C_8H_8O_2$
• Benzeneacetic acid [103-82-2]
Phenylacetic acid
Group-member nr.: 44-038/S1
• Methyl benzoate [93-58-3]
Methyl ester benzoic acid
Group-member nr.: 45-048/B+S1
• 2-Methylbenzoic acid [118-90-1]
o-Toluic acid
Group-member nr.: 44-017
• 3-Methylbenzoic acid [99-04-7]
m-Toluic acid
Group-member nr.: 44-018
• 4-Methylbenzoic acid [99-94-5]
p-Toluic acid

Group-member nr.: 44-019

$C_8H_8O_3$
- Methyl 2-hydroxybenzoate [119-36-8]
  Methyl salicylate
  Group-member nr.: 47-029
- 3a,4,7,7a-Tetrahydro-1,3-isobenzofurandione [85-43-8]
  4-Cyclohexene-1,2-dicarboxylic acid anhydride
  1,2,3,6-Tetrahydrophthalic anhydride
  Group-member nr.: 44-020

$C_8H_9NO_2$
- *N*-(2-Hydroxyphenyl)acetamide [614-80-2]
  o-Hydroxyacetanilide
  Group-member nr.: 62-076
- Methyl ester phenylcarbamic acid [2603-10-3]
  Methyl phenylcarbamate
  Methyl ester carbanilic acid
  Group-member nr.: 62-077

C_8H_{10}
- 1,2-Dimethylbenzene [95-47-6]
  o-Xylene
  Group-member nr.: 14-018/B+S1
- 1,3-Dimethylbenzene [108-38-3]
  m-Xylene
  Group-member nr.: 14-019/B+S1
- 1,4-Dimethylbenzene [106-42-3]
  p-Xylene
  Group-member nr.: 14-020/B+S1
- Ethylbenzene [100-41-4]
  Phenylethane
  Group-member nr.: 14-021/B+S1

$C_8H_{10}N_2$
- Phenylhydrazone acetaldehyde [935-07-9]
  Group-member nr.: 34-009

$C_8H_{10}O$
- Benzeneethanol [60-12-8]
  Phenethyl alcohol
  2-Phenylethanol
  Group-member nr.: 42-066
- Ethoxybenzene [103-73-1]
  Ethyl phenyl ether
  Phenetole
  Group-member nr.: 41-032
- 1-Methoxy-4-methylbenzene [104-93-8]
  Methyl 4-methylphenyl ether
  p-Methylanisole
  Methyl *p*-tolyl ether
  p-Cresol methyl ether
  Group-member nr.: 41-033

$C_8H_{10}O_2$
- 2-Phenoxyethanol [122-99-6]
  Ethylene glycol monophenyl ether
  Group-member nr.: 47-030

$C_8H_{10}O_4$
- Di-2-propenyl ethanedioate [615-99-6]
  Di-2-propenyl ester ethanedioic acid
  Diallyl oxalate
  Group-member nr.: 45-049

$C_8H_{11}Cl_3OS$
- *O*-Pentyl ester 2,3,3-trichloro-2-propenethioic acid [76619-94-8]
  O-Pentyl ester trichlorothioacrylic acid
  n-Amyl trichlorothioacrylate
  Group-member nr.: 64-039/S1

$C_8H_{11}N$
- Benzeneethanamine [64-04-0]
  2-Phenylethylamine
  Phenethylamine
  Group-member nr.: 31-032
- *endo*-Bicyclo[2.2.1]heptane-2-carbonitrile [3211-87-8]
  endo-2-Cyanobicyclo[2.2.1]heptane
  endo-2-Norbornanecarbonitrile
  Group-member nr.: 32-025/B+S1
- *exo*-Bicyclo[2.2.1]heptane-2-carbonitrile [3211-90-3]
  exo-2-Cyanobicyclo[2.2.1]heptane
  exo-2-Norbornanecarbonitrile
  Group-member nr.: 32-026/B+S1
- *N*,*N*-Dimethylbenzenamine [121-69-7]
  N,*N*-Dimethylaniline
  Group-member nr.: 31-033/B+S1^E
- 2,4-Dimethylbenzenamine [95-68-1]
  2,4-Dimethylaniline
  2,4-Xylidine
  Group-member nr.: 31-048/S1
- 2,5-Dimethylbenzenamine [95-78-3]
  2,5-Dimethylaniline
  2,5-Xylidine
  Group-member nr.: 31-049/S1
- 2,6-Dimethylbenzenamine [87-62-7]
  2,6-Dimethylaniline
  2,6-Xylidine
  Group-member nr.: 31-034/B+S1^E
- *N*-Ethylbenzenamine [103-69-5]
  N-Ethylaniline
  Ethylphenylamine
  Group-member nr.: 31-050/S1
- 2-Ethylbenzenamine [578-54-1]
  2-Ethylphenylamine
  2-Ethylaniline
  Group-member nr.: 31-051/S1
- α-Methylbenzenemethanamine [618-36-0]
  α-Methylbenzylamine
  Group-member nr.: 31-052/S1
- 2,3,6-Trimethylpyridine [1462-84-6]
  2,3,6-Collidine
  Group-member nr.: 33-031
- 2,4,6-Trimethylpyridine [108-75-8]
  2,4,6-Collidine
  Group-member nr.: 33-032

$C_8H_{11}NO$
- 4-Ethoxybenzenamine [156-43-4]
  p-Phenetidine

Group-member nr.: 62-161/S1

C_8H_{12}
- Bicyclo[2.2.2]oct-2-ene [931-64-6]
  Group-member nr.: 14-022
- 1,5-Cyclooctadiene (unspecified stereoisomer) [111-78-4]
  Group-member nr.: 14-023

$C_8H_{12}N_2$
- 1,6-Diisocyanohexane [929-57-7]
  1,6-Hexamethylene isocyanide
  1,6-Hexamethylene diisocyanide
  Group-member nr.: 34-010

$C_8H_{12}N_2O_2$
- 1,6-Diisocyanatohexane [822-06-0]
  Hexamethylene diisocyanate
  Hexamethylene ester isocyanic acid
  Group-member nr.: 62-078

$C_8H_{12}O$
- 2-(1,1-Dimethylethyl)furan [7040-43-9]
  2-*tert*-Butylfuran
  Group-member nr.: 46-030/S1

C_8H_{14}
- Bicyclo[2.2.2]octane [280-33-1]
  Group-member nr.: 12-020
- *cis*-Bicyclo[4.2.0]octane [28282-35-1]
  Group-member nr.: 12-021
- Cyclooctene (unspecified stereoisomer) [931-88-4]
  Group-member nr.: 14-024
- Ethenylcyclohexane [695-12-5]
  Vinylcyclohexane
  Group-member nr.: 12-125/S1
- Ethylidenecyclohexane [1003-64-1]
  Group-member nr.: 12-022
- *endo*-2-Methylbicyclo[2.2.1]heptane [765-90-2]
  endo-2-Methylnorbornane
  Group-member nr.: 12-023
- *exo*-2-Methylbicyclo[2.2.1]heptane [872-78-6]
  exo-2-Methylnorbornane
  Group-member nr.: 12-024
- *cis*-Octahydropentalene [1755-05-1]
  cis-Bicyclo[3.3.0]octane
  Group-member nr.: 12-025
- *trans*-Octahydropentalene [5597-89-7]
  trans-Bicyclo[3.3.0]octane
  Group-member nr.: 12-026
- (2-Propenyl)cyclopentane [3524-75-2]
  Allylcyclopentane
  Group-member nr.: 12-027

$C_8H_{14}O$
- 6-Methyl-5-hepten-2-one [110-93-0]
  Group-member nr.: 43-037
- 3-Oxabicyclo[3.2.2]nonane [283-27-2]
  Group-member nr.: 46-021

$C_8H_{14}O_2$
- Butyl 2-methyl-2-propenoate [97-88-1]
  Butyl methacrylate
  Group-member nr.: 45-050/B+S1
- 2-Propenyl pentanoate [6321-45-5]
  Allyl valerate
  Group-member nr.: 45-051

$C_8H_{14}O_4$
- Diethyl butanedioate [123-25-1]
  Diethyl ester butanedioic acid
  Diethyl succinate
  Group-member nr.: 45-052
- Dipropyl ethanedioate [615-98-5]
  Dipropyl ester ethanedioic acid
  Dipropyl oxalate
  Group-member nr.: 45-053
- 1,2-Ethanediol dipropionate [123-80-8]
  1,2-Ethanediyl ester propanoic acid
  Ethylene glycol dipropionate
  Group-member nr.: 45-054

$C_8H_{14}O_6$
- Diethyl ester 2,3-dihydroxy-[R-(R*,R*)]-butanedioic acid [87-91-2]
  Diethyl $L(+)$-tartarate
  Group-member nr.: 47-031

$C_8H_{15}N$
- 3-Azabicyclo[3.2.2]nonane [283-24-9]
  Group-member nr.: 33-033

$C_8H_{15}O_2Tl$
- Thallium(1+) salt octanoic acid [18993-50-5]
  Thallium(I) octanoate
  Group-member nr.: 74-027/S1

C_8H_{16}
- Cyclooctane [292-64-8]
  Group-member nr.: 12-028
- 1,1-Dimethylcyclohexane [590-66-9]
  Group-member nr.: 12-029
- *cis*-1,2-Dimethylcyclohexane [2207-01-4]
  Group-member nr.: 12-030
- *trans*-1,2-Dimethylcyclohexane [6876-23-9]
  Group-member nr.: 12-031
- *cis*-1,3-Dimethylcyclohexane [638-04-0]
  Group-member nr.: 12-032
- *trans*-1,3-Dimethylcyclohexane [2207-03-6]
  Group-member nr.: 12-033
- *cis*-1,4-Dimethylcyclohexane [624-29-3]
  Group-member nr.: 12-034
- *trans*-1,4-Dimethylcyclohexane [2207-04-7]
  Group-member nr.: 12-035
- Ethylcyclohexane [1678-91-7]
  Group-member nr.: 12-036
- 1-Octene [111-66-0]
  1-Octylene
  1-Caprylene
  Group-member nr.: 13-031
- Propylcyclopentane [2040-96-2]
  Group-member nr.: 12-037
- 2,4,4-Trimethyl-1-pentene [107-39-1]

Group-member nr.: 13-032
- 2,4,4-Trimethyl-2-pentene [107-40-4]
  Group-member nr.: 13-033

$C_8H_{16}O$
- Octanal [124-13-0]
  Octyl aldehyde
  Caprilic aldehyde
  Group-member nr.: 43-038
- 2-Octanone [111-13-7]
  Hexyl methyl ketone
  Group-member nr.: 43-039

$C_8H_{16}O_2$
- Butyl butanoate [109-21-7]
  Butyl butyrate
  Group-member nr.: 45-055
- Ethyl hexanoate [123-66-0]
  Ethyl caproate
  Group-member nr.: 45-056
- (±)-2-Ethylhexanoic acid [83829-68-9]
  Group-member nr.: 44-039/S1
- Hexyl acetate [142-92-7]
  Hexyl ethanoate
  Group-member nr.: 45-057/B+S1
- 3-Methylbutyl propanoate [105-68-0]
  Isoamyl propionate
  Isopentyl propionate
  Group-member nr.: 45-059
- Methyl heptanoate [106-73-0]
  Methyl enanthoate
  Group-member nr.: 45-058
- 2-Methylpropyl butanoate [539-90-2]
  Isobutyl butyrate
  Group-member nr.: 45-060
- 2-Methylpropyl 2-methylpropanoate [97-85-8]
  Isobutyl isobutyrate
  Group-member nr.: 45-061
- Octanoic acid [124-07-2]
  Caprylic acid
  Group-member nr.: 44-021
- Pentyl propanoate [624-54-4]
  Amyl propionate
  Group-member nr.: 45-062
- Propyl pentanoate [141-06-0]
  Propyl valerate
  Group-member nr.: 45-063

$C_8H_{16}O_4$
- 2-(2-Ethoxyethoxy)ethanol acetate [112-15-2]
  2-(2-Ethoxyethoxy)ethyl acetate
  Diethylene glycol ethyl ether acetate
  Group-member nr.: 47-032
- 1,4,7,10-Tetraoxacyclododecane [294-93-9]
  Group-member nr.: 46-022

$C_8H_{17}Br$
- 1-Bromooctane [111-83-1]
  n-Octyl bromide
  Group-member nr.: 23-037/B+S1

$C_8H_{17}Cl$
- 1-Chlorooctane [111-85-3]
  n-Octyl chloride
  Group-member nr.: 22-063/S1

$C_8H_{17}NO$
- *N*,*N*-Dipropylacetamide [1116-24-1]
  Group-member nr.: 62-079

C_8H_{18}
- 2,3-Dimethylhexane [584-94-1]
  Group-member nr.: 11-025
- 2,5-Dimethylhexane [592-13-2]
  Group-member nr.: 11-026
- 3,3-Dimethylhexane [563-16-6]
  Group-member nr.: 11-027
- 3-Ethyl-2-methylpentane [609-26-7]
  Group-member nr.: 11-028
- 2-Methylheptane [592-27-8]
  Group-member nr.: 11-029
- 3-Methylheptane [589-81-1]
  Group-member nr.: 11-030
- 4-Methylheptane [589-53-7]
  Methyldipropylmethane
  Group-member nr.: 11-031
- Octane [111-65-9]
  Group-member nr.: 11-032/B+S1^E
- 2,2,3,3-Tetramethylbutane [594-82-1]
  Group-member nr.: 11-033
- 2,2,4-Trimethylpentane [540-84-1]
  Isooctane
  Group-member nr.: 11-034/B+S1^E
- 2,3,3-Trimethylpentane [560-21-4]
  Group-member nr.: 11-035
- 2,3,4-Trimethylpentane [565-75-3]
  Group-member nr.: 11-036

$C_8H_{18}N_2O$
- Bis(1,1-dimethylethyl)diazene 1-oxide [16649-52-8]
  Di-*tert*-butyldiazene *N*-oxide
  Group-member nr.: 62-080

$C_8H_{18}O$
- 2-Ethyl-1-hexanol [104-76-7]
  Group-member nr.: 42-067/B+S1
- 2-Methyl-1-heptanol [106-67-2]
  Group-member nr.: 42-068
- 2-Methyl-2-heptanol [625-25-2]
  Group-member nr.: 42-069
- 2-Methyl-4-heptanol [21570-35-4]
  Group-member nr.: 42-070
- 3-Methyl-2-heptanol [31367-46-1]
  Group-member nr.: 42-071
- 4-Methyl-2-heptanol [56298-90-9]
  Group-member nr.: 42-072
- 4-Methyl-3-heptanol [14979-39-6]
  Group-member nr.: 42-073
- 4-Methyl-4-heptanol [598-01-6]

Group-member nr.: 42-074
- 5-Methyl-1-heptanol [7212-53-5]
  Group-member nr.: 42-075
- 5-Methyl-2-heptanol [54630-50-1]
  Group-member nr.: 42-076
- 6-Methyl-2-heptanol [4730-22-7]
  Group-member nr.: 42-077
- 6-Methyl-3-heptanol [18720-66-6]
  Group-member nr.: 42-078
- 1-Octanol [111-87-5]
  Octyl alcohol
  Group-member nr.: 42-079/B+S1
- 2-Octanol [123-96-6]
  Group-member nr.: 42-080
- 3-Octanol [589-98-0]
  Group-member nr.: 42-081
- 4-Octanol [589-62-8]
  Group-member nr.: 42-082
- 1,1′-Oxybisbutane [142-96-1]
  Dibutyl ether
  Group-member nr.: 41-034/B+S1

$C_8H_{18}O_2$
- Bis(1,1-dimethylethyl) peroxide [110-05-4]
  tert-Butyl peroxide
  Group-member nr.: 47-062/S1
- 1,2-Dipropoxyethane [18854-56-3]
  4,7-Dioxadecane
  Ethylene glycol dipropyl ether
  Group-member nr.: 41-035

$C_8H_{18}O_3$
- 2-(2-Butoxyethoxy)ethanol [112-34-5]
  Diethylene glycol monobutyl ether
  Group-member nr.: 47-033/B+S1
- 1,1′-Oxybis(2-ethoxyethane) [112-36-7]
  3,6,9-Trioxaundecane
  Diethylene glycol diethyl ether
  Group-member nr.: 41-036

$C_8H_{18}O_4$
- 2,5,8,11-Tetraoxadodecane [112-49-2]
  Triethylene glycol dimethyl ether
  Triglyme
  Group-member nr.: 41-037/B+S1

$C_8H_{18}O_5$
- 2,2′-[Oxybis(2,1-ethanediyloxy)]bisethanol [112-60-7]
  Tetraethylene glycol
  Group-member nr.: 47-034/B+S1[E]

$C_8H_{18}S$
- 2-(Methylthio)heptane [54063-12-6]
  3-Methyl-2-thiaoctane
  Methyl 1-methylhexyl sulfide
  Group-member nr.: 51-020
- 1,1′-Thiobisbutane [544-40-1]
  Dibutyl sulfide
  Group-member nr.: 51-021

$C_8H_{19}Al$
- Hydrobis(2-methylpropyl)aluminum [1191-15-7]
  Diisobutylaluminium hydride
  Group-member nr.: 73-038/S1

$C_8H_{19}N$
- 2-Methyl-*N*-(2-methylpropyl)-1-propanamine [110-96-3]
  Diisobutylamine
  Group-member nr.: 31-035
- 1-Octanamine [111-86-4]
  Octylamine
  Group-member nr.: 31-053/S1

$C_8H_{19}NO$
- 2-[Bis(1-methylethyl)aminoethanol [96-80-0]
  Diisopropylethanolamine
  2-Diisopropylaminoethanol
  Group-member nr.: 62-162/S1

$C_8H_{19}NO_2$
- 2,2′-(Butylimino)bisethanol [102-79-4]
  Butyldiethanolamine
  2-[Butyl(2-hydroxyethyl)amino]ethanol
  Group-member nr.: 62-163/S1
- 2,2′-[(1,1-Dimethylethyl)imino]bisethanol [2160-93-2]
  tert-Butyldiethanolamine
  2-[*tert*-Butyl(2-hydroxyethyl)amino]ethanol
  Group-member nr.: 62-164/S1

$C_8H_{19}NSi$
- 1-[2-(Trimethylsilyl)ethyl]azetidine [42525-64-4]
  N-(β-Trimethylsilylethyl)trimethylenimine
  Group-member nr.: 71-020

$C_8H_{20}Ge$
- Tetraethylgermane [597-63-7]
  Group-member nr.: 73-024

$C_8H_{20}N_4$
- 1,4-Piperazinediethanamine [6531-38-0]
  1,4-Bis(2-aminoethyl)piperazine
  Group-member nr.: 33-034
- *N*-[2-(1-Piperazinyl)ethyl]-1,2-ethanediamine [24028-46-4]
  1-[2-[(2-Aminoethyl)amino]ethyl]piperazine
  Group-member nr.: 33-035

$C_8H_{20}OZn$
- Diethyl[1,1′-oxybis(ethane)]zinc [58482-38-5]
  Group-member nr.: 73-039/S1

$C_8H_{20}O_4Si$
- Tetraethyl ester silicic acid [78-10-4]
  Tetraethyl orthosilicate
  Tetraethoxysilane
  Group-member nr.: 71-021

$C_8H_{20}Pb$
- Tetraethylplumbane [78-00-2]
  Tetraethyllead
  TEL
  Group-member nr.: 73-025

$C_8H_{20}Si$
- Tetraethylsilane [631-36-7]
  Group-member nr.: 71-022/B+S1

$C_8H_{20}Sn$
- Tetraethylstannane [597-64-8]
  Tetraethyltin
  Group-member nr.: 73-026

$C_8H_{20}TeZn$
- Diethyl[1,1′-tellurobis(ethane)]zinc [132851-15-1]
  Complex dithylzinc with diethyltellurium
  Group-member nr.: 73-040/S1

$C_8H_{23}N_5$
- *N*-(2-Aminoethyl)-*N*′-[2-[(2-aminoethyl)amino]ethyl]-1,2-ethanediamine [112-57-2]
  Tetraethylenepentamine
  Group-member nr.: 31-036

$C_8H_{24}O_2Si_3$
- Octamethyltrisiloxane [107-51-7]
  Group-member nr.: 71-063/S1

$C_8H_{24}O_4Si_4$
- Octamethylcyclotetrasiloxane [556-67-2]
  Group-member nr.: 71-023

$C_8H_{28}N_4Si_4$
- 2,2,4,4,6,6,8,8-Octamethylcyclotetrasilazane [1020-84-4]
  Dimethylaminosilane tetramer
  Group-member nr.: 71-024

$C_9H_4O_5$
- 1,3-Dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid [552-30-7]
  1,2,4-Benzenetricarboxylic 1:2 anhydride
  Trimellitic anhydride
  Group-member nr.: 47-035

$C_9H_6N_2O_2$
- 2,4-Diisocyanato-1-methylbenzene [584-84-9]
  4-Methyl-*m*-phenyl diisocyanate
  4-Methyl-1,3-phenylene ester isocyanic acid
  2,4-Diisocyanate tolylene
  Group-member nr.: 62-081

C_9H_7ClO
- 2-Chloro-3-phenyl-2-propenal [18365-42-9]
  α-Chlorocinnamaldehyde
  Group-member nr.: 61-046

C_9H_7N
- Isoquinoline [119-65-3]
  Benzo[*c*]pyridine
  Group-member nr.: 33-036
- Quinoline [91-22-5]
  Benzo[*b*]pyridine
  Group-member nr.: 33-037

C_9H_8
- 1*H*-Indene [95-13-6]
  Group-member nr.: 14-025

$C_9H_8N_2$
- 1-Phenyl-1*H*-imidazole [7164-98-9]
  Group-member nr.: 33-053/S1
- 1-Phenyl-1*H*-pyrazole [1126-00-7]
  Group-member nr.: 33-054/S1

C_9H_8O
- 3-Phenyl-2-propenal [104-55-2]
  Cinnamaldehyde
  Group-member nr.: 43-040

C_9H_{10}
- 2,3-Dihydroindene [496-11-7]
  Indan
  Group-member nr.: 14-026
- (1-Methylethenyl)benzene [98-83-9]
  Isopropenylbenzene
  α-Methylstyrene
  Group-member nr.: 14-027/B+S1

$C_9H_{10}O$
- 3,4-Dihydro-1*H*-2-benzopyran [493-05-0]
  Isochroman
  Group-member nr.: 46-023
- 3,4-Dihydro-2*H*-1-benzopyran [493-08-3]
  Chroman
  Group-member nr.: 46-024
- 1-Phenyl-1-propanone [93-55-0]
  Ethyl phenyl ketone
  Propiophenone
  Group-member nr.: 43-041

$C_9H_{10}O_2$
- Ethyl benzoate [93-89-0]
  Ethyl ester benzoic acid
  Group-member nr.: 45-064/B+S1
- (Phenoxymethyl)oxirane [122-60-1]
  Phenyl glycidyl ether
  Group-member nr.: 47-036/B+S1
- Phenylmethyl acetate [140-11-4]
  Phenylmethyl ester acetic acid
  Benzyl acetate
  Group-member nr.: 45-065

$C_9H_{10}O_3$
- 3a,4,7,7a-Tetrahydro-4-methyl-1,3-isobenzofurandione [5333-84-6]
  3-Methyl-4-cyclohexene-1,2-dicarboxylic acid anhydride
  3-Methyl-1,2,3,6-tetrahydrophthalic anhydride
  Group-member nr.: 44-022

$C_9H_{11}N$
- 1,2,3,4-Tetrahydroquinoline [635-46-1]
  Group-member nr.: 33-038
- 5,6,7,8-Tetrahydroquinoline [10500-57-9]
  2,3-Cyclohexenopyridine
  Group-member nr.: 33-039

$C_9H_{11}NO$
- 4-(Dimethylamino)benzaldehyde [100-10-7]
  Group-member nr.: 62-165/S1

$C_9H_{11}NO_2$
- Ethyl ester phenylcarbamic acid [101-99-5]
  Ethyl phenylcarbamate
  Ethyl ester carbanilic acid
  Group-member nr.: 62-082

C_9H_{12}
- 5-Ethenylbicyclo[2.2.1]hept-2-ene [3048-64-4]
  5-Vinylnorbornene
  Group-member nr.: 14-101/S1
- (*Z*)-5-Ethylidenebicyclo[2.2.1]hept-2-ene [28304-66-7]
  cis-5-Ethylidene-2-norbornene
  Group-member nr.: 14-102/S1
- (1-Methylethyl)benzene [98-82-8]
  Isopropylbenzene
  Cumene
  Group-member nr.: 14-028/B+S1^E
- Propylbenzene [103-65-1]
  Group-member nr.: 14-029/B+S1^E
- 1,2,3-Trimethylbenzene [526-73-8]
  Hemimellitene
  Group-member nr.: 14-030
- 1,2,4-Trimethylbenzene [95-63-6]
  Pseudocumene
  Group-member nr.: 14-031
- 1,3,5-Trimethylbenzene [108-67-8]
  Mesitylene
  Group-member nr.: 14-032/B+S1^E

$C_9H_{12}O$
- Benzenepropanol [122-97-4]
  3-Phenyl-1-propanol
  Phenylethyl carbinol
  Hydrocinnamyl alcohol
  Group-member nr.: 42-083
- 1-Ethoxy-4-methylbenzene [622-60-6]
  Ethyl-4-methylphenyl ether
  p-Methylphenetole
  Ethyl *p*-tolyl ether
  Group-member nr.: 41-038
- 1-Methoxy-2,4-dimethylbenzene [6738-23-4]
  Methyl 2,4-dimethylphenyl ether
  2,4-Dimethylanisole
  Group-member nr.: 41-039
- Propoxybenzene [622-85-5]
  Phenyl propyl ether
  Group-member nr.: 41-040

$C_9H_{13}N$
- Benzenepropanamine [2038-57-5]
  3-Phenylpropylamine
  Group-member nr.: 31-037
- α,α-Dimethylbenzenemethanamine [585-32-0]
  α,α-Dimethylbenzylamine
  Group-member nr.: 31-054/S1
- *N*,*N*-Dimethylbenzenemethanamine [103-83-3]
  N,*N*-Dimethylbenzylamine
  Group-member nr.: 31-055/S1
- 2-(1-Methylethyl)benzenamine [643-28-7]
  2-Isopropylphenylamine
  2-Isopropylaniline
  Group-member nr.: 31-056/S1
- *N*,*N*,2-Trimethylbenzenamine [609-72-3]
  N,*N*-Dimethyl-*o*-toluidine
  Group-member nr.: 31-038

$C_9H_{14}O$
- 2,5,6-Trimethyl-2-cyclohexen-1-one [20030-30-2]
  Group-member nr.: 43-042

$C_9H_{14}O_6$
- 1,2,3-Propanetriol triacetate [102-76-1]
  1,2,3-Propanetriyl ester acetic acid
  Triacetin
  Group-member nr.: 45-066

C_9H_{16}
- *cis*-Bicyclo[6.1.0]nonane [13757-43-2]
  Group-member nr.: 12-038
- Octahydro-1*H*-indene [496-10-6]
  Hexahydroindan
  Hydrindan (unspecified stereoisomer)
  Group-member nr.: 12-039
- *cis*-Octahydro-1*H*-indene [4551-51-3]
  cis-Hexahydroindan
  cis-Hydrindan
  Group-member nr.: 12-040
- *trans*-Octahydro-1*H*-indene [3296-50-2]
  trans-Hexahydroindan
  trans-Hydrindan
  Group-member nr.: 12-041
- (2-Propenyl)cyclohexane [2114-42-3]
  Allylcyclohexane
  Group-member nr.: 12-042

$C_9H_{16}O_2$
- Ethyl cyclohexanecarboxylate [3289-28-9]
  Ethyl ester cyclohexanecarboxylic acid
  Group-member nr.: 45-067

$C_9H_{16}O_4$
- Dipropyl propanedioate [1117-19-7]
  Dipropyl ester propanedioic acid
  Dipropyl malonate
  Group-member nr.: 45-068

$C_9H_{17}N$
- *trans*-(±)-Decahydroquinoline [105728-23-2]
  trans-(*R*,*S*)-Decahydroquinoline
  Group-member nr.: 33-055/S1

C_9H_{18}
- Butylcyclopentane [2040-95-1]
  Group-member nr.: 12-043
- 1-Nonene [124-11-8]
  Group-member nr.: 13-034/B+S1^E
- Propylcyclohexane [1678-92-8]
  Group-member nr.: 12-044

$C_9H_{18}O$
- 2,6-Dimethyl-4-heptanone [108-83-8]

Diisobutyl ketone
Group-member nr.: 43-043
• Nonanal [124-19-6]
Nonyl aldehyde
Pelargonic aldehyde
Group-member nr.: 43-044
• 5-Nonanone [502-56-7]
Dibutyl ketone
Group-member nr.: 43-045

$C_9H_{18}O_2$
• Butyl pentanoate [591-68-4]
Butyl valerate
Group-member nr.: 45-069
• Heptyl acetate [112-06-1]
Group-member nr.: 45-137/S1
• 3-Methylbutyl butanoate [106-27-4]
Isoamyl butyrate
Isopentyl butyrate
Group-member nr.: 45-071
• 3-Methylbutyl 2-methylpropanoate [2050-01-3]
Isoamyl isobutyrate
Isopentyl isobutyrate
Group-member nr.: 45-072
• Methyl octanoate [111-11-5]
Methyl caprylate
Group-member nr.: 45-070
• 2-Methylpropyl pentanoate [10588-10-0]
Isobutyl valerate
Group-member nr.: 45-073
• Nonanoic acid [112-05-0]
Pelargonic acid
Group-member nr.: 44-023
• Pentyl butanoate [540-18-1]
Pentyl butyrate
Amyl butyrate
Group-member nr.: 45-074

$C_9H_{18}O_4$
• 2-(2′-Hydroxyethoxy)ethyl ester 2,2-dimethylpropanoic acid [20267-21-4]
2-(2′-Hydroxyethoxy)ethyl pivalate
Group-member nr.: 47-063/S1

$C_9H_{19}Br$
• 1-Bromononane [693-58-3]
n-Nonyl bromide
Group-member nr.: 23-038

$C_9H_{19}NOS$
• *S*-Ethyl ester dipropylcarbamothionic acid [759-94-4]
S-Ethyl dipropylthiocarbamate
Group-member nr.: 64-026

C_9H_{20}
• 3,3-Diethylpentane [1067-20-5]
Group-member nr.: 11-037
• Nonane [111-84-2]
Group-member nr.: 11-038/B+S1
• 2,2,3,3-Tetramethylpentane [7154-79-2]
Group-member nr.: 11-039
• 2,2,4,4-Tetramethylpentane [1070-87-7]
Group-member nr.: 11-040

$C_9H_{20}N_2O$
• Tetraethyl urea [1187-03-7]
Tetraethylcarbamide
Group-member nr.: 62-083

$C_9H_{20}O$
• 1-Nonanol [143-08-8]
Nonyl alcohol
Group-member nr.: 42-084/B+S1

$C_9H_{20}O_4$
• 1,1′-[(1-Methyl-1,2-ethanediyl)bis(oxy)]bis-2-propanol [1638-16-0]
Tri(propylene glycol)
Group-member nr.: 47-064/S1

$C_9H_{21}Al$
• Tripropylaluminium [102-67-0]
Group-member nr.: 73-027/B+S1

$C_9H_{21}ClO_3Si$
• (3-Chloropropyl)triethoxysilane [5089-70-3]
Group-member nr.: 71-025

$C_9H_{23}NO_3Si$
• 3-(Triethoxysilyl)-1-propanamine [919-30-2]
3-(Triethoxysilyl)propylamine
3-Aminopropyltriethoxysilane
Group-member nr.: 71-026

$C_9H_{24}Si_2$
• 1,3-Propanediylbis[trimethylsilane] [2295-05-8]
2,2,6,6-Tetramethyl-2,6-disilaheptane
Hexamethyldisilylpropane
Group-member nr.: 71-027

$C_9H_{24}Si_3$
• 1,1,3,3,5,5-Hexamethyl-1,3,5-trisilacyclohexane [1627-99-2]
Group-member nr.: 71-028

$C_{10}F_{16}$
• Hexadecafluoro-1,2,3,4,5,6,7,8-octahydronaphthalene [54939-04-7]
Group-member nr.: 21-030

$C_{10}F_{18}$
• *cis*-Octadecafluorodecahydronaphthalene [60433-11-6]
cis-Perfluorodecaline
Group-member nr.: 21-031
• *trans*-Octadecafluorodecahydronaphthalene [60433-12-7]
trans-Perfluorodecaline
Group-member nr.: 21-032

$C_{10}H_2O_6$
• 1*H*,3*H*-Benzo[1,2-*c*:4,5-*c*′]difuran-1,3,5,7-tetrone [89-32-7]
1,2,4,5-Benzenetetracarboxylic 1,2:4,5 dianhydride
Pyromellitic dianhydride
Group-member nr.: 44-024

$C_{10}H_6O_2S$
- 1-Oxide naphtho[1,8-*cd*]-1,2-dithiole [49833-12-7]
  Naphthalene 1,8-disulfide-*S*-oxide
  Group-member nr.: 63-005

$C_{10}H_7Cl$
- 1-Chloronaphthalene [90-13-1]
  Group-member nr.: 22-044/B+S1
- 2-Chloronaphthalene [91-58-7]
  Group-member nr.: 22-045

$C_{10}H_7NO_2$
- 1-Nitronaphthalene [86-57-7]
  α-Nitronaphthalene
  Group-member nr.: 62-084

$C_{10}H_8$
- Naphthalene [91-20-3]
  Group-member nr.: 14-033/B+S1

$C_{10}H_8O$
- 1-Naphthol [90-15-3]
  α-Naphthol
  Group-member nr.: 42-085
- 2-Naphthol [135-19-3]
  β-Naphthol
  Group-member nr.: 42-086

$C_{10}H_9N$
- 1-Naphthalenamine [134-32-7]
  1-Aminonaphthalene
  α-Naphthylamine
  Group-member nr.: 31-057/S1
- 2-Naphthalenamine [91-59-8]
  2-Aminonaphthalene
  β-Naphthalenamine
  Group-member nr.: 31-039

$C_{10}H_{10}$
- Tricyclo[3.3.2.0^{2,8}]deca-3,6,9-triene [1005-51-2]
  Group-member nr.: 14-034

$C_{10}H_{10}Fe$
- Ferrocene [102-54-5]
  Dicyclopentadienyliron
  Group-member nr.: 73-028

$C_{10}H_{10}N_2$
- 1-(Phenylmethyl)-1*H*-pyrazole [10199-67-4]
  1-Benzylpyrazole
  Group-member nr.: 33-056/S1

$C_{10}H_{10}O$
- 3,4-Dihydro-1(2*H*)-naphthalenone [529-34-0]
  α-Tetralone
  1,2,3,4-Tetrahydro-1-naphthalenone
  Group-member nr.: 43-066/S1

$C_{10}H_{10}O_2$
- 2-Propenyl benzoate [583-04-0]
  2-Propenyl ester benzoic acid
  Allyl benzoate
  Group-member nr.: 45-075

$C_{10}H_{10}O_4$
- Dimethyl 1,2-benzenedicarboxylate [131-11-3]
  Dimethyl phthalate
  Dimethyl ester 1,2-benzenedicarboxylic acid
  Group-member nr.: 45-076/B+S1
- Dimethyl 1,3-benzenedicarboxylate [1459-93-4]
  Dimethyl isophthalate
  Dimethyl ester 1,3-benzenedicarboxylic acid
  Group-member nr.: 45-138/S1
- Dimethyl 1,4-benzenedicarboxylate [120-61-6]
  Dimethyl terephthalate
  Dimethyl ester 1,4-benzenedicarboxylic acid
  Group-member nr.: 45-077

$C_{10}H_{12}$
- 1-Methylenepropylbenzene [2039-93-2]
  α-Ethylstyrene
  Group-member nr.: 14-103/S1
- (3aα,4α,7α,7aα)-3a,4,7,7a-Tetrahydro-4,7-methano-1*H*-indene [1755-01-7]
  endo-Dicyclopentadiene
  Group-member nr.: 14-104/S1
- 1,2,3,4-Tetrahydronaphthalene [119-64-2]
  Tetralin
  Group-member nr.: 14-035/B+S1

$C_{10}H_{12}O$
- 1-(4-Ethylphenyl)ethanone [937-30-4]
  4′-Ethylacetophenone
  Group-member nr.: 43-046
- 1-Methoxy-4-(1-propenyl)benzene [104-46-1]
  p-Propenylanisole
  Anethole
  Group-member nr.: 41-041

$C_{10}H_{12}O_2$
- 2-Methoxy-4-(2-propenyl)phenol [97-53-0]
  4-Allyl-2-methoxyphenol
  Eugenol
  Group-member nr.: 47-037
- Propyl benzoate [2315-68-6]
  Propyl ester benzoic acid
  Group-member nr.: 45-078

$C_{10}H_{13}NO_2$
- Propyl ester phenylcarbamic acid [5532-90-1]
  Propyl phenylcarbamate
  Propyl ester carbanilic acid
  Group-member nr.: 62-085

$C_{10}H_{14}$
- Butylbenzene [104-51-8]
  1-Phenylbutane
  Group-member nr.: 14-036
- (1,1-Dimethylethyl)benzene [98-06-6]
  tert-Butylbenzene
  2-Methyl-2-phenylpropane
  Group-member nr.: 14-037
- 1-Methyl-4-(1-methylethyl)benzene [99-87-6]
  1-Isopropyl-4-methylbenzene

p-Cymene
Group-member nr.: 14-038
• (1-Methylpropyl)benzene [135-98-8]
sec-Butylbenzene
2-Phenylbutane
Group-member nr.: 14-039
• 1,2,3,4-Tetramethylbenzene [488-23-3]
Prehnitene
Group-member nr.: 14-040
• 1,2,3,5-Tetramethylbenzene [527-53-7]
Isodurene
Group-member nr.: 14-041
• 1,2,4,5-Tetramethylbenzene [95-93-2]
Durene
Group-member nr.: 14-042

$C_{10}H_{14}O$
• 2-(1,1-Dimethylethyl)phenol [88-18-6]
2-*tert*-Butylphenol
1-*tert*-Butyl-2-hydroxybenzene
Group-member nr.: 42-112/S1
• (±)-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one [22327-39-5]
(±)-*p*-Mentha-6,8-dien-2-one
dl-Carvone
Group-member nr.: 43-067/S1
• (*R*)-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one [6485-40-1]
(*R*)-*p*-Mentha-6,8-dien-2-one
l-Carvone
Group-member nr.: 43-068/S1
• 2-Methyl-5-(1-methylethyl)phenol [499-75-2]
5-Isopropyl-2-methylphenol
Carvacrol
Group-member nr.: 42-087

$C_{10}H_{14}O_2$
• 4-(1,1-Dimethylethyl)-1,2-benzenediol [98-29-3]
4-*tert*-Butylcatechol
4-*tert*-Butylpyrocatechol
Group-member nr.: 42-113/S1

$C_{10}H_{14}O_4$
• Di-2-propenyl butanedioate [925-16-6]
Di-2-propenyl ester butanedioic acid
Diallyl succinate
Group-member nr.: 45-079

$C_{10}H_{14}Si$
• Ethenyldimethylphenylsilane [1125-26-4]
Group-member nr.: 71-029
• 1-Methyl-1-phenylsilacyclobutane [3944-08-9]
Group-member nr.: 71-064/S1

$C_{10}H_{15}N$
• *N*,*N*-Diethylbenzenamine [91-66-7]
N,*N*-Diethylaniline
Group-member nr.: 31-040
• 2,6-Diethylbenzenamine [579-66-8]
2,6-Diethylphenylamine
2,6-Diethylaniline
Group-member nr.: 31-058/S1
• 2-(1,1-Dimethylethyl)benzenamine [6310-21-0]
2-*tert*-Butylphenylamine
2-*tert*-Butylaniline
Group-member nr.: 31-059/S1

$C_{10}H_{15}NO$
• (*E*)-(*R*,*S*)-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one oxime [55658-55-4]
dl-Carvoxime
Group-member nr.: 62-086
• [*R*-(*E*)]-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one oxime [60827-56-7]
l-Carvoxime
Group-member nr.: 62-087

$C_{10}H_{16}$
• 6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane [127-91-3]
β-Pinene
Nopinene
Terebenthene
Group-member nr.: 12-045/B+S1
• 4-Methylene-1-(1-methylethyl)bicyclo[3.1.0]hexane [3387-41-5]
Sabinene
Group-member nr.: 12-046
• 1-Methyl-4-(1-methylethenyl)cyclohexene [138-86-3]
Limonene
Group-member nr.: 14-043/B+S1
• (*R*)-1-Methyl-4-(1-methylethenyl)cyclohexene [5989-27-5]
d-Limonene
Group-member nr.: 14-105/S1
• Octahydro-4,7-methano-1*H*-indene [6004-38-2]
Hexahydro-4,7-methanoindan
Tricyclo[5.2.1.0^{2,6}]decane
Tetrahydrodicyclopentadiene
Group-member nr.: 12-047
• (3aα,4β,7β,7aα)-Octahydro-4,7-methano-1*H*-indene [2825-82-3]
exo-Tetrahydrodicyclopentadiene
Group-member nr.: 12-126/S1
• Tricyclo[3.3.1.1^{3,7}]decane [281-23-2]
Adamantane
Group-member nr.: 12-127/S1
• 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene [80-56-8]
α-Pinene
(*DL*)-Pin-2-ene
Group-member nr.: 14-106/S1

$C_{10}H_{16}O$
• Camphor [76-22-2]
1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one
Group-member nr.: 43-047
• 3,7-Dimethyl-2,6-octadienal [5392-40-5]

Citral
Group-member nr.: 43-048
• 3,7-Dimethyl-6-octen-1-yn-3-ol [29171-20-8]
Dehydrolynalol
Group-member nr.: 42-088
• 5-Methyl-2-(1-methylethylidene)cyclohexanone [15932-80-6]
p-Menth-4(8)-en-3-one
1-Isopropylidene-4-methylcyclohexan-2-on
Pulegone
Group-member nr.: 43-049

$C_{10}H_{18}$
• 1,1′-Bicyclopentyl [1636-39-1]
Cyclopentylcyclopentane
Group-member nr.: 12-048
• *cis*-Decahydroazulene [16189-46-1]
cis-Perhydroazulene
cis-Bicyclo[5.3.0]decane
Group-member nr.: 12-049
• Decahydronaphthalene [91-17-8]
Decalin (unspecified stereoisomer)
Group-member nr.: 12-050
• *cis*-Decahydronaphthalene [493-01-6]
cis-Decalin
Group-member nr.: 12-051
• *trans*-Decahydronaphthalene [493-02-7]
trans-Decalin
Group-member nr.: 12-052
• Octahydromethyl-1*H*-indene [unknown]
Hexahydromethylindan
Methylhydrindan (unspecified isomer)
Group-member nr.: 12-053
• 2,6,6-Trimethylbicyclo[3.1.1]heptane [473-55-2]
Pinane
Group-member nr.: 12-054

$C_{10}H_{18}O$
• 3,7-Dimethyl-1,6-octadien-3-ol [78-70-6]
Linalol
Group-member nr.: 42-089

$C_{10}H_{18}O_4$
• Bis(2-methylpropyl) ethanedioate [2050-61-5]
Bis(2-methylpropyl) ester ethanedioic acid
Diisobutyl oxalate
Group-member nr.: 45-080
• Dipropyl butanedioate [925-15-5]
Dipropyl ester butanedioic acid
Dipropyl succinate
Group-member nr.: 45-081
• 1,2-Ethanediyl dibutanoate [105-72-6]
1,2-Ethanediyl ester butanoic acid
1,2-Ethanediol dibutyrate
Ethylene glycol dibutyrate
Group-member nr.: 45-082

$C_{10}H_{18}Si$
• Bicyclo[2.2.1]hept-5-en-2-yltrimethylsilane [17985-13-6]
5-Trimethylsilyl-2-norbornene
Group-member nr.: 71-065/S1

$C_{10}H_{20}$
• Butylcyclohexane [1678-93-9]
Group-member nr.: 12-055
• 1-Decene [872-05-9]
1-Decylene
α-Decylene
Group-member nr.: 13-035/B+S1^{E}
• Diethylcyclohexane (unspecified isomer) [1331-43-7]
Group-member nr.: 12-056
• 1,4-Diethylcyclohexane [1679-00-1]
Group-member nr.: 12-057
• (1,1-Dimethylethyl)cyclohexane [3178-22-1]
tert-Butylcyclohexane
Group-member nr.: 12-058

$C_{10}H_{20}O$
• Decanal [112-31-2]
Decyl aldehyde
Capric aldehyde
Group-member nr.: 43-050
• (1α,2β,5α)-5-Methyl-2-(1-methylethyl)cyclohexanol [89-78-1]
(±)-Menthol
p-Menthan-3-ol
(±)-2-Isopropyl-5-methylcyclohexanol
Group-member nr.: 42-114/S1

$C_{10}H_{20}O_2$
• Decanoic acid [334-48-5]
Capric acid
Group-member nr.: 44-025
• Hexyl butanoate [2639-63-6]
Hexyl butyrate
Group-member nr.: 45-083
• 3-Methylbutyl pentanoate [2050-09-1]
Isoamyl valerate
Isopentyl valerate
Group-member nr.: 45-084
• Octyl acetate [112-14-1]
Group-member nr.: 45-085/B+S1

$C_{10}H_{20}O_4$
• 2-(2-Butoxyethoxy)ethanol acetate [124-17-4]
2-(2-Butoxyethoxy)ethyl acetate
Diethylene glycol butyl ether acetate
Group-member nr.: 47-038

$C_{10}H_{20}O_5$
• 1,4,7,10,13-Pentaoxacyclopentadecane [33100-27-5]
Group-member nr.: 46-025

$C_{10}H_{21}NO$
• *N*,*N*-Dibutylacetamide [1563-90-2]
Group-member nr.: 62-088

$C_{10}H_{22}$
• Decane [124-18-5]
Group-member nr.: 11-041/B+S1
• 2,7-Dimethyloctane [1072-16-8]

Group-member nr.: 11-042
- 2-Methylnonane [871-83-0]
  Isodecane
  Group-member nr.: 11-043
- 3-Methylnonane [5911-04-6]
  Group-member nr.: 11-044
- 4-Methylnonane [17301-94-9]
  Group-member nr.: 11-045
- 5-Methylnonane [15869-85-9]
  Group-member nr.: 11-046

$C_{10}H_{22}N_4$
- 1,1′-(1,2-Ethanediyl)bispiperazine [19479-83-5]
  Dipiperazinylethane
  Group-member nr.: 33-040

$C_{10}H_{22}O$
- 1-Decanol [112-30-1]
  Decyl alcohol
  Group-member nr.: 42-090/B+S1
- 5-Decanol [5205-34-5]
  Group-member nr.: 42-091
- 3,7-Dimethyl-1-octanol [106-21-8]
  Group-member nr.: 42-092
- 4-Propyl-4-heptanol [2198-72-3]
  Group-member nr.: 42-093

$C_{10}H_{22}O_2$
- 1,10-Decanediol [112-47-0]
  Group-member nr.: 42-115/S1
- 1,1′-[1,2-Ethanediylbis(oxy)]bisbutane [112-48-1]
  1,2-Dibutoxyethane
  Ethylene glycol dibutyl ether
  Group-member nr.: 41-042
- 1,1′-[Ethylidenebis(oxy)]bisbutane [871-22-7]
  1,1-Dibutoxyethane
  Acetaldehyde dibutylacetal
  6-Methyl-5,7-dioxaundecane
  Group-member nr.: 41-043

$C_{10}H_{22}O_5$
- 2,5,8,11,14-Pentaoxapentadecane [143-24-8]
  Bis(methoxyethoxyethyl) ether
  Tetraethylene glycol dimethyl ether
  Group-member nr.: 41-044/B+S1

$C_{10}H_{22}O_6$
- 3,6,9,12-Tetraoxatetradecane-1,14-diol [4792-15-8]
  Pentaethylene glycol
  Group-member nr.: 47-039

$C_{10}H_{22}S$
- 1-Decanethiol [143-10-2]
  1-Decyl mercaptan
  Group-member nr.: 52-018/B+S1^E
- 1-Ethylthiooctane [3698-94-0]
  Ethyl *n*-octyl sulfide
  Group-member nr.: 51-029/S1
- 1,1′-Thiobispentane [872-10-6]
  6-Thiaundecane
  Dipentyl sulfide
  Group-member nr.: 51-022

$C_{10}H_{22}Te$
- 1,1′-Tellurobispentane [71475-88-2]
  Group-member nr.: 73-041/S1

$C_{10}H_{23}N$
- 1-Decanamine [2016-57-1]
  n-Decylamine
  Group-member nr.: 31-061/S1
- *N*,*N*-Dimethyloctanamine [7378-99-6]
  Dimethyloctylamine
  Group-member nr.: 31-060/S1

$C_{10}H_{24}N_4$
- Octamethylethenetetramine [996-70-3]
  Tetrakis(dimethylamino)ethylene
  Group-member nr.: 31-062/S1

$C_{10}H_{25}N_5$
- *N*-(2-Aminoethyl)-1,4-piperazinediethanamine [31295-54-2]
  1-(2-Aminoethyl)-4-[2-[(2-aminoethyl)amino]ethyl]piperazine
  Group-member nr.: 33-041

$C_{10}H_{25}O_5U$
- Pentaethoxyuranium [unknown]
  Uranium pentaethylate
  Group-member nr.: 73-042/S1

$C_{10}H_{26}O_3Si_3$
- 2,2,4,4-Tetraethyl-6,6-dimethylcyclotrisiloxane [110505-51-6]
  Group-member nr.: 71-030

$C_{11}H_{10}$
- 1-Methylnaphthalene [90-12-0]
  α-Methylnaphthalene
  Group-member nr.: 14-044
- 2-Methylnaphthalene [91-57-6]
  β-Methylnaphthalene
  Group-member nr.: 14-045

$C_{11}H_{12}O_2$
- Ethyl 3-phenyl-2-propenoate [103-36-6]
  Ethyl ester 3-phenyl-2-propenoic acid
  Ethyl cinnamate (unspecified stereoisomer)
  Group-member nr.: 45-086
- Methyl ester pentacyclo[4.3.0.0^{2,5}.0^{3,8}.0^{4,7}]nonane-4-carboxylic acid [40317-63-3]
  4-Carbomethoxyhomocubane
  Group-member nr.: 45-139/S1
- Phenylmethyl 2-methyl-2-propenoate [2495-37-6]
  Phenylmethyl ester 2-methyl-2-propenoic acid
  Benzyl methacrylate
  Group-member nr.: 45-087

$C_{11}H_{14}$
- 1,1-Dimethylindan [4912-92-9]
  Group-member nr.: 14-046
- 4,6-Dimethylindan [1685-82-1]

Group-member nr.: 14-047
• 4,7-Dimethylindan [6682-71-9]
Group-member nr.: 14-048
• (2-Methyl-1-methylenepropyl)benzene [17498-71-4]
α-Isopropylstyrene
Group-member nr.: 14-107/S1
• Octahydro-1,2,4-ethanylylidene-1*H*-cyclobuta [*cd*]pentalene [4421-32-3]
Pentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]undecane
Group-member nr.: 12-128/S1

$C_{11}H_{14}O_2$
• Butyl benzoate [136-60-7]
Group-member nr.: 45-140/S1
• Ethyl benzenepropanoate [2021-28-5]
Ethyl ester benzenepropanoic acid
Ethyl 3-phenylpropanoate
Ethyl hydrocinnamate
Group-member nr.: 45-088

$C_{11}H_{14}O_3$
• 1,1-Dimethylethyl ester benzenecarboperoxoic acid [614-45-9]
tert-Butyl peroxybenzoate
tert-Butyl perbenzoate
Group-member nr.: 47-065/S1

$C_{11}H_{16}$
• Pentamethylbenzene [700-12-9]
Group-member nr.: 14-049

$C_{11}H_{16}O$
• 2-(1,1-Dimethylethyl)-5-methylphenol [88-60-8]
2-*tert*-Butyl-5-methylphenol
Group-member nr.: 42-116/S1

$C_{11}H_{16}Si$
• Ethenyldimethyl(phenylmethyl)silane [18001-46-2]
Benzyldimethylvinylsilane
Group-member nr.: 71-031

$C_{11}H_{19}NO_2$
• Ethyl ester 2-cyano-3-methyl-2-(1-methylethyl)butanoic acid [62391-95-1]
Ethyl ester 2-cyano-2-isopropyl-3-methylbutyric acid
Group-member nr.: 62-166/S1

$C_{11}H_{20}$
• Decahydro-1-methylnaphthalene [2958-75-0]
α-Methyldecalin
Group-member nr.: 12-059
• Decahydro-2-methylnaphthalene [2958-76-1]
β-Methyldecalin
Group-member nr.: 12-060
• Ethyloctahydro-1*H*-indene [95098-51-4]
Ethylhexahydroindan
Ethylhydrindan (unspecified isomer)
Group-member nr.: 12-061

$C_{11}H_{20}O_2$
• Oxacyclododecan-2-one [1725-03-7]
Undecanolide
Undecanolactone
Group-member nr.: 47-040

$C_{11}H_{22}$
• 1-Undecene [821-95-4]
α-Undecene
Group-member nr.: 13-036

$C_{11}H_{22}O_2$
• Methyl decanoate [110-42-9]
Methyl caprate
Group-member nr.: 45-089
• Nonyl acetate [143-13-5]
Group-member nr.: 45-141/S1
• Undecanoic acid [112-37-8]
Undecylic acid
Group-member nr.: 44-026

$C_{11}H_{24}$
• 2-Methyldecane [6975-98-0]
Group-member nr.: 11-047
• Undecane [1120-21-4]
Hendecane
Group-member nr.: 11-048

$C_{11}H_{24}O$
• 1-Methoxydecane [7289-52-3]
Decyl methyl ether
Group-member nr.: 41-045
• 1-Undecanol [112-42-5]
Undecyl alcohol
Decyl carbinol
1-Hendecanol
Group-member nr.: 42-094

$C_{12}F_{10}$
• 2,2′,3,3′,4,4′,5,5′,6,6′-Decafluoro-1,1′-biphenyl [434-90-2]
Decafluorobiphenyl
Perfluorobiphenyl
Group-member nr.: 21-033

$C_{12}F_{26}$
• Hexacosafluorododecane [307-59-5]
Perfluorododecane
Group-member nr.: 21-052/S1

$C_{12}H_8$
• Acenaphthylene [208-96-8]
Group-member nr.: 14-050

$C_{12}H_8Cl_2O_2S$
• 1,1′-Sulfonylbis(4-chlorobenzene) [80-07-9]
Bis(*p*-chlorophenyl)sulfone
4,4′-Dichlorodiphenyl sulfone
Group-member nr.: 64-027

$C_{12}H_8N_2O_5$
• 1,1′-Oxybis(4-nitrobenzene) [101-63-3]
Bis(*p*-nitrophenyl) ether
4,4′-Dinitrodiphenyl ether
Group-member nr.: 62-089

$C_{12}H_8O$
- Dibenzofuran [132-64-9]
  Diphenylene oxide
  Group-member nr.: 46-026/B+S1[E]

$C_{12}H_8OS$
- Phenoxathiin [262-20-4]
  Group-member nr.: 63-007/S1

$C_{12}H_8OS_2$
- Dibenzo[*c*,*e*][1,2]dithiin-5-oxide [49833-13-8]
  Diphenylene 2,2′-disulfide-*S*-oxide
  Group-member nr.: 63-006

$C_{12}H_8S$
- Dibenzothiophene [132-65-0]
  Group-member nr.: 53-013/B+S1

$C_{12}H_8S_2$
- Thianthrene [92-85-3]
  Group-member nr.: 53-014/S1

$C_{12}H_9Cl$
- 2-Chloro-1,1′-biphenyl [2051-60-7]
  o-Chlorobiphenyl
  o-Chlorodiphenyl
  Group-member nr.: 22-046
- 4-Chloro-1,1′-biphenyl [2051-62-9]
  p-Chlorobiphenyl
  p-Chlorodiphenyl
  Group-member nr.: 22-047

$C_{12}H_9Cl_3Si$
- [1,1′-Biphenyl]-2-yltrichlorosilane [18030-62-1]
  o-(Trichlorosilyl)biphenyl
  o-Trichlorosilanediphenyl
  Group-member nr.: 71-032
- [1,1′-Biphenyl]-4-yltrichlorosilane [18030-61-0]
  p-(Trichlorosilyl)biphenyl
  p-Trichlorosilanediphenyl
  Group-member nr.: 71-033

$C_{12}H_{10}$
- Acenaphthene [83-32-9]
  1,8-Dihydroacenaphthalene
  Ethylenenaphthalene
  Group-member nr.: 14-051
- 1,1′-Biphenyl [92-52-4]
  Diphenyl
  Group-member nr.: 14-052/B+S1[E]

$C_{12}H_{10}N_2$
- Diphenyldiazene [103-33-3]
  Azobenzene
  Diphenyldiimide (unspecified stereoisomer)
  Group-member nr.: 34-011/B+S1
- (*E*)-Diphenyldiazene [17082-12-1]
  trans-Azobenzene
  trans-Diphenyldiimide
  Group-member nr.: 34-012/B+S1

$C_{12}H_{10}N_2O$
- 1-Oxide diphenyldiazene [495-48-7]
  N,*N*-Diphenyldiazene *N*-oxide
  Azoxybenzene
  Group-member nr.: 62-167/S1

$C_{12}H_{10}O$
- 1,1′-Oxybisbenzene [101-84-8]
  Diphenyl ether
  Diphenyl oxide
  Group-member nr.: 41-046

$C_{12}H_{10}S$
- 1,1′-Thiobisbenzene [139-66-2]
  Diphenyl sulfide
  Phenyl sulfide
  Group-member nr.: 51-023/B+S1

$C_{12}H_{10}Te$
- Diphenyltelluride [1202-36-4]
  Group-member nr.: 73-043/S1

$C_{12}H_{11}N$
- (1,1′-Biphenyl)-2-amine [90-41-5]
  2-Aminobiphenyl
  Group-member nr.: 31-041
- *N*-Phenylbenzenamine [122-39-4]
  Diphenylamine
  Group-member nr.: 31-042/B+S1

$C_{12}H_{12}$
- 1,8-Dimethylnaphthalene [569-41-5]
  Group-member nr.: 14-053
- 2,3-Dimethylnaphthalene [581-40-8]
  Group-member nr.: 14-054
- 2,6-Dimethylnaphthalene [581-42-0]
  Group-member nr.: 14-055
- 2,7-Dimethylnaphthalene [582-16-1]
  Group-member nr.: 14-056/B+S1

$C_{12}H_{12}Ge$
- Diphenylgermane [1675-58-7]
  Group-member nr.: 73-029

$C_{12}H_{12}N_2O$
- 4,4′-Oxybisbenzenamine [101-80-4]
  4,4′-Oxydianiline
  4,4′-Diaminodiphenyl ether
  Group-member nr.: 62-090

$C_{12}H_{12}N_2O_2S$
- 4,4′-Sulfonylbisbenzenamine [80-08-0]
  4,4′-Sulfonyldianiline
  4-Aminophenyl sulfone
  Dapsone
  Group-member nr.: 64-028

$C_{12}H_{14}N_4O$
- 4,4′-Oxybis-1,2-benzenediamine [2676-59-7]
  3,3′,4,4′-Tetraaminodiphenyl oxide
  3,3′,4,4′-Tetraaminodiphenyl ether
  Group-member nr.: 62-168/S1

$C_{12}H_{14}O_4$
- Diethyl 1,2-benzenedicarboxylate [84-66-2]

Diethyl phthalate
Diethyl ester 1,2-benzenedicarboxylic acid
Group-member nr.: 45-090/B+S1

- Diethyl 1,4-benzenedicarboxylate [636-09-9]
Diethyl terephthalate
Diethyl ester 1,4-benzenedicarboxylic acid
Group-member nr.: 45-091
- Monobutyl ester 1,2-benzenedicarboxylic acid [131-70-4]
Monobutyl phthalate
Group-member nr.: 45-142/S1

$C_{12}H_{16}$

- Cyclohexylbenzene [827-52-1]
Phenylcyclohexane
Group-member nr.: 14-057
- (2,2-Dimethyl-1-methylenepropyl)benzene [5676-29-9]
α-*tert*-Butylstyrene
Group-member nr.: 14-108/S1

$C_{12}H_{18}$

- 1,3-Bis(1-methylethyl)benzene [99-62-7]
1,3-Diisopropylbenzene
m-Diisopropylbenzene
Group-member nr.: 14-109/S1
- 1,4-Bis(1-methylethyl)benzene [100-18-5]
1,4-Diisopropylbenzene
p-Diisopropylbenzene
Group-member nr.: 14-110/S1
- (E,E,Z)-1,5,9-Cyclododecatriene [706-31-0]
trans,trans,cis-1,5,9-Cyclododecatriene
Group-member nr.: 14-058
- Decahydrodimethanonaphthalene [unknown]
Dimethanodecalin (unspecified isomer)
Group-member nr.: 12-062
- Hexamethylbenzene [87-85-4]
Mellitene
Group-member nr.: 14-059
- Hexylbenzene [1077-16-3]
1-Phenylhexane
Group-member nr.: 14-060
- 1,3,5-Triethylbenzene [102-25-0]
Group-member nr.: 14-111/S1

$C_{12}H_{18}O$

- 2,6-Bis(1-methylethyl)phenol [2078-54-8]
2,6-Diisopropylphenol
Group-member nr.: 42-117/S1
- 2-(1,1-Dimethylethyl)-4,6-dimethylphenol [1879-09-0]
2-*tert*-Butyl-4,6-dimethylphenol
Group-member nr.: 42-118/S1

$C_{12}H_{19}N$

- 2,6-Bis(1-methylethyl)benzenamine [24544-04-5]
2,6-Diisopropylphenylamine
2,6-Diisopropylaniline
Group-member nr.: 31-063/S1

$C_{12}H_{20}$

- 1,3-Dimethyltricyclo[3.3.1.1^{3,7}]decane [702-79-4]
1,3-Dimethyladamantane
Group-member nr.: 12-063/B+S1
- Dodecahydroacenaphtylene [2146-36-3]
Perhydroacenaphthylene
Tricyclo[7.2.1.0^{5,12}]dodecane (mixture of stereoisomers)
Group-member nr.: 12-129/S1
- (3aα,4β,7β,7aα)-Octahydrodimethyl-4,7-methano-1*H*-indene [28014-61-1]
exo-Tetrahydrodi(methylcyclopentadiene)
Group-member nr.: 12-130/S1
- Tricyclo[6.2.1.1^{3,6}]dodecane [281-84-5]
Group-member nr.: 12-064

$C_{12}H_{20}O$

- 2,5-Bis(1,1-dimethylethyl)furan [4789-40-6]
2,5-Di-*tert*-butylfuran
Group-member nr.: 46-031/S1

$C_{12}H_{20}O_6$

- 1,2,3-Propanetriyl tripropanoate [139-45-7]
1,2,3-Propanetriyl ester propanoic acid
Tripropionin
Group-member nr.: 45-092

$C_{12}H_{22}$

- 1,1′-Bicyclohexyl [92-51-3]
Cyclohexylcyclohexane
Dodecahydrobiphenol
Group-member nr.: 12-065
- Decahydrodimethylnaphthalene [28777-88-0]
Dimethyldecalin (unspecified isomer)
Group-member nr.: 12-066
- Ethyldecahydronaphthalene [25551-49-9]
Ethyldecalin (unspecified isomer)
Group-member nr.: 12-067
- 1-Ethyldecahydronaphthalene [1008-17-9]
1-Ethyldecalin
α-Ethyldecalin (unspecified stereoisomer)
Group-member nr.: 12-068
- 2-Ethyldecahydronaphthalene [1618-23-1]
2-Ethyldecalin
β-Ethyldecalin (unspecified stereoisomer)
Group-member nr.: 12-069
- Octahydro(1-methylethyl)-1*H*-indene [88889-26-3]
Hexahydroisopropylindan
Isopropylhydrindan (unspecified isomer)
Group-member nr.: 12-070

$C_{12}H_{22}O$

- *trans*-[1,1′-Bicyclohexyl]-2-ol [58879-21-3]
trans-2-Cyclohexylcyclohexanol
Group-member nr.: 42-119/S1

$C_{12}H_{22}O_2$

- Nonyl 2-propenoate [2664-55-3]
Nonyl ester 2-propenoic acid
Nonyl acrylate
Group-member nr.: 45-093
- Octyl 2-methyl-2-propenoate [2157-01-9]
Octyl ester 2-methyl-2-propenoic acid
Octyl methacrylate

Group-member nr.: 45-094

$C_{12}H_{22}O_4$
- Bis(3-methylbutyl) ethanedioate [2051-00-5]
  Bis(3-methylbutyl) ester ethanedioic acid
  Diisoamyl oxalate
  Group-member nr.: 45-095
- Bis(2-methylpropyl) butanedioate [925-06-4]
  Bis(2-methylpropyl) ester butanedioic acid
  Diisobutyl succinate
  Group-member nr.: 45-096
- Dibutyl butanedioate [141-03-7]
  Dibutyl ester butanedioic acid
  Dibutyl succinate
  Group-member nr.: 45-097

$C_{12}H_{22}O_4Pb$
- Lead(2+) salt hexanoic acid [15773-53-2]
  Lead(II) hexanoate
  Lead(II) caproate
  Group-member nr.: 74-004

$C_{12}H_{22}S$
- 1,1′-Thiobiscyclohexane [7133-46-2]
  Dicyclohexyl sulfide
  Group-member nr.: 51-030/S1

$C_{12}H_{24}$
- 1-Dodecene [112-41-4]
  α-Dodecylene
  Group-member nr.: 13-037

$C_{12}H_{24}N_2O_2$
- *N*,*N*′-Dipropylhexanediamine [10263-96-4]
  N,*N*′-Dipropyladipamide
  Group-member nr.: 62-091

$C_{12}H_{24}O_2$
- Decyl acetate [112-17-4]
  Group-member nr.: 45-098/B+S1
- Dodecanoic acid [143-07-7]
  Lauric acid
  Group-member nr.: 44-027

$C_{12}H_{25}NO$
- *N*,*N*-Dipentylacetamide [16238-16-7]
  Group-member nr.: 62-092

$C_{12}H_{26}$
- Dodecane [112-40-3]
  Group-member nr.: 11-049/B+S1^E
- 2,2,4,6,6-Pentamethylheptane [13475-82-6]
  Group-member nr.: 11-050

$C_{12}H_{26}O$
- 1-Dodecanol [112-53-8]
  Dodecyl alcohol
  Lauryl alcohol
  Group-member nr.: 42-095/B+S1

$C_{12}H_{26}O_3$
- 1,1′-[Oxybis(2,1-ethanediyloxy)]bisbutane [112-73-2]
  Bis(2-butoxyethyl)ether
  Diethylene glycol dibutyl ether
  5,8,11-Trioxapentadecane
  Group-member nr.: 41-047/B+S1

$C_{12}H_{26}O_5$
- 2-[2-[2-(2-Hydroxypropoxy)propoxy]propoxy]-1-propanol [24800-25-7]
  Tetra(propylene glycol)
  Group-member nr.: 47-066/S1

$C_{12}H_{26}O_7$
- 3,6,9,12,15-Pentaoxaheptadecane-1,17-diol [2615-15-8]
  Hexa(ethylene glycol)
  Group-member nr.: 47-067/S1

$C_{12}H_{26}S$
- 1,1′-Thiobishexane [6294-31-1]
  7-Thiatridecane
  Dihexyl sulfide
  Group-member nr.: 51-024

$C_{12}H_{27}O_4P$
- Tributyl ester phosphoric acid [126-73-8]
  Tributyl phosphate
  Group-member nr.: 72-019/S1

$C_{12}H_{28}O_4Si$
- Tetrapropyl ester silicic acid [682-01-9]
  Tetrapropyl orthosilicate
  Tetrapropoxysilane
  Group-member nr.: 71-034

$C_{12}H_{30}OSi_2$
- Hexaethyldisiloxane [994-49-0]
  Group-member nr.: 71-035

$C_{12}H_{30}O_3Si_3$
- Hexaethylcyclotrisiloxane [2031-79-0]
  Group-member nr.: 71-036

$C_{13}H_9F_3N_2O_2$
- 2-[[3-(Trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid [4394-00-7]
  Niflumic acid
  Group-member nr.: 64-040/S1

$C_{13}H_9N$
- Acridine [260-94-6]
  Benzo[*b*]quinoline
  2,3,5,6-Dibenzopyridine
  Group-member nr.: 33-042
- Benzo[*h*]quinoline [230-27-3]
  7,8-Benzoquinoline
  Group-member nr.: 33-043
- Phenanthridine [229-87-8]
  Benzo[*c*]quinoline
  Group-member nr.: 33-044

$C_{13}H_{10}$
- 9*H*-Fluorene [86-73-7]
  α-Diphenylenemethane
  Group-member nr.: 14-061/B+S1

$C_{13}H_{10}N_2$
- *N*,*N*′-Methanetetraylbisbenzenamine [622-16-2]

Diphenylcarbodiimide
Group-member nr.: 34-013

$C_{13}H_{10}O$
• Diphenyl methanone [119-61-9]
Diphenyl ketone
Benzophenone
Group-member nr.: 43-051

$C_{13}H_{10}O_3$
• Phenyl ester 2-hydroxybenzoic acid [118-55-8]
Phenyl salicylate
Salol
Group-member nr.: 47-041

$C_{13}H_{11}Cl$
• 1,1′-(Chloromethylene)bisbenzene [90-99-3]
Diphenylchloromethane
Group-member nr.: 22-048

$C_{13}H_{11}N$
• 9-Methyl-9*H*-carbazole [1484-12-4]
Group-member nr.: 33-045

$C_{13}H_{12}$
• 1,1′-Methylenebisbenzene [101-81-5]
Diphenylmethane
Benzylbenzene
Group-member nr.: 14-062

$C_{13}H_{13}N$
• *N*-Methyl-*N*-phenylbenzenamine [552-82-9]
N-Methyldiphenylamine
Group-member nr.: 31-043

$C_{13}H_{14}N_2$
• 4,4′-Methylenebisbenzenamine [101-77-9]
4,4′-Methylenedianiline
Bis-(4-aminophenyl)methane
Group-member nr.: 31-044

$C_{13}H_{15}N$
• 2,3,4,9-Tetrahydro-9-methyl-1*H*-carbazole [6303-88-4]
1,2,3,4-Tetrahydro-9-methylcarbazole
Group-member nr.: 33-046

$C_{13}H_{15}NO$
• 1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl)benzene [2094-99-7]
m-Isopropenyl-α,α-dimethylbenzyl ester isocyanic acid
Group-member nr.: 62-093
• 1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl)benzene [2889-58-9]
p-Isopropenyl-α,α-dimethylbenzyl ester isocyanic acid
Group-member nr.: 62-094

$C_{13}H_{18}$
• 1,1,4,6-Tetramethylindan [941-60-6]
Group-member nr.: 14-063
• 1,1,4,7-Tetramethylindan [1078-04-2]
Group-member nr.: 14-064

$C_{13}H_{19}NO_2$
• Hexyl ester phenylcarbamic acid [7461-26-9]
Hexyl phenylcarbamate
Hexyl ester carbanilic acid
Group-member nr.: 62-095

$C_{13}H_{20}$
• Heptylbenzene [1078-71-3]
1-Phenylheptane
Group-member nr.: 14-065

$C_{13}H_{20}O$
• 6,10-Dimethyl-3,5,9-undecatriene-2-one [141-10-6]
Pseudoionone
ψ-Ionone
Group-member nr.: 43-052
• 6,10-Dimethyl-4,5,9-undecatriene-2-one [16647-05-5]
Group-member nr.: 43-053
• 4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one [14901-07-6]
β-Ionone
Group-member nr.: 43-054

$C_{13}H_{22}$
• 1,3,5-Trimethyltricyclo[3.3.1.1^{3,7}]decane [707-35-7]
1,3,5-Trimethyladamantane
Group-member nr.: 12-071

$C_{13}H_{24}$
• Decahydro(1-methylethyl)naphthalene [27193-29-9]
Isopropyldecalin (unspecified isomer)
Group-member nr.: 12-072
• Decahydro-1-(1-methylethyl)naphthalene [1010-74-8]
Decahydro-1-isopropylnaphthalene
α-Isopropyldecalin
Group-member nr.: 12-073
• Decahydro-1-propylnaphthalene [91972-45-1]
1-Propyldecalin
α-Propyldecalin
Group-member nr.: 12-074
• 2-Methyl-1,1′-bicyclohexyl [66324-47-8]
1-Methylcyclohexylcyclohexane
Group-member nr.: 12-075
• 1,1′-Methylenebiscyclohexane [3178-23-2]
Dicyclohexylmethane
Group-member nr.: 12-076

$C_{13}H_{24}O_2$
• Nonyl 2-methyl-2-propenoate [2696-43-7]
Nonyl ester 2-methyl-2-propenoic acid
Nonyl methacrylate
Group-member nr.: 45-099
• Oxacyclotetradecan-2-one [1725-04-8]
Tridecanolide
Tridecanolactone
Group-member nr.: 47-042

$C_{13}H_{25}NO_3$
• α-[(Cyclohexyloxy)methyl]-4-morpholineethanol [95639-17-1]
1-Morpholino-3-cyclohexyloxy-2-propanol
Group-member nr.: 62-169/S1

$C_{13}H_{26}$
- Heptylcyclohexane [5617-41-4]
  Group-member nr.: 12-077

$C_{13}H_{26}O$
- 6,10-Dimethyl-2-undecanone [1604-34-8]
  Hexahydropseudoionone
  Group-member nr.: 43-055

$C_{13}H_{26}O_2$
- Tridecanoic acid [638-53-9]
  Tridecylic acid
  Group-member nr.: 44-028
- Undecyl acetate [1731-81-3]
  Group-member nr.: 45-143/S1

$C_{13}H_{26}O_2Si_3$
- 1,1,1,3,5,5,5-Heptamethyl-3-phenyltrisiloxane [546-44-1]
  Group-member nr.: 71-037

$C_{13}H_{28}$
- Tridecane [629-50-5]
  Group-member nr.: 11-051

$C_{13}H_{28}O$
- 5-Butyl-5-nonanol [597-93-3]
  Group-member nr.: 42-096
- 1-Tridecanol [112-70-9]
  n-Tridecyl alcohol
  Group-member nr.: 42-097/B+S1^E

$C_{14}F_{30}$
- Triacontafluorotetradecane [307-62-0]
  Perfluorotetradecane
  Group-member nr.: 21-053/S1

$C_{14}H_8O_2$
- 9,10-Anthracenedione [84-65-1]
  9,10-Antraquinone
  Group-member nr.: 43-056

$C_{14}H_{10}$
- Anthracene [120-12-7]
  Group-member nr.: 14-066/B+S1^E
- 1,1′-(1,2-Ethynediyl)bisbenzene [501-65-5]
  1,2-Diphenylacetylene
  Tolan
  Group-member nr.: 14-067
- Phenanthrene [85-01-8]
  Group-member nr.: 14-068/B+S1^E

$C_{14}H_{12}$
- (*E*)-1,1′-(1,2-Ethenediyl)bisbenzene [103-30-0]
  trans-1,2-Diphenylethylene
  Stilbene
  Toluylene
  Group-member nr.: 14-070
- 1,1′-Ethenylidenebisbenzene [530-48-3]
  1,1-Diphenylethylene
  Group-member nr.: 14-071/B+S1^E
- 9,10-Dihydroanthracene [613-31-0]
  Group-member nr.: 14-112/S1
- 9,10-Dihydrophenanthrene [776-35-2]
  Group-member nr.: 14-069

$C_{14}H_{12}O$
- (3-Methylphenyl)phenylmethanone [643-65-2]
  3-Methylbenzophenone
  Phenyl *m*-tolyl ketone
  Group-member nr.: 43-057

$C_{14}H_{12}O_4$
- Dimethyl ester 2,6-naphthalenedicarboxylic acid [840-65-3]
  Group-member nr.: 45-144/S1

$C_{14}H_{14}$
- 2,2′-Dimethyl-1,1′-biphenyl [605-39-0]
  2,2′-Dimethylbiphenyl
  Group-member nr.: 14-113/S1
- 1,1′-(1,2-Ethanediyl)bisbenzene [103-29-7]
  Bibenzyl
  1,2-Diphenylethane
  sym-Diphenylethane
  Dibenzyl
  Group-member nr.: 14-072
- 2-Ethyl-1,1′-biphenyl [1812-51-7]
  2-Ethylbiphenyl
  Group-member nr.: 14-114/S1
- 1,1′-Ethylidenebisbenzene [612-00-0]
  1,1-Diphenylethane
  unsym-Diphenylethane
  Group-member nr.: 14-073/B+S1^E
- 1-Methyl-2-(phenylmethyl)benzene [713-36-0]
  Phenyl-*o*-tolylmethane
  Group-member nr.: 14-115/S1
- 1,2,3,4-Tetrahydroanthracene [2141-42-6]
  Group-member nr.: 14-116/S1
- 1,2,3,4-Tetrahydrophenanthrene [1013-08-7]
  Group-member nr.: 14-117/S1

$C_{14}H_{14}N_2O_3$
- Bis(4-methoxyphenyl)diazene-1-oxide [1562-94-3]
  4,4′-Dimethoxyazoxybenzene
  p-Azoxyanisole
  Group-member nr.: 62-096

$C_{14}H_{14}O$
- 1,1′-[Oxybis(methylene)]bisbenzene [103-50-4]
  Dibenzyl ether
  Group-member nr.: 41-050/S1

$C_{14}H_{16}$
- Dodecahydro-1,3,4,6-ethanediylidenedicyclopenta-[*cd*,*gh*]pentalene [17872-39-8]
  Heptacyclo[6.6.0^{2,6}.0^{3,13}.0^{4,11}.0^{5,9}.0^{10,14}]tetradecane
  Group-member nr.: 12-131/S1

$C_{14}H_{16}N_2O_2$
- 1,3-Bis(1-isocyanato-1-methylethyl)benzene [2778-42-9]
  $\alpha,\alpha,\alpha',\alpha'$-Tetramethyl-*m*-xylylene ester isocyanic acid
  Group-member nr.: 62-097
- 1,4-Bis(1-isocyanato-1-methylethyl)benzene [2778-41-8]
  $\alpha,\alpha,\alpha',\alpha'$-Tetramethyl-*p*-xylylene ester isocyanic acid
  Group-member nr.: 62-098

$C_{14}H_{18}$
• Dodecahydro-4,7-methano-2,3,8-methenocyclopent[*a*]indene (stereoisomer HNN) [66289-74-5]
Hexacyclic *endo,endo*-dihydrodinorbornadiene
Group-member nr.: 12-132/S1
• Dodecahydro-4,7-methano-2,3,8-methenocyclopent[*a*]indene (stereoisomer HXN) [66289-73-4]
Hexacyclic *exo,endo*-dihydronorbornadiene
Group-member nr.: 12-133/S1
• Dodecahydro-4,7-methano-2,3,8-methenocyclopent[*a*]indene (stereoisomer HXX) [64162-49-8]
Hexacyclic *exo,exo*-dihydrodinorbornadiene
Group-member nr.: 12-134/S1
• 1,2,3,4,5,6,7,8-Octahydroanthracene [1079-71-6]
Group-member nr.: 14-074

$C_{14}H_{20}$
• Decahydro-3,5,1,7-[1,2,3,4]butanetetraylnaphthalene [2292-79-7]
Diamantane
Group-member nr.: 12-078
• Dodecahydro-1,4:5,8-dimethanobiphenylene [25079-41-8]
Pentacyclic *exo,trans,exo*-tetrahydrodinorbornadiene
Group-member nr.: 12-135/S1

$C_{14}H_{20}O_3$
• 1-[4-(1,1-Diethoxyethyl)phenyl]ethanone [64533-95-5]
p-Diacetylbenzene diethyl ketal
Group-member nr.: 47-043

$C_{14}H_{22}$
• Octylbenzene [2189-60-8]
1-Phenyloctane
Group-member nr.: 14-075

$C_{14}H_{22}N_2O$
• 1-Anilino-3-piperidino-2-propanol [14585-29-6]
Group-member nr.: 62-170/S1

$C_{14}H_{23}NO_2$
• Decyl ester 2-cyano-2-propenoic acid [3578-07-2]
n-Decyl α-cyanacrylate
Group-member nr.: 62-171/S1

$C_{14}H_{24}$
• Dodecahydro-9-methylfluorene [92431-75-9]
9-Methylperhydrofluorene
Group-member nr.: 12-079
• Tetradecahydrophenanthrene [5743-97-5]
Perhydrophenanthrene
Perhydrophenanthrene
Tricyclo[8.4.0.0^{2,7}]tetradecane (mixture of stereoisomers)
Group-member nr.: 12-080/B+S1
• (4aα,4bα,8aα,10aβ)-Tetradecahydrophenanthrene [27425-35-0]
cis-syn-trans-Perhydrophenantrene
Group-member nr.: 12-081
• (4aα,4bβ,8aα,10aα)-Tetradecahydrophenanthrene [27389-73-7]
trans-anti-cis-Perhydrophenanthrene
Group-member nr.: 12-082
• (4aα,4bβ,8aα,10aβ)-Tetradecahydrophenanthrene [2108-89-6]
trans-anti-trans-Perhydrophenanthrene
Group-member nr.: 12-083

$C_{14}H_{26}$
• 1-Butyldecahydronaphthalene [92369-80-7]
1-Butyldecalin
α-Butyldecalin
Group-member nr.: 12-084
• 1-(Cyclohexylmethyl)-2-methylcyclohexane [66826-96-8]
Cyclohexyl(2-methylcyclohexyl)methane
Group-member nr.: 12-085
• Decahydro-1-(1-methylpropyl)naphthalene [92369-82-9]
1-*sec*-Butyldecahydronaphthalene
α-*sec*-Butyldecalin
Group-member nr.: 12-086
• Decahydro-1-(2-methylpropyl)naphthalene [92369-83-0]
Decahydro-1-isobutylnaphthalene
α-Isobutyldecalin
Group-member nr.: 12-087
• (1,1-Dimethylethyl)decahydronaphthalene [27193-30-2]
tert-Butyldecalin (unspecified isomer)
Group-member nr.: 12-088
• 1,1′-(1,2-Ethanediyl)biscyclohexane [3321-50-4]
1,2-Dicyclohexylethane
Group-member nr.: 12-089
• 2-Ethyl-1,1′-bicyclohexyl [66826-94-6]
2-Ethylcyclohexylcyclohexane
Group-member nr.: 12-090
• 1,1′-Ethylidenebiscyclohexane [2319-61-1]
1,1-Dicyclohexylethane
Group-member nr.: 12-091

$C_{14}H_{26}O$
• 2-(1,2-Dimethylpropyl)-5,6-dimethyl-2-heptenal [99914-84-8]
Group-member nr.: 43-058
• 2-Pentyl-2-nonenal [3021-89-4]
Group-member nr.: 43-059

$C_{14}H_{26}O_2$
• Decyl 2-methyl-2-propenoate [3179-47-3]
Decyl ester 2-methyl-2-propenoic acid
Decyl methacrylate
Group-member nr.: 45-100

$C_{14}H_{26}O_4$
• Bis(3-methylbutyl) butanedioate [818-04-2]
Bis(3-methylbutyl) ester butanedioic acid
Diisoamyl succinate
Group-member nr.: 45-101
• Dibutyl ester hexanedioic acid [105-99-7]
Dibutyl adipate
Group-member nr.: 45-145/S1

$C_{14}H_{26}O_4Pb$
• Lead(2+) salt heptanoic acid [16180-10-2]
Lead(II) heptanoate
Lead(II) oenanthate
Group-member nr.: 74-028/S1

$C_{14}H_{27}NO_2$
• α-[(Cyclohexyloxy)methyl]-1-piperidineethanol [96450-92-9]
1-Piperidino-3-cyclohexoxy-2-propanol
Group-member nr.: 62-172/S1

$C_{14}H_{28}O$
• 2-Tetradecanone [2345-27-9]
Dodecyl methyl ketone
Group-member nr.: 43-060

$C_{14}H_{28}O_2$
• Dodecyl acetate [112-66-3]
Group-member nr.: 45-146/S1
• Tetradecanoic acid [544-63-8]
Myristic acid
Group-member nr.: 44-029

$C_{14}H_{30}$
• Tetradecane [629-59-4]
Group-member nr.: 11-052/B+S1[E]

$C_{14}H_{30}O$
• 1-Tetradecanol [112-72-1]
n-Tetradecyl alcohol
Myristyl alcohol
Group-member nr.: 42-098/B+S1

$C_{14}H_{30}S$
• 1,1′-Thiobisheptane [629-65-2]
8-Thiapentadecane
Diheptyl sulfide
Group-member nr.: 51-025

$C_{15}H_{10}N_2O_2$
• 1,1′-Methylenebis[4-isocyanatobenzene] [101-68-8]
Methylenedi-*p*-phenylene ester isocyanic acid
Diphenylmethane-4,4′-diisocyanate
Group-member nr.: 62-099/B+S1

$C_{15}H_{12}$
• 4-Methylphenanthrene [832-64-4]
Group-member nr.: 14-076

$C_{15}H_{16}$
• (1-Methylethyl)-1,1′-biphenyl [25640-78-2]
Isopropylbiphenyl
Isopropyldiphenyl (unspecified isomer)
Group-member nr.: 14-077
• 1,1′-(1,3-Propanediyl)bisbenzene [1081-75-0]
1,3-Diphenylpropane
Group-member nr.: 14-118/S1

$C_{15}H_{16}N_2O_3$
• (4-Ethoxyphenyl)(4-methoxyphenyl)diazene-*N*-oxide [56095-14-8]
4-Ethoxy-4′-methoxyazoxybenzene
p-Azoxyanisoylphenetole
Group-member nr.: 62-100

$C_{15}H_{16}O_2$
• 4,4′-(1-Methylethylidene)bisphenol [80-05-7]
4,4′-Isopropylidenediphenol
4,4′-Dihydroxydiphenyl-2,2-propane
Group-member nr.: 42-099

$C_{15}H_{16}S_2$
• 1,1′-[(1-Methylethylidene)bis(thio)]bisbenzene [14252-46-1]
2,2′-Bis(phenylthio)propane
Group-member nr.: 51-031/S1

$C_{15}H_{24}$
• 1,3,5-Tris(1-methylethyl)benzene [717-74-8]
1,3,5-Triisopropylbenzene
Group-member nr.: 14-119/S1

$C_{15}H_{26}$
• 1,1′:3′,1″-Tercyclopentane [6051-40-7]
1,3-Dicyclopentylcyclopentane
Group-member nr.: 12-092

$C_{15}H_{26}O_6$
• 1,2,3-Propanetriyl tributanoate [60-01-5]
1,2,3-Propanetriyl ester butanoic acid
Tributyrin
Group-member nr.: 45-102

$C_{15}H_{28}$
• Cyclohexyl(ethylcyclohexyl)methane (unspecified isomer) [97239-02-6]
Group-member nr.: 12-093
• 1-(Cyclohexylmethyl)-2-ethylcyclohexane [66374-71-8]
Cyclohexyl(2-ethylcyclohexyl)methane
Group-member nr.: 12-094
• 1,2-Dicyclohexylpropane [41851-34-7]
Group-member nr.: 12-095
• (1-Methylethyl)-1,1′-bicyclohexyl [31624-59-6]
Isopropylbicyclohexyl
Isopropylcyclohexylcyclohexane (unspecified isomer and stereoisomer)
Group-member nr.: 12-096

$C_{15}H_{28}O$
• 3,7,11-Trimethyl-1-dodecyn-3-ol [1604-35-9]
Group-member nr.: 42-100

$C_{15}H_{28}O_2$
• Oxacyclohexadecan-2-one [106-02-5]
Pentadecanolide
Pentadecanolactone
15-Hydroxypentadecanoic acid lactone
Group-member nr.: 47-044

$C_{15}H_{30}$
• Decylcyclopentane [1795-21-7]
Cyclopentyldecane
Group-member nr.: 12-097

$C_{15}H_{30}InN_3S_6$
• Tri(diethylcarbamodithioato-*S*,*S*′)indium [15741-07-8]

Group-member nr.: 73-044/S1

$C_{15}H_{30}O$
- 2-Pentadecanone [2345-28-0]
  Methyl tridecyl ketone
  Group-member nr.: 43-061

$C_{15}H_{30}O_2$
- Methyl tetradecanoate [124-10-7]
  Methyl myristate
  Group-member nr.: 45-103
- Pentadecanoic acid [1002-84-2]
  Pentadecylic acid
  Group-member nr.: 44-030

$C_{15}H_{32}$
- Pentadecane [629-62-9]
  Group-member nr.: 11-053

$C_{15}H_{32}O$
- 1-Pentadecanol [629-76-5]
  n-Pentadecyl alcohol
  Group-member nr.: 42-101

$C_{15}H_{32}O_6$
- 2,5,8,11-Tetramethyl-3,6,9,12-tetraoxapentadecane-1,14-diol [21482-12-2]
  Penta(propylene glycol)
  Group-member nr.: 47-068/S1

$C_{16}F_{34}$
- Tetratriacontafluorohexadecane [355-49-7]
  Perfluorohexadecane
  Group-member nr.: 21-054/S1

$C_{16}H_{10}$
- Fluoranthene [206-44-0]
  Group-member nr.: 14-078/B+S1^E
- Pyrene [129-00-0]
  Group-member nr.: 14-079/B+S1^E

$C_{16}H_{12}Ge$
- Diethynyldiphenylgermane [1675-59-8]
  Group-member nr.: 73-030

$C_{16}H_{12}Si$
- Diethynyldiphenylsilane [1675-57-6]
  Group-member nr.: 71-038

$C_{16}H_{14}$
- 4,5,9,10-Tetrahydropyrene [781-17-9]
  Group-member nr.: 14-120/S1

$C_{16}H_{14}O_2$
- 1,4-Diphenyl-1,4-butanedione [495-71-6]
  1,2-Dibenzoylethane
  Group-member nr.: 43-062

$C_{16}H_{15}N$
- 4′-Propyl[1,1′-biphenyl]-4-carbonitrile [58743-76-3]
  4′-Propylbiphenyl-4-carbonitrile
  Group-member nr.: 32-029/S1

$C_{16}H_{16}$
- 1,2,3,6,7,8-Hexahydropyrene [1732-13-4]
  Group-member nr.: 14-121/S1

$C_{16}H_{16}N_2O_2$
- [(4-Methoxyphenyl)methylene]hydrazone-4-methoxybenzaldehyde [2299-73-2]
  p-Anisaldehydeazine
  Anisaldazine
  Group-member nr.: 62-101

$C_{16}H_{18}$
- 1,1′-(2-Methylpropylidene)bisbenzene [1634-11-3]
  2-Methyl-1,1-diphenylpropane
  Group-member nr.: 14-122/S1

$C_{16}H_{18}N_2O_3$
- Bis(4-ethoxyphenyl)diazene-1-oxide [4792-83-0]
  4,4′-Diethoxyazoxybenzene
  p-Azoxyphenetole
  Group-member nr.: 62-102

$C_{16}H_{20}Cr$
- Bis[(1,2,3,4,5,6-η)-ethylbenzene]chromium [12212-68-9]
  Bis(ethylbenzene)chromium
  Group-member nr.: 73-045/S1

$C_{16}H_{22}OSi_2$
- 1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane [56-33-7]
  Group-member nr.: 71-039/B+S1

$C_{16}H_{22}O_3Si_3$
- 2,2,4,4-Tetramethyl-6,6-diphenylcyclotrisiloxane [1693-51-2]
  Group-member nr.: 71-040

$C_{16}H_{22}O_4$
- Dibutyl 1,2-benzenedicarboxylate [84-74-2]
  Dibutyl ester 1,2-benzenedicarboxylic acid
  Dibutyl phthalate
  Group-member nr.: 45-104/B+S1

$C_{16}H_{25}NO_2$
- Nonyl phenylcarbamate [33689-71-3]
  Nonyl ester phenylcarbamic acid
  Nonyl ester carbanilic acid
  Group-member nr.: 62-103

$C_{16}H_{27}N$
- [*trans(trans)*]-4′-Propyl-[1,1′-bicyclohexyl]-4-carbonitrile [65355-35-3]
  trans,trans-4′-Propylbicyclohexyl-4-carbonitrile
  Group-member nr.: 32-030/S1

$C_{16}H_{28}$
- 1-Cyclohexyloctahydro-3-methyl-1*H*-indene [2320-05-0]
  1-Cyclohexyl-3-methylhydrindan
  Group-member nr.: 12-098
- 2-Ethyltetradecahydrophenanthrene [90591-84-7]
  2-Ethylperhydrophenanthrene
  Group-member nr.: 12-099

$C_{16}H_{30}$
- Cyclohexyl[(1-methylethyl)cyclohexyl]methane [97676-41-0]
  Cyclohexyl(isopropylcyclohexyl)methane (unspecified isomer)

Group-member nr.: 12-101
• 1,1′-(1-Methyl-1,3-propanediyl)biscyclohexane [41851-35-8]
1,3-Dicyclohexylbutane
Group-member nr.: 12-100

$C_{16}H_{30}HgO_4$
• Mercury(2+) salt octanoic acid [28043-54-1]
Mercury(II) octanoate
Mercury(II) caprylate
Group-member nr.: 74-005

$C_{16}H_{30}O_4Pb$
• Lead(2+) salt octanoic acid [7319-86-0]
Lead(II) octanoate
Lead(II) caprylate
Group-member nr.: 74-006

$C_{16}H_{32}$
• Decylcyclohexane [1795-16-0]
Cyclohexyldecane
Group-member nr.: 12-102
• 1-Hexadecene [629-73-2]
α-Hexadecylene
Cetene
Group-member nr.: 13-038

$C_{16}H_{32}O_2$
• Hexadecanoic acid [57-10-3]
Palmitic acid
Group-member nr.: 44-031/B+S1
• Tetradecyl acetate [638-59-5]
Group-member nr.: 45-147/S1

$C_{16}H_{34}$
• 2,2,4,4,6,8,8-Heptamethylnonane [4390-04-9]
Group-member nr.: 11-054/B+S1
• Hexadecane [544-76-3]
Cetane
Group-member nr.: 11-055/B+S1^E

$C_{16}H_{34}O$
• 1-Hexadecanol [36653-82-4]
n-Hexadecyl alcohol
Cetyl alcohol
Group-member nr.: 42-102/B+S1
• 1,1′-Oxybisoctane [629-82-3]
Dioctyl ether
Group-member nr.: 41-051/S1

$C_{16}H_{34}S$
• 1,1′-Thiobisoctane [2690-08-6]
9-Thiaheptadecane
Dioctyl sulfide
Group-member nr.: 51-026/B+S1

$C_{16}H_{35}N$
• *N*,*N*-Dimethyl-2-pentyl-1-nonanamine [99916-30-0]
N,*N*-Dimethyl-2-pentylnonylamine
Group-member nr.: 31-045
• *N*-Octyl-1-octanamine [1120-48-5]
N,*N*-Dioctylamine
Group-member nr.: 31-064/S1

$C_{16}H_{36}Ge$
• Tetrabutylgermane [1067-42-1]
Group-member nr.: 73-031

$C_{16}H_{36}O_4Si$
• Tetrabutyl ester silicic acid [4766-57-8]
Tetrabutyl orthosilicate
Tetrabutoxysilane
Group-member nr.: 71-041

$C_{16}H_{36}O_4Ti$
• Titanium(4+) salt 1-butanol [5593-70-4]
Tetrabutoxytitanium
Group-member nr.: 74-007

$C_{16}H_{40}O_4Si_4$
• Octaethylcyclotetrasiloxane [1451-99-6]
Group-member nr.: 71-042

$C_{17}H_{14}N_2O_2$
• (1-Methylethylidene)di-1,4-phenylene ester cyanic acid [1156-51-0]
2,2-Bis(4-cyanatophenyl)propane
Group-member nr.: 62-173/S1

$C_{17}H_{30}$
• Cyclopentylbicyclohexyl (unspecified isomer) [26447-22-3]
Group-member nr.: 12-103

$C_{17}H_{32}$
• Bis(ethylcyclohexyl)methane (unspecified isomer) [98028-64-9]
Group-member nr.: 12-104
• 1-Cyclohexyl-1-(1-methylethyl)cyclohexylethane [26637-18-3]
1-Cyclohexyl-1-(isopropylcyclohexyl)ethane (unspecified isomer)
Group-member nr.: 12-105

$C_{17}H_{34}O_2$
• Heptadecanoic acid [506-12-7]
Margaric acid
Group-member nr.: 44-032
• 1-Methylethyl ester tetradecanoic acid [110-27-0]
Isopropyl myristate
Group-member nr.: 45-148/S1

$C_{17}H_{36}$
• Heptadecane [629-78-7]
Group-member nr.: 11-056/B+S1

$C_{18}HF_{15}Ge$
• Tris[2,3,4,5,6-pentafluorophenyl]germane [42371-50-6]
Tri(pentafluorophenyl)germane
Group-member nr.: 73-046/S1

$C_{18}H_{12}$
• Triphenylene [217-59-4]
9,10-Benzophenanthrene
Group-member nr.: 14-080

$C_{18}H_{14}$
- 1,1′:2′,1″-Terphenyl [84-15-1]
  o-Terphenyl
  Group-member nr.: 14-081
- 1,1′:3′,1″-Terphenyl [92-06-8]
  m-Terphenyl
  Group-member nr.: 14-082
- 1,1′:4′,1″-Terphenyl [92-94-4]
  p-Terphenyl
  Group-member nr.: 14-083/B+S1^{E}

$C_{18}H_{15}ClSi$
- Chlorotriphenylsilane [76-86-8]
  Group-member nr.: 71-044

$C_{18}H_{15}OP$
- Triphenylphosphine oxide [791-28-6]
  Oxotriphenylphosphorane
  Oxotriphenylphosphorus
  Group-member nr.: 72-012

$C_{18}H_{15}O_4P$
- Triphenyl ester phosphoric acid [115-86-6]
  Triphenyl phosphate
  Group-member nr.: 72-013

$C_{18}H_{18}$
- 1-Methyl-7-(1-methylethyl)phenanthrene [483-65-8]
  7-Isopropyl-1-methylphenanthrene
  Retene
  Group-member nr.: 14-084

$C_{18}H_{18}N_2O_5$
- Diethyl ester 4,4′-azoxybisbenzoic acid [6421-04-1]
  Diethyl 4,4′-azoxybisbenzoate
  Ethyl-p,p-azoxybenzoate
  Group-member nr.: 62-104

$C_{18}H_{21}NO$
- 4-Butyl-*N*-[(4-methoxyphenyl)methylene]benzenamine [26227-73-6]
  N-(*p*-Methoxybenzylidene)-*p*-butylaniline
  MBBA
  Group-member nr.: 62-105

$C_{18}H_{21}NO_2$
- 2-[[(4-Butylphenyl)imino]methyl]-4-methoxyphenol [52218-22-1]
  N-(*o*-Hydroxy-*p*-methoxybenzylidene-*p*-butylaniline
  2,4-OHMBBA
  Group-member nr.: 62-106

$C_{18}H_{22}$
- *ar*,*ar*′-Bis(1-methylethyl)-1,1′-biphenyl [36876-13-8]
  Diisopropylbiphenyl (unspecified isomer)
  Group-member nr.: 14-085

$C_{18}H_{22}N_2O$
- (*E*)-(4-Butylphenyl)(4-ethoxyphenyl)diazene [98644-12-3]
  Group-member nr.: 62-107

$C_{18}H_{22}N_2O_3$
- Bis(4-propoxyphenyl)diazene-1-oxide [23315-55-1]
  4,4′-Dipropoxyazoxybenzene
  Group-member nr.: 62-108

$C_{18}H_{28}O_2Si_3$
- 1,1,1,5,5,5-Hexamethyl-3,3-diphenyltrisiloxane [797-77-3]
  Group-member nr.: 71-045

$C_{18}H_{28}O_4Si_4$
- 2,2,4,4,6,6-Hexamethyl-8,8-diphenylcyclotetrasiloxane [30026-85-8]
  Group-member nr.: 71-046

$C_{18}H_{30}$
- Dodecylbenzene [123-01-3]
  1-Phenyldodecane
  Group-member nr.: 14-123/S1
- 3-Ethylhexadecahydropyrene [94262-24-5]
  3-Ethylperhydropyrene
  Group-member nr.: 12-106

$C_{18}H_{30}O_4$
- 1,4-Bis(1,1-diethoxyethyl)benzene [47189-08-2]
  p-Diacetylbenzene tetraethyl ketal
  Ethylacetal *p*-diacetyl benzene
  Group-member nr.: 41-048

$C_{18}H_{32}$
- 1-Cyclohexyloctahydro-1,3,3-trimethyl-1*H*-indene [22236-61-9]
  1-Cyclohexyl-1,3,3-trimethylhydrindan
  Group-member nr.: 12-107
- 1,1′:2′,1″-Tercyclohexane [2456-43-1]
  o-Tercyclohexane
  Group-member nr.: 12-108
- 1,1′:3′,1″-Tercyclohexane [1706-50-9]
  m-Tercyclohexane
  Group-member nr.: 12-109
- 1,1′:4′,1″-Tercyclohexane [1795-19-3]
  p-Tercyclohexane
  Group-member nr.: 12-110

$C_{18}H_{32}O$
- 6,10,14-Trimethyl-3,5-pentadecadien-2-one [1604-32-6]
  Group-member nr.: 43-063

$C_{18}H_{34}$
- 1,1,-Bis(dimethylcyclohexyl)ethane (unspecified isomer) [98803-06-6]
  Group-member nr.: 12-112
- 1,1-Bis(ethylcyclohexyl)ethane (unspecified isomer) [98803-07-7]
  Group-member nr.: 12-111

$C_{18}H_{34}O_2$
- (*Z*)-9-Octadecenoic acid [112-80-1]
  Oleic acid
  Group-member nr.: 44-033/B+S1

$C_{18}H_{34}O_4$
- Dibutyl decanedioate [109-43-3]
  Dibutyl ester decanedioic acid
  Dibutyl sebacate
  Group-member nr.: 45-105

$C_{18}H_{34}O_4Pb$
• Lead(2+) salt nonanoic acid [63400-08-8]
Lead(II) nonanoate
Lead(II) pelargonate
Group-member nr.: 74-029/S1

$C_{18}H_{36}$
• Dodecylcyclohexane [1795-17-1]
Cyclohexyldodecane
Group-member nr.: 12-113
• Hexaethylcyclohexane (unspecified isomer) [98803-61-3]
Group-member nr.: 12-114

$C_{18}H_{36}N_2O_2$
• *N*,*N*′-Dihexylhexanediamide [21150-82-3]
N,*N*′-Dihexyladipamide
Group-member nr.: 62-109

$C_{18}H_{36}O$
• (*Z*)-9-Octadecen-1-ol [143-28-2]
Oleyl alcohol
Group-member nr.: 42-120/S1
• 6,10,14-Trimethyl-2-pentadecanone [502-69-2]
Phytone
Group-member nr.: 43-064

$C_{18}H_{36}O_2$
• Octadecanoic acid [57-11-4]
Stearic acid
Group-member nr.: 44-034/B+S1

$C_{18}H_{37}Cl$
• 1-Chlorooctadecane [3386-33-2]
Group-member nr.: 22-049

$C_{18}H_{38}$
• Octadecane [593-45-3]
Group-member nr.: 11-057/B+S1

$C_{18}H_{38}O$
• 1-Octadecanol [112-92-5]
n-Octadecyl alcohol
Stearyl alcohol
Group-member nr.: 42-103/B+S1

$C_{18}H_{38}O_7$
• 2,5,8,11,14-Pentamethyl-3,6,9,12,15-pentaoxaoctadecane [74388-92-4]
Hexa(propylene glycol)
Group-member nr.: 47-069/S1

$C_{18}H_{38}S$
• 1,1′-Thiobisnonane [929-98-6]
10-Thianonadecane
Dinonyl sulfide
Group-member nr.: 51-027

$C_{19}H_{15}Cl$
• 1,1′,1″-(Chloromethylidene)trisbenzene [76-83-5]
Triphenylchloromethane
Group-member nr.: 22-064/S1

$C_{19}H_{16}$
• 1,1′,1″-Methylidynetrisbenzene [519-73-3]
Triphenylmethane
Tritane
Group-member nr.: 14-086

$C_{19}H_{20}F_3N_3O_3$
• 2-(4-Morpholinyl)ethyl ester 2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid [65847-85-0]
Morniflumate
Group-member nr.: 64-041/S1

$C_{19}H_{20}O_4$
• Butyl phenylmethyl ester 1,2-benzenedicarboxylic acid [85-68-7]
Benzyl butyl phthalate
Group-member nr.: 45-149/S1

$C_{19}H_{22}ClNO$
• 4-Chloro-*N*-[[4-(hexyloxy)phenyl]methylene]benzenamine [5219-48-7]
p-*n*-Hexyloxybenzylideneamino-*p*′-chlorobenzene
Group-member nr.: 64-029

$C_{19}H_{22}FNO$
• 4-Fluoro-*N*-[[4-(hexyloxy)]methylene]benzenamine [56544-26-4]
p-*n*-Hexyloxybenzylideneamino-*p*′-fluorobenzene
Group-member nr.: 64-030

$C_{19}H_{23}NO$
• 4-Butyl-*N*-[(4-ethoxyphenyl)methylene]benzenamine [29743-08-6]
p-Butyl-*N*-(*p*-ethoxybenzylidene)aniline
Group-member nr.: 62-110
• *N*-[[4-(Hexyloxy)phenyl]methylene]benzenamine [5219-49-8]
p-*n*-Hexyloxybenzylideneaniline
Group-member nr.: 62-111

$C_{19}H_{36}$
• Bis(2,4,6-trimethylcyclohexyl)methane [94380-80-0]
Group-member nr.: 12-115
• 4-Heptyl-1,1′-bicyclohexyl [96667-88-8]
4-Heptylcyclohexylcyclohexane
Group-member nr.: 12-116
• 1,1′-Heptylidenebiscyclohexane [2090-15-5]
1,1-Dicyclohexylheptane
Group-member nr.: 12-117

$C_{19}H_{38}O_2$
• 1-Methylethyl ester hexadecanoic acid [142-91-6]
Isopropyl palmitate
Group-member nr.: 45-150/S1
• Nonadecanoic acid [646-30-0]
Nonadecylic acid
Group-member nr.: 44-035

$C_{19}H_{40}$
• Nonadecane [629-92-5]
Group-member nr.: 11-058/B+S1
• 2,6,10,14-Tetramethylpentadecane [1921-70-6]
Pristane

Group-member nr.: 11-059

$C_{19}H_{40}O$
• 1-Nonadecanol [1454-84-8]
Group-member nr.: 42-121/S1

$C_{20}F_{42}$
• Dotetracontafluoroeicosane [37589-57-4]
Perfluoroeicosane
Group-member nr.: 21-055/S1

$C_{20}H_{12}$
• Benzo[*a*]pyrene [50-32-8]
3,4-Benzopyrene
Group-member nr.: 14-124/S1
• Perylene [198-55-0]
Group-member nr.: 14-087/B+S1^{E}

$C_{20}H_{14}$
• 9,10-Dihydro-9,10[1′,2′]-benzenoanthracene [477-75-8]
Triptycene
Group-member nr.: 14-088

$C_{20}H_{22}N_2O$
• 4-[[[4-(Hexyloxy)phenyl]methylene]amino]benzonitrile [35280-78-5]
p-*n*-Hexyloxybenzylideneamino-*p*′-benzonitrile
Group-member nr.: 62-112

$C_{20}H_{24}N_2O_3$
• (*E*)-4-[(4-Methoxyphenyl)azo]phenyl ester heptanoic acid [97402-83-0]
Group-member nr.: 62-113

$C_{20}H_{25}NO$
• *N*-[[4-(Hexyloxy)phenyl]methylene]-4-methylbenzenamine [25959-51-7]
p-*n*-Hexyloxybenzylidene-*p*′-toluidine
Group-member nr.: 62-114

$C_{20}H_{26}N_2O_3$
• Bis(4-butoxyphenyl)diazene-1-oxide [17051-01-3]
4,4′-Dibutoxyazoxybenzene
Group-member nr.: 62-115

$C_{20}H_{30}O_3Si_3$
• 2,2,4,4-Tetraethyl-6,6-diphenylcyclotrisiloxane [108543-32-4]
Group-member nr.: 71-047

$C_{20}H_{34}$
• Diethylhexadecahydropyrene [26446-93-5]
Diethylperhydropyrene
Group-member nr.: 12-118

$C_{20}H_{34}O_5Si_5$
• Octamethyldiphenylcyclopentasiloxane (unspecified isomer) [51134-26-0]
Group-member nr.: 71-048

$C_{20}H_{38}HgO_4$
• Mercury(2+) salt decanoic acid [27394-49-6]
Mercury(II) decanoate
Mercury(II) caprate
Group-member nr.: 74-008

$C_{20}H_{38}O$
• 3,7,11,15-Tetramethyl-1-hexadecyn-3-ol [29171-23-1]
Group-member nr.: 42-104

$C_{20}H_{38}PbO_4$
• Lead(2+) salt decanoic acid [15773-52-1]
Lead(II) decanoate
Lead(II) caprate
Group-member nr.: 74-009

$C_{20}H_{40}O$
• 3,7,11,15-Tetramethyl-1-hexadecen-3-ol [505-32-8]
Isophytol
Group-member nr.: 42-105

$C_{20}H_{40}O_2$
• Eicosanoic acid [506-30-9]
Icosanic acid
Arachidic acid
Group-member nr.: 44-036

$C_{20}H_{42}$
• Eicosane [112-95-8]
Icosane
Group-member nr.: 11-060/B+S1

$C_{20}H_{42}O$
• 1-Eicosanol [629-96-9]
Group-member nr.: 42-122/S1
• 2-Octyl-1-dodecanol [5333-42-6]
9-Hydroxymethylnonadecane
Group-member nr.: 42-123/S1

$C_{20}H_{42}O_6$
• 3,6,9,12,15-Pentaoxapentacosan-1-ol [23244-49-7]
Pentaoxyethylene glycol decyl ether
Group-member nr.: 47-070/S1

$C_{20}H_{42}S$
• 1,1′-Thiobisdecane [693-83-4]
11-Thiaheneicosane
11-Thiahenicosane
Didecyl sulfide
Group-member nr.: 51-028

$C_{20}H_{44}Sn$
• Tetrapentylstannane [3765-65-9]
Tetrapentyltin
Group-member nr.: 73-032

$C_{21}H_{14}N_2O_4$
• 1,1′-(Methylenedi-4,1-phenylene)bis-1*H*-pyrrole-2,5-dione [13676-54-5]
Bis-(4-maleic acidimidphenyl)methane
Group-member nr.: 62-116

$C_{21}H_{16}$
• 1-(2-Naphthalenylmethyl)naphthalene [611-48-3]
1,2′-Dinaphthylmethane
Group-member nr.: 14-089

$C_{21}H_{21}O_4P$
• Tris(methylphenyl)ester phosphoric acid [1330-78-5]
Tricresyl phosphate

Tritolyl phosphate (unspecified isomer)
Group-member nr.: 72-014

$C_{21}H_{24}O_3Si_3$
• (2α,4α,6α)-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane [3424-57-5]
cis-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane
Group-member nr.: 71-049
• (2α,4α,6β)-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane [6138-53-0]
trans-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane
Group-member nr.: 71-050

$C_{21}H_{24}O_4$
• 2,2′-[(1-Methylethylidene)bis(4,1-phenyleneoxymethylene)]bisoxirane [1675-54-3]
Group-member nr.: 47-045

$C_{21}H_{38}$
• 9-(2-Ethylhexyl)dodecahydrofluorene [95135-48-1]
9-(2-Ethylhexyl)perhydrofluorene
Group-member nr.: 12-119
• 1,1′,1″-(1-Propanyl-2-ylidene)triscyclohexane [55682-89-8]
1,1,3-Tricyclohexylpropane
Group-member nr.: 12-120

$C_{21}H_{38}O_6$
• 1,2,3-Propanetriyl ester hexanoic acid [621-70-5]
1,2,3-Propanetriyl trihexanoate
Trihexanoin
Tricaproin
Group-member nr.: 45-106

$C_{21}H_{40}$
• 4-Nonyl-1,1′-bicyclohexyl [95135-87-8]
4-Nonylcyclohexylcyclohexane
Group-member nr.: 12-121

$C_{21}H_{40}O_4$
• 1-Methyl-1,2-ethanediyl ester nonanoic acid [41395-83-9]
Propylene dinonanoate
Propyleneglycol dipelargonate
Group-member nr.: 45-151/S1

$C_{21}H_{42}InN_3S_6$
• Tris[bis(1-methylethyl)carbamodithioato-*S*,*S*′]indium [85883-33-6]
Group-member nr.: 73-047/S1
• Tris(dipropylcarbamodithiato-*S*,*S*′)indium [87052-01-5]
Group-member nr.: 73-048/S1

$C_{21}H_{42}O_4$
• 2,3-Dihydroxypropyl ester octadecanoic acid [123-94-4]
1-Monostearin
Group-member nr.: 47-046

$C_{21}H_{44}$
• Heneicosane [629-94-7]
Henicosane
Group-member nr.: 11-061

$C_{22}H_{14}$
• Pentacene [135-48-8]
2,3,6,7-Dibenzoanthracene
Group-member nr.: 14-090/B+S1[E]

$C_{22}H_{14}O_4$
• 1,1′-(1,4-Phenylene)bis[2-phenylethanedione] [3363-97-1]
1,4-Bis(phenylglyoxaloyl)benzene
Group-member nr.: 43-069/S1

$C_{22}H_{24}O_6$
• *trans*-Bis(4-methoxyphenyl)ester 1,4-cyclohexanedicarboxylic acid [26379-55-5]
Di(*p*-methoxyphenyl)-*trans*-cyclohexane-1,4-dicarboxylate
Group-member nr.: 47-047

$C_{22}H_{29}NO$
• 4-Butyl-*N*-[[4-(pentyloxy)phenyl]methylene]benzenamine [29743-10-0]
N-*p*-*n*-Pentyloxybenzylidene-*p*′-*n*-butylaniline
Group-member nr.: 62-117

$C_{22}H_{30}N_2O_3$
• Bis(4-pentyloxyphenyl)diazene-1-oxide [19482-05-4]
4,4′-Bis(pentyloxy)azoxybenzene
Group-member nr.: 62-118

$C_{22}H_{42}O_4$
• Bis(2-ethylhexyl) hexanedioate [103-23-1]
Bis(2-ethylhexyl) adipate
Bis(2-ethylhexyl) ester hexanedioic acid
Group-member nr.: 45-107/B+S1[E]
• Dihexyl decanedioate [2449-10-7]
Dihexyl ester decanedioic acid
Dihexyl sebacate
Group-member nr.: 45-108

$C_{22}H_{42}O_4Pb$
• Lead(2+) salt undecanoic acid [63400-07-7]
Lead(II) undecanoate
Group-member nr.: 74-030/S1

$C_{22}H_{44}N_2O_2$
• *N*,*N*′-Dihexyldecanediamine [31827-03-9]
N,*N*′-Dihexylsebacamide
Group-member nr.: 62-119

$C_{22}H_{44}O_2$
• Butyl octadecanoate [123-95-5]
Butyl ester octadecanoic acid
Butyl stearate
Group-member nr.: 45-109

$C_{22}H_{45}Br$
• 1-Bromodocosane [6938-66-5]
n-Docosyl bromide
Group-member nr.: 23-039

$C_{22}H_{46}$
• Docosane [629-97-0]
Group-member nr.: 11-062

$C_{22}H_{46}O$
• 1-Docosanol [661-19-8]
Group-member nr.: 42-124/S1

$C_{22}H_{46}O_6$
• 3,6,9,12,15-Pentaoxaheptacosan-1-ol [3055-95-6]
Pentaoxyethylene glycol dodecyl ether
Group-member nr.: 47-071/S1

$C_{22}H_{46}O_7$
• 3,6,9,12,15,18-Hexaoxaoctacosan-1-ol [5168-89-8]
Hexaoxyethylene glycol decyl ether
Group-member nr.: 47-072/S1

$C_{23}H_{31}NO$
• 4-Butyl-*N*-[[4-(hexyloxy)phenyl]methylene]benzenamine [29743-11-1]
N-*p*-*n*-Hexyloxybenzylidene-*p*′-*n*-butylaniline
Group-member nr.: 62-120

$C_{23}H_{44}O_5$
• 3-(Acetyloxy)-2-hydroxypropyl ester octadecanoic acid [820-17-7]
3-Aceto-1-stearin
Group-member nr.: 47-048

$C_{23}H_{48}$
• Tricosane [638-67-5]
Group-member nr.: 11-063

$C_{24}F_{50}$
• Pentacontafluorotetracosane [1766-41-2]
Perfluorotetracosane
Group-member nr.: 21-056/S1

$C_{24}H_{18}$
• 5′-Phenyl-1,1′:3′,1″-terphenyl [612-71-5]
1,3,5-Triphenylbenzene
Group-member nr.: 14-091
• 1,1′:3′,1″:3″,1‴-Quaterphenyl [1166-18-3]
m-Quaterphenyl
Group-member nr.: 14-092

$C_{24}H_{32}O_3$
• 4-(Heptyloxy)phenyl ester 4-butylbenzoic acid [38454-35-2]
p-(Heptyloxy)phenyl *p*-butylbenzoate
Group-member nr.: 47-049

$C_{24}H_{34}$
• 1,1-Diphenyldodecane [1603-53-8]
Group-member nr.: 14-093

$C_{24}H_{34}N_2O_3$
• Bis(4-hexyloxyphenyl)diazene-1-oxide [2587-42-0]
4,4′-Bis(hexyloxy)azoxybenzene
Group-member nr.: 62-121

$C_{24}H_{36}Cr$
• Bis[(1,2,3,4,5,6-η)-bis(1-methylethyl)benzene]chromium [38744-20-6]
Bis[diisopropylbenzene]chromium
Group-member nr.: 73-049/S1

$C_{24}H_{38}O_4$
• Bis(2-ethylhexyl)-1,2-benzenedicarboxylate [117-81-7]
Bis(2-ethylhexyl) ester phthalic acid
Group-member nr.: 45-110/B+S1

$C_{24}H_{40}$
• (1-Cyclohexyldodecyl)benzene [62155-50-4]
1-Cyclohexyl-1-phenyldodecane
Group-member nr.: 14-094

$C_{24}H_{46}CdO_4$
• Cadmium salt dodecanoic acid [2605-44-9]
Cadmium dodecanoate
Cadmium laurate
Group-member nr.: 74-010

$C_{24}H_{46}HgO_4$
• Mercury(2+) salt dodecanoic acid [23186-25-6]
Mercury(II) dodecanoate
Mercury(II) laurate
Group-member nr.: 74-011

$C_{24}H_{46}O_4Pb$
• Lead(2+) salt dodecanoic acid [15773-55-4]
Lead(II) dodecanoate
Lead(II) laurate
Group-member nr.: 74-012

$C_{24}H_{50}$
• Tetracosane [646-31-1]
Group-member nr.: 11-064

$C_{24}H_{50}O_7$
• 3,6,9,12,15,18-Hexaoxatriacontan-1-ol [3055-96-7]
Hexaoxyethylene glycol dodecyl ether
Group-member nr.: 47-073/S1

$C_{24}H_{51}N$
• *N*,*N*-Dioctyl-1-octanamine [1116-76-3]
N,*N*,*N*-Trioctylamine
Group-member nr.: 31-065/S1

$C_{24}H_{52}ClNO_4$
• *N*,*N*,*N*-Trihexyl-1-hexanaminium perchlorate [4656-81-9]
Tetrahexylammonium perchlorate
Group-member nr.: 74-013

$C_{24}H_{52}O_4Si$
• Tetrakis(2-ethylbutyl) ester silicic acid [78-13-7]
Tetrakis(2-ethylbutyl) orthosilicate
Tetrakis(2-ethylbutoxy)silane
Group-member nr.: 71-051

$C_{25}H_{34}O_2S$
• *S*-(4-Pentylphenyl) ester 4-(heptyloxy)benzenecarbothioic acid [61519-00-4]
4-*n*-Pentylphenyl-4′-heptyloxythiobenzoate
Group-member nr.: 63-008/S1

$C_{25}H_{42}O_3$
• 4-(Octadecyloxy)benzoic acid [15872-50-1]
p-*n*-Octadecyloxybenzoic acid
Group-member nr.: 47-074/S1

$C_{25}H_{44}$
• Nonadecylbenzene [29136-19-4]
Group-member nr.: 14-125/S1

$C_{25}H_{46}$
• 4′-Heptyl-1,1′:3′,1″-tercyclohexane [unknown]

4-Heptyl-*m*-tercyclohexyl
Group-member nr.: 12-122

$C_{25}H_{46}O_6$
• 2,3-Bis(acetyloxy)propyl ester octadecanoic acid [33599-07-4]
1,2-Diacetostearin
Group-member nr.: 45-111

$C_{25}H_{48}O_4$
• Bis(2-ethylhexyl) nonanedioate [103-24-2]
Bis(2-ethylhexyl) azelate
Bis(2-ethylhexyl) ester nonanedioic acid
Group-member nr.: 45-112

$C_{25}H_{50}$
• Nonadecylcyclohexane [22349-03-7]
Group-member nr.: 12-136/S1

$C_{25}H_{52}$
• Pentacosane [629-99-2]
Group-member nr.: 11-065

$C_{26}H_{18}$
• 9,10-Diphenylanthracene [1499-10-1]
Group-member nr.: 14-095/B+S1^{E}

$C_{26}H_{26}OSi_2$
• 1,3-Dimethyl-1,1,3,3-tetraphenyldisiloxane [807-28-3]
Group-member nr.: 71-052

$C_{26}H_{36}O_3Si_3$
• 2,2-Dimethyl-4,4,6,6-tetraphenylcyclotrisiloxane [1438-86-4]
Group-member nr.: 71-053

$C_{26}H_{38}N_2O_3$
• Bis(4-heptyloxyphenyl)diazene-1-oxide [2635-26-9]
4,4′-Bis(heptyloxy)azoxybenzene
Group-member nr.: 62-122

$C_{26}H_{50}O_4$
• Dioctyl decanedioate [2432-87-3]
Dioctyl ester decanedioic acid
Dioctyl sebacate
Group-member nr.: 45-113

$C_{26}H_{50}O_4Pb$
• Lead(2+) salt tridecanoic acid [50354-80-8]
Lead(II) tridecanoate
Group-member nr.: 74-031/S1

$C_{26}H_{54}$
• Hexacosane [630-01-3]
Group-member nr.: 11-066

$C_{26}H_{54}O_9$
• 3,6,9,12,15,18,21,24-Octaoxatetratriacontan-1-ol [24233-81-6]
Octaoxyethylene glycol decyl ether
Group-member nr.: 47-075/S1

$C_{27}H_{46}O$
• Cholesterol [57-88-5]
5-Cholesten-3β-ol
Group-member nr.: 42-125/S1

$C_{27}H_{48}$
• (5α)-Cholestane [481-21-0]
17-(1,5-Dimethylhexyl)-10,13-dimethylhexahydro-1*H*-cyclopenta[*a*]phenanthrene
Group-member nr.: 12-137/S1
• 11-Phenylheneicosane [6703-80-6]
(1-Decylundecyl)benzene
11-Phenylhenicosane
Group-member nr.: 14-096

$C_{27}H_{50}$
• 4′-Nonyl-1,1′:3′,1″-tercyclohexane [unknown]
4-Nonyl-*m*-tercyclohexyl
Group-member nr.: 12-123

$C_{27}H_{50}O_6$
• 1,2,3-Propanetriyl ester octanoic acid [538-23-8]
1,2,3-Propanetriyl trioctanoate
Trioctanoin
Group-member nr.: 45-114

$C_{27}H_{54}$
• (1-Decylundecyl)cyclohexane [6703-99-7]
11-Cyclohexylheneicosane
11-Cyclohexylhenicosane
Group-member nr.: 12-124

$C_{27}H_{54}AsN_3S_6$
• Tris(dibutylcarbamodithioato-*S*,*S*′)arsenic [48233-55-2]
Group-member nr.: 73-050/S1

$C_{27}H_{54}BiN_3S_6$
• Tris(dibutylcarbamodithioato-*S*,*S*′)bismuth [34410-99-6]
Group-member nr.: 73-051/S1

$C_{27}H_{54}InN_3S_6$
• Tris[bis(2-methylpropyl)carbamodithiato-*S*,*S*′]indium [85129-27-7]
Group-member nr.: 73-052/S1
• Tris(dibutylcarbamodithioato-*S*,*S*′)indium [23467-56-3]
Group-member nr.: 73-053/S1

$C_{27}H_{54}N_3PS_6$
• Tris(anhydrosulfide) with phosphorotrithious acid dibutylcarbamodithioic acid [69267-83-0]
Group-member nr.: 72-020/S1

$C_{27}H_{54}N_3S_6Sb$
• Tris(dibutylcarbamodithioato-*S*,*S*′)antimony [14907-93-8]
Group-member nr.: 73-054/S1

$C_{27}H_{56}$
• Heptacosane [593-49-7]
Group-member nr.: 11-067

$C_{28}H_{28}P$
• 1,4-Butanediylbis(diphenylphosphine) [7688-25-7]
1,4-Bis(diphenylphosphino)butane
Tetramethylenebis(diphenylphosphine)
Group-member nr.: 72-015

$C_{28}H_{32}O_4Si_4$
• 2,2,4,4-Tetramethyl-6,6,8,8-tetraphenylcyclotetrasiloxane [1693-47-6]

Group-member nr.: 71-054
• 2,4,6,8-Tetramethyl-2,4,6,8-tetraphenylcyclotetrasiloxane [77-63-4]
Group-member nr.: 71-055

$C_{28}H_{42}N_2O_3$
• Bis(4-octyloxyphenyl)diazene-1-oxide [25729-12-8]
4,4′-Bis(octyloxy)azoxybenzene
Group-member nr.: 62-123

$C_{28}H_{54}CdO_4$
• Cadmium salt tetradecanoic acid [10196-67-5]
Cadmium tetradecanoate
Cadmium myristate
Group-member nr.: 74-014

$C_{28}H_{54}HgO_4$
• Mercury(2+) salt tetradecanoic acid [36215-49-3]
Mercury(II) tetradecanoate
Mercury(II) myristate
Group-member nr.: 74-015

$C_{28}H_{54}O_2$
• Decyl ester (*Z*)-9-octadecenoic acid [3687-46-5]
Decyl oleate
Group-member nr.: 45-152/S1

$C_{28}H_{54}O_4Pb$
• Lead(2+) salt tetradecanoic acid [32112-52-0]
Lead(II) tetradecanoate
Lead(II) myristate
Group-member nr.: 74-016

$C_{28}H_{58}$
• Octacosane [630-02-4]
Group-member nr.: 11-068

$C_{29}H_{42}O_4$
• 4-(Hexyloxy)phenyl ester 4-(decyloxy)benzoic acid [68162-09-4]
4-Hexyloxyphenyl-4′-*n*-decyloxybenzoate
Group-member nr.: 47-050

$C_{30}H_{32}P_2$
• 1,6-Hexanediyl[diphenylphosphine] [19845-69-3]
1,6-Bis(diphenylphosphino)hexane
Group-member nr.: 72-021/S1

$C_{30}H_{46}N_2O_3$
• Bis(4-nonyloxyphenyl)diazene-1-oxide [25729-13-9]
4,4′-Bis(nonyloxy)azoxybenzene
Group-member nr.: 62-124

$C_{30}H_{58}O_4$
• Didecyl decanedioate [2432-89-5]
Didecyl ester decanedioic acid
Didecyl sebacate
Group-member nr.: 45-115

$C_{30}H_{61}Br$
• 1-Bromotriacontane [4209-22-7]
n-Triacontyl bromide
Group-member nr.: 23-040

$C_{30}H_{62}$
• 2,6,10,15,19,23-Hexamethyltetracosane [111-01-3]
Squalane
Group-member nr.: 11-069
• Triacontane [638-68-6]
Group-member nr.: 11-070

$C_{31}H_{32}O_2P_2$
• [[(4*R*,5*R*)-2,2-Dimethyl-1,3-dioxolane-4,5-diyl]bis(methylene)]bis[diphenylphosphine] [32305-98-9]
(−)-2,3-*O*-Isopropylidene-2,3-dihydroxy-1,4-bis(diphenylphosphino)butane
Group-member nr.: 72-022/S1

$C_{31}H_{52}O_3$
• 3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol acetate [7695-91-2]
α-Tocopherol acetate
Group-member nr.: 47-051

$C_{31}H_{62}O$
• 16-Hentriacontanone [502-73-8]
Dipentadecyl ketone
Group-member nr.: 43-070/S1

$C_{31}H_{64}$
• 11-Decylheneicosane [55320-06-4]
11-Decylhenicosane
Group-member nr.: 11-071
• Hentriacontane [630-04-6]
Unatriacontane
Group-member nr.: 11-072

$C_{32}H_{50}N_2O_3$
• Bis(4-decyloxyphenyl)diazene-1-oxide [2312-12-1]
4,4′-Bis(decyloxy)azoxybenzene
Group-member nr.: 62-125

$C_{32}H_{54}O_4$
• Bis(2,4-diethyloctyl) ester 1,2-benzenedicarboxylic acid [40989-56-8]
Diisododecyl phthalate
Group-member nr.: 45-153/S1

$C_{32}H_{62}CdO_4$
• Cadmium salt hexadecanoic acid [6427-86-7]
Cadmium hexadecanoate
Cadmium palmitate
Group-member nr.: 74-017

$C_{32}H_{62}HgO_4$
• Mercury(2+) salt hexadecanoic acid [16888-60-1]
Mercury(II) hexadecanoate
Mercury(II) palmitate
Group-member nr.: 74-018

$C_{32}H_{62}O_4Pb$
• Lead(2+) salt hexadecanoic acid [15773-56-5]
Lead(II) hexadecanoate
Lead(II) palmitate
Group-member nr.: 74-019

$C_{32}H_{66}$
• Dotriacontane [544-85-4]
Group-member nr.: 11-073

$C_{33}H_{62}O_6$
• 1,2,3-Propanetriyl ester decanoic acid [621-71-6]
1,2,3-Propanetriyl tridecanoate
Tridecanoin
Group-member nr.: 45-116

$C_{33}H_{68}$
• Tritriacontane [630-05-7]
Group-member nr.: 11-074

$C_{34}H_{54}N_2O_3$
• Bis[4-(undecyloxy)phenyl]diazene-1-oxide [2312-13-2]
4,4′-Bis(undecyloxy)azoxybenzene
Group-member nr.: 62-126

$C_{34}H_{66}O_4$
• Didodecyl decanedioate [2432-88-4]
Didodecyl ester decanedioic acid
Didodecyl sebacate
Group-member nr.: 45-117

$C_{34}H_{70}$
• Tetratriacontane [14167-59-0]
Group-member nr.: 11-075

$C_{35}H_{72}$
• Pentatriacontane [630-07-9]
Group-member nr.: 11-076

$C_{36}H_{24}$
• 1,1′,1″-(1,3,5-Benzenetriyl)trisnaphthalene [7059-70-3]
1,3,5-Tri-α-naphthylbenzene
Group-member nr.: 14-097

$C_{36}H_{48}N_2O_2$
• (*E*,*E*)-*N*,*N*′-Bis[[4-(octyloxy)phenyl]methylene]-1,4-benzenediamine [29273-90-3]
N,*N*′-Bis(4-*n*-octyloxybenzal)-1,4-phenylenediamine
Group-member nr.: 62-174/S1

$C_{36}H_{58}N_2O_3$
• Bis[4-(dodecyloxy)phenyl]diazene-1-oxide [2312-14-3]
4,4′-Bis(dodecyloxy)azoxybenzene
Group-member nr.: 62-127

$C_{36}H_{68}O_2$
• (*Z*)-9-Octadecenyl ester (*Z*)-9-octadecenoic acid [3687-45-4]
Oleyl oleate
Group-member nr.: 45-154/S1

$C_{36}H_{70}CdO_4$
• Cadmium salt octadecanoic acid [2223-93-0]
Cadmium octadecanoate
Cadmium stearate
Group-member nr.: 74-020

$C_{36}H_{70}HgO_4$
• Mercury(2+) salt octadecanoic acid [645-99-8]
Mercury(II) octadecanoate
Mercury(II) stearate
Group-member nr.: 74-021

$C_{36}H_{70}O_4Pb$
• Lead(2+) salt octadecanoic acid [1072-35-1]
Lead(II) octadecanoate
Lead(II) stearate
Group-member nr.: 74-022

$C_{36}H_{74}$
• Hexatriacontane [630-06-8]
Group-member nr.: 11-077/B+S1

$C_{37}H_{54}Si$
• Tribenzylhexadecylsilane [4033-52-7]
Group-member nr.: 71-056

$C_{38}H_{70}O_8$
• 1,6-Hexanediyldihexyl ester decanedioic acid [55205-81-7]
Dihexyl hexamethylenesebacate
Group-member nr.: 45-118

$C_{38}H_{74}O_4$
• Ditetradecyl decanedioate [26719-47-1]
Ditetradecyl ester decanedioic acid
Ditetradecyl sebacate
Group-member nr.: 45-119

$C_{39}H_{74}O_6$
• 1,2,3-Propanetriyl ester dodecanoic acid [538-24-9]
1,2,3-Propanetriyl tridodecanoate
Trilaurin
Group-member nr.: 45-120/B+S1

$C_{39}H_{78}O$
• 20-Nonatriacontanone [22986-70-5]
Dinonadecyl ketone
Group-member nr.: 43-071/S1

$C_{40}H_{82}$
• Tetracontane [4181-95-7]
Group-member nr.: 11-078

$C_{41}H_{72}O_2$
• Cholest-5-en-3-ol (3β) tetradecanoate [1989-52-2]
Cholesterol myristate
Group-member nr.: 45-121

$C_{42}H_{66}O_{12}$
• 1,2,3,4,5,6-Benzenehexayl ester hexanoic acid [65201-69-6]
Benzene hexa-*n*-hexanoate
Group-member nr.: 45-122

$C_{42}H_{82}O_4$
• Dihexadecyl decanedioate [26719-48-2]
Dihexadecyl ester decanedioic acid
Dihexadecyl sebacate
Group-member nr.: 45-123

$C_{42}H_{86}$
• Dotetracontane [7098-20-6]
Group-member nr.: 11-079

$C_{43}H_{88}$
• Tritetracontane [7098-21-7]

Group-member nr.: 11-080

$C_{44}H_{90}$
• Tetratetracontane [7098-22-8]
Group-member nr.: 11-081

$C_{45}H_{86}O_6$
• 1,2,3-Propanetriyl ester tetradecanoic acid [555-45-3]
1,2,3-Propanetriyl tritetradecanoate
Trimyristin
Group-member nr.: 45-124/B+S1

$C_{46}H_{90}O_4$
• Dioctadecyl decanedioate [3072-03-5]
Dioctadecyl ester decanedioic acid
Dioctadecyl sebacate
Group-member nr.: 45-125

$C_{47}H_{90}O_6$
• 2,3-Bis[(1-oxotetradecyl)oxy]propyl ester hexadecanoic acid [60138-13-8]
1,2-Dimyristoyl-3-palmitoyl triglyceride
Group-member nr.: 45-155/S1

$C_{48}H_{40}P_2$
• [1,1′-Binaphthalene]-2,2′-diylbis[bis(4-methylphenyl)phosphine] [153305-67-0]
2,2′-Bis(di-*p*-toluenephosphino)-1,1′-binaphthyl
Group-member nr.: 72-023/S1

$C_{48}H_{78}O_{12}$
• 1,2,3,4,5,6-Benzenehexayl ester heptanoic acid [65201-70-9]
Benzene hexa-*n*-heptanoate
Group-member nr.: 45-126

$C_{48}H_{98}$
• Octatetracontane [7098-26-2]
Group-member nr.: 11-082

$C_{49}H_{92}O_6$
• 2,3-Bis[(1-oxotetradecyl)oxy]propyl ester (*Z*)-9-octadecenoic acid [74160-01-3]
1,2-Dimyristoyl-3-oleoyl triglyceride
Group-member nr.: 45-156/S1

$C_{50}H_{102}$
• Pentacontane [6596-40-3]
Group-member nr.: 11-083

$C_{51}H_{98}O_6$
• 1,2,3-Propanetriyl ester hexadecanoic acid [555-44-2]
1,2,3-Propanetriyl trihexadecanoate
Tripalmitin
Group-member nr.: 45-127/B+S1

$C_{53}H_{100}O_6$
• 2,3-Bis[(1-oxohexadecyl)oxy]propyl ester (*Z*)-9-octadecenoic acid [1867-91-0]
1,2-Dipalmitoyl-3-oleoyl triglyceride
Group-member nr.: 45-157/S1

$C_{54}H_{90}O_{12}$
• 1,2,3,4,5,6-Benzenehexayl ester octanoic acid [65201-71-0]
Benzene hexa-*n*-octanoate
Group-member nr.: 45-128

$C_{54}H_{98}O_{12}$
• 10,19,28,37-Tetraoxodihexyl ester 11,18,29,36-tetraoxahexatetracosanedioic acid [55205-82-8]
Dihexyl bis(hexamethylenesebacate)
Group-member nr.: 45-129

$C_{55}H_{102}O_6$
• 1-[[(1-Oxohexadecyl)oxy]methyl]-1,2-ethanediyl ester (*Z*)-9-octadecenoic acid [2190-30-9]
1,2-Dioleoyl-3-palmitoyl triglyceride
3-Palmito-1,2-diolein
Group-member nr.: 45-158/S1

$C_{57}H_{92}O_6$
• (9*Z*,9′*Z*,9″*Z*,12*Z*,12′*Z*,12″*Z*,15*Z*,15′*Z*,15″*Z*)-1,2,3-Propanetriyl ester 9,12,15-octadecatrienoic acid [14465-68-0]
Trilinolein
Group-member nr.: 45-159/S1

$C_{57}H_{110}O_6$
• 1,2,3-Propanetriyl ester octadecanoic acid [555-43-1]
1,2,3-Propanetriyl trioctadecanoate
Tristearin
Group-member nr.: 45-130/B+S1

$C_{66}H_{96}O_{12}$
• 2,3,6,7,10,11-Triphenylenehexayl ester octanoic acid [70351-94-9]
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
Group-member nr.: 45-160/S1

ClD
• Hydrochlorid acid-*d* [7698-05-7]
Deuterium chloride
Group-member nr.: 02-030

$ClFO_3$
• Perchloryl fluoride ($(ClO_3)F$) [7616-94-6]
Group-member nr.: 02-031/B+S1

ClF_3
• Chlorine fluoride (ClF_3) [13637-63-3]
Chlorine trifluoride
Group-member nr.: 02-032

ClH
• Hydrochlorid acid [7647-01-0]
Hydrogen chloride
Group-member nr.: 02-033

$ClHO_4$
• Perchloric acid [7601-90-3]
Group-member nr.: 02-034

ClI
• Iodine chloride [7790-99-0]
Iodine monochloride
Group-member nr.: 02-035

$ClNaO_3$
• Sodium salt chloric acid [7775-09-9]

Sodium chlorate
Group-member nr.: 02-036

Cl_2
• Chlorine [7782-50-5]
Group-member nr.: 01-004

Cl_2OS
• Thionyl chloride [7719-09-7]
Group-member nr.: 02-037

Cl_2O_2S
• Sulfuryl chloride [7791-25-5]
Group-member nr.: 02-038

$Cl_2O_5S_2$
• Disulfuryl chloride [7791-27-7]
Pyrosulfuryl chloride
Group-member nr.: 02-039

Cl_2S_2
• Sulfur chloride (S_2Cl_2) [10025-67-9]
Sulfur monochloride
Group-member nr.: 02-040

Cl_2Sn
• Tin chloride ($SnCl_2$) [7772-99-8]
Group-member nr.: 02-041

Cl_3HSi
• Trichlorosilane [10025-78-2]
Group-member nr.: 02-042

Cl_3OP
• Phosphoryl chloride [10025-87-3]
Group-member nr.: 02-043

Cl_3P
• Phosphorous trichloride [7719-12-2]
Phosphorus chloride (PCl_3)
Group-member nr.: 02-044

Cl_4Ge
• Tetrachlorogermane [10038-98-9]
Germanium tetrachloride
Group-member nr.: 02-045

Cl_4Si
• Tetrachlorosilane [10026-04-7]
Silicon chloride
Group-member nr.: 02-046

Cl_4Sn
• Tetrachlorostannane [7646-78-8]
Tin(IV) chloride
Tin tetrachloride
Group-member nr.: 02-047

Cl_4Te
• Tellurium chloride ($TeCl_4$) [10026-07-0]
Tellurium tetrachloride
Group-member nr.: 02-048

Cl_4Ti
• Titanium chloride ($TiCl_4$) [7550-45-0]
Titanium tetrachloride
Titanic chloride
Group-member nr.: 02-049

$Cl_6N_3P_3$
• 2,2,4,4,6,6-Hexachloro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine [940-71-6]
Hexachlorocyclotriphosphazene
Group-member nr.: 02-104/S1

$Cl_8N_4P_4$
• 2,2,4,4,6,6,8,8-Octachloro-2,2,4,4,6,6,8,8-octahydro-1,3,5,7,2,4,6,8-tetrazatetraphosphorine [2950-45-0]
Octachlorocyclotetraphosphazene
Group-member nr.: 02-105/S1

Cs
• Cesium [7440-46-2]
Group-member nr.: 01-005

CsF_2H
• Cesium fluoride ($Cs(HF_2)$) [12280-52-3]
Cesium hydrogen difluoride
Group-member nr.: 02-050

DH
• Deuterium molecule with hydrogen [13983-20-5]
Hydrogen deuteride
Group-member nr.: 02-051

DI
• Hydroiodic acid-*d* [14104-45-1]
Deuterium iodide
Group-member nr.: 02-052

D_2
• Deuterium (D_2) [7782-39-0]
Group-member nr.: 01-006/B+S1^E
• ortho-Deuterium (D_2) [unknown]
Group-member nr.: 01-007

D_2O
• Water-d_2 [7789-20-0]
Heavy water
Deuterium oxide
Group-member nr.: 02-053

D_2O_2
• Hydrogen-d_2 peroxide [6909-54-2]
Deuterium peroxide
Group-member nr.: 02-054

D_2S
• Hydrogen sulfide-d_2 [13536-94-2]
Deuterium sulfide
Group-member nr.: 02-055

D_2Se
• Hydrogen selenide-d_2 [13536-95-3]
Deuterium selenide
Group-member nr.: 02-056

D_3N
• Ammonia-d_3 [13550-49-7]
Deuterium ammonia
Trideuterated ammonia

Group-member nr.: 02-057

FH
- Hydrofluoric acid [7664-39-3]
  Hydrogen fluoride
  Group-member nr.: 02-058

F_2
- Fluorine [7782-41-4]
  Group-member nr.: 01-008

F_2HRb
- Rubidium fluoride ($Rb(HF_2)$) [12280-64-7]
  Rubidium hydrogen difluoride
  Group-member nr.: 02-059

F_2H_5N
- Ammonium fluoride ($(NH_4)(HF_2)$) [1341-49-7]
  Ammonium hydrogen difluoride
  Group-member nr.: 02-060

F_2O
- Oxygen fluoride [7783-41-7]
  Group-member nr.: 02-061

F_2OS
- Thionyl fluoride [7783-42-8]
  Group-member nr.: 02-062

F_2O_2S
- Sulfuryl fluoride [2699-79-8]
  Group-member nr.: 02-063/B+S1^E

F_3N
- Nitrogen fluoride (NF_3) [7783-54-2]
  Nitrogen trifluoride
  Group-member nr.: 02-064

F_3OP
- Phosphoryl fluoride [13478-20-1]
  Group-member nr.: 02-065

F_3P
- Phosphorous trifluoride [7783-55-3]
  Phosphorus trifluoride
  Phosphorous fluoride (PF_3)
  Group-member nr.: 02-066

F_4Si
- Tetrafluorosilane [7783-61-1]
  Silicon tetrafluoride
  Group-member nr.: 02-106/S1

F_5I
- Iodine fluoride (IF_5) [7783-66-6]
  Iodine pentafluoride
  Group-member nr.: 02-067

F_5Nb
- Niobium fluoride (NbF_5) [7783-68-8]
  Niobium pentafluoride
  Group-member nr.: 02-068

F_6Mo
- Molybdenum fluoride (MoF_6) [7783-77-9]
  Molybdenum hexafluoride
  Group-member nr.: 02-069

F_6S
- Sulfur fluoride (SF_6) [2551-62-4]
  Sulfur hexafluoride
  Group-member nr.: 02-070/B+S1

F_6Se
- Selenium fluoride (SeF_6) [7783-79-1]
  Hexafluoroselenium
  Group-member nr.: 02-107/S1

F_6U
- Uranium(VI) fluoride [7783-81-5]
  Uranium hexafluoride
  Group-member nr.: 02-071

F_6W
- Tungsten fluoride (WF_6) [69175-55-9]
  Hexafluorotungsten
  Group-member nr.: 02-108/S1

Ga
- Gallium [7440-55-3]
  Group-member nr.: 01-009

GeH_4
- Germane [7782-65-2]
  Group-member nr.: 02-072/B+S1

HI
- Hydroiodic acid [10034-85-2]
  Hydrogen iodide
  Group-member nr.: 02-073

HNO_3
- Nitric acid [7697-37-2]
  Group-member nr.: 02-074

H_2
- Hydrogen [1333-74-0]
  Group-member nr.: 01-010
- para-Hydrogen [unknown]
  Group-member nr.: 01-011

H_2O
- Water [7732-18-5]
  Group-member nr.: 02-075

$H_2{}^{18}O$
- Water-^{18}O [14314-42-2]
  Heavy Oxygen Water
  Group-member nr.: 02-109/S1

H_2O_2
- Hydrogen peroxide [7722-84-1]
  Group-member nr.: 02-076

H_2O_4S
- Sulfuric acid [7664-93-9]
  Group-member nr.: 02-077

$H_2O_7S_2$
- Disulfuric acid [7783-05-3]
  Pyrosulfuric acid
  Group-member nr.: 02-078

H_2S
- Hydrogen sulfide [7783-06-4]
  Group-member nr.: 02-079

H_2S_2
- Hydrogen sulfide (H_2S_2) [13465-07-1]
  Dihydrogen disulfide
  Group-member nr.: 02-080

H_2S_3
- Hydrogen sulfide (H_2S_3) [13845-23-3]
  Dihydrogen trisulfide
  Group-member nr.: 02-081

H_2S_4
- Hydrogen sulfide (H_2S_4) [13845-25-5]
  Dihydrogen tetrasulfide
  Group-member nr.: 02-082

H_2S_5
- Hydrogen sulfide (H_2S_5) [13845-24-4]
  Dihydrogen pentasulfide
  Group-member nr.: 02-083

H_2S_6
- Hydrogen sulfide (H_2S_6) [13845-51-7]
  Dihydrogen hexasulfide
  Group-member nr.: 02-084

H_2Se
- Hydrogen selenide [7783-07-5]
  Group-member nr.: 02-085

H_3N
- Ammonia [7664-41-7]
  Group-member nr.: 02-086/B+S1

H_3O_4P
- Phosphoric acid [7664-38-2]
  Group-member nr.: 02-087

H_3P
- Phosphine [7803-51-2]
  Group-member nr.: 02-088

H_4N_2
- Hydrazine [302-01-2]
  Group-member nr.: 02-089

H_4Si
- Silane [7803-62-5]
  Group-member nr.: 02-090

H_5NO
- Ammonium hydroxide [1336-21-6]
  Group-member nr.: 02-091

$H_5N_3O_3$
- Hydrazine mononitrate [13464-97-6]
  Hydrazine nitrate
  Group-member nr.: 02-092

H_8N_2O
- Ammonium oxide [12161-77-2]
  Group-member nr.: 02-093

He
- Helium (isotope of mass 3) [14762-55-1]
  Group-member nr.: 01-013
- Helium [7440-59-7]
  Group-member nr.: 01-012

Hg
- Mercury [7439-97-6]
  Group-member nr.: 01-014

HgI_2
- Mercury iodide (HgI_2) [7774-29-0]
  Group-member nr.: 02-094

I_2
- Iodine [7553-56-2]
  Group-member nr.: 01-015

I_4Sn
- Tetraiodostannane [7790-47-8]
  Tin iodide
  Stannic iodide
  Group-member nr.: 02-095

In
- Indium [7440-74-6]
  Group-member nr.: 01-016

K
- Potassium [7440-09-7]
  Kalium
  Group-member nr.: 01-017

Kr
- Krypton [7439-90-9]
  Group-member nr.: 01-018

Li
- Lithium [7439-93-2]
  Group-member nr.: 01-019

$LiNO_3$
- Lithium salt nitric acid [7790-69-4]
  Lithium nitrate
  Group-member nr.: 02-096

NO
- Nitrogen oxide (NO) [10102-43-9]
  Nitrogen monoxide
  Nitric oxide
  Group-member nr.: 02-097

NO_2
- Nitrogen oxide (NO_2) [10102-44-0]
  Nitrogen dioxide
  Group-member nr.: 02-098

N_2
- Nitrogen [7727-37-9]
  Group-member nr.: 01-020

N_2O
- Nitrogen oxide (N_2O) [10024-97-2]
  Dinitrogen monoxide
  Nitrous oxide
  Group-member nr.: 02-099/B+S1[E]

N_2O_4
- Nitrogen oxide (N_2O_4) [10544-72-6]
  Dinitrogen tetroxide
  Nitrogen peroxide
  Nitrogen tetroxide
  Group-member nr.: 02-100

Na
- Sodium [7440-23-5]
  Natrium
  Group-member nr.: 01-021

Ne
- Neon [7440-01-9]
  Group-member nr.: 01-022

O_2
- Oxygen [7782-44-7]
  Group-member nr.: 01-023

O_2S
- Sulfur dioxide [7446-09-5]
  Group-member nr.: 02-101

O_3
- Ozone [10028-15-6]
  Group-member nr.: 01-024

O_3S
- Sulfur trioxide [7446-11-9]
  Group-member nr.: 02-102

O_6P_4
- Phosphorus oxide (P_4O_6) [12440-00-5]
  Group-member nr.: 02-103

P_4
- Phosphorus mol.(P_4) [12185-10-3]
  Group-member nr.: 01-025

Rb
- Rubidium [7440-17-7]
  Group-member nr.: 01-026

S
- Sulfur [7704-34-9]
  Group-member nr.: 01-027

Se
- Selenium [7782-49-2]
  Group-member nr.: 01-028

Sn
- Tin [7440-31-5]
  Stannane
  Group-member nr.: 01-029

Xe
- Xenon [7440-63-3]
  Group-member nr.: 01-030

Name: Deuterium (D_2)
Formula: D_2

CAS-RN: 7782-39-0
Group No.: 1-006
Molar Mass: 4.03

Table 1.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
35CLU/BAR	N	19.4–21.7	8	nosp	99.7	estim	sat	BSIO	36CLU/GOL
64GRE/WHI	N	19.9–22.0	3	1.20	not specified		sat	BSAO	64GRE/WHI

35CLU/BAR content of HD 0.3%
64GRE/WHI sample contained 78.7% para-Deuterium

Name: Trifluoroborane
Formula: BF_3

CAS-RN: 7637-07-2
Group No.: 2-008
Molar Mass: 67.81

Table 2.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
38EUC/SCH		145.0–173.0	5 S	nosp	99.3	melpt	*p*	BSAO	38EUC/SCH
58KOS/SAM	N	145.8–149.0	4	nosp	99.79	melpt	*p*	BSAO	54STR/ICK

58KOS/SAM data from a graph only

Table 2.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
38EUC/SCH	145.0–173.0	5	0.80 #	0.027	2.72–3	0.02	3.67–4	1
58KOS/SAM	147.0–149.0	3	0.80 #	0.251	2.49–2	0.20	−5.11–4	−1

Table 2.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	9	8	0.179	1.78–2	0.14	3.78–5	0

Temp. range K	A_1	A_2	Level of uncertainty
145.0–173.0	1.08324+1	1.04203	IV

Name: Carbon dioxide
Formula: CO_2

CAS-RN: 124-38-9
Group No.: 2-026
Molar Mass: 44.01

Table 2.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
26MAA/BAR	N	257.5	1	nosp	not specified		avg	DSIO	20MAA/HAT
28EUC/HAU		220.0–290.0	8 S	nosp	not specified		sat	BSIO	28EUC/HAU
86MAG/ELY		220.4–303.0	77	0.50	99.9946	chrom	sat	BSAO	61GOO
94HAA/TIL	N	295.4–304.0	11	nosp	not specified		sat	not specified	

26MAA/BAR average value in temperature range 217–298 K
94HAA/TIL calorimeter described in Tillmann W.: Dissertation, Aachen (1993)

Table 2.26.2. Correlated heat capacities

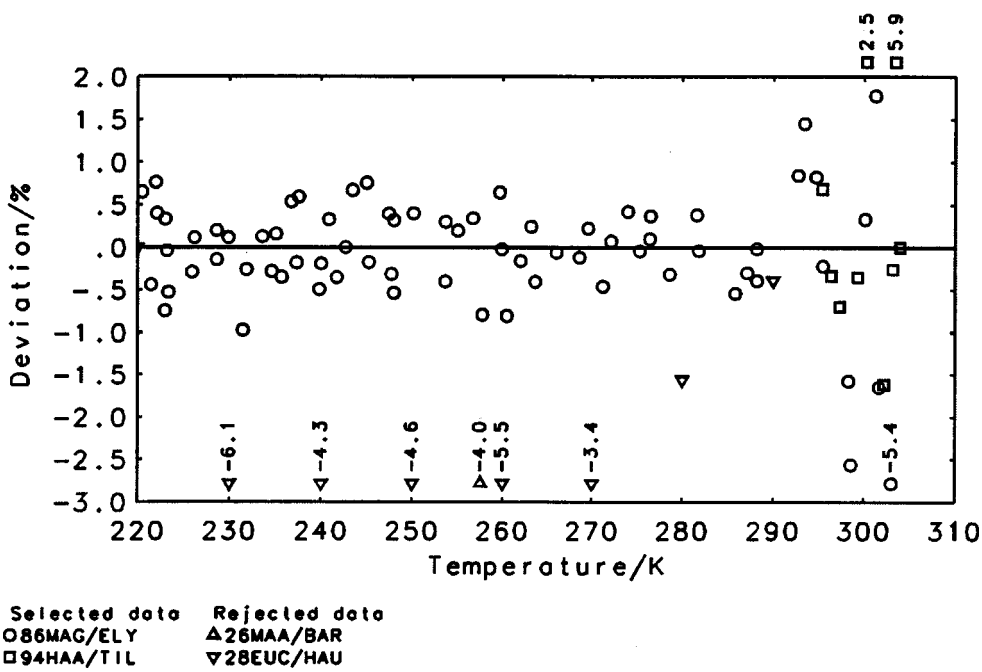
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
86MAG/ELY	220.4–303.0	77	0.70 #	1.251	4.99–1	0.88	−6.17–2	−6
94HAA/TIL	295.4–303.4	10	0.70 #	3.408	2.01	2.39	6.81–1	−2
			Rejected data					
26MAA/BAR	(4.57–1,4.05,−4.57–1,−1)		28EUC/HAU	(4.56–1,4.18,−4.15–1,−7)				

Table 2.26.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	97	87	1.720	8.63–1	1.20	2.37–2	−8

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
220.4–270.0	−1.78373+2	2.47895+2	−1.09362+2	1.62199+1	IV
270.0–290.0	−5.20709+3	5.83536+3	−2.17879+3	2.71705+2	IV
290.0–300.0	−2.21391+5	2.29474+5	−7.92955+4	9.13570+3	V
300.0–303.4	−3.06917+7	3.06998+7	−1.02361+7	1.13767+6	V

2-026



Name: Perchloryl fluoride ($(ClO_3)F$)
Formula: $ClFO_3$

CAS-RN: 7616-94-6
Group No.: 2-031
Molar Mass: 102.45

Table 2.31.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
58JAR/FRI	N	226.1–360.2	33	nosp	99.9	anal	sat	BSAO	58JAR/FRI
58KOE/GIA		130.5–223.3	15	nosp	99.999	melpt	sat	BSIO	28GIA/WIEl

58JAR/FRI uncertainty estimated by authors is 0.5% up to 340 K and 3% at 360 K

Table 2.31.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
58JAR/FRI	226.1–360.2	33	1.00 #	1.972	3.95–1	1.97	5.18–2	13
58KOE/GIA	130.5–223.3	15	0.40 #	1.047	4.69–2	0.42	−1.19–2	−3

Table 2.31.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	48	48	1.856	3.51–1	1.77	3.19–2	10
sat	48	48	1.664	3.08–1	1.59	2.66–2	8

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
130.5–250.0	1.62679+1	−9.29989	4.61991	−6.19907–1	IV
250.0–350.0	−8.47500+1	1.11922+2	−4.38687+1	5.84524	V
350.0–360.2	−5.96396+5	5.11236+5	−1.46079+5	1.39140+4	VI
130.5–250.0	1.52656+1	−7.70718	3.81068	−4.89344–1	IV
250.0–350.0	−4.91040+1	6.95364+1	−2.70868+1	3.63031	V
350.0–360.2	−4.56439+5	3.91261+5	−1.11796+5	1.06483+4	VI

Name: Sulfuryl fluoride
Formula: F_2O_2S

CAS-RN: 2699-79-8
Group No.: 2-063
Molar Mass: 102.06

Table 2.63.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
60BOC/PET	142.3–209.6	20	0.10	99.71	melpt	sat	BSAO	55PAC/PIE
76MOU/WEI	137.3–138.4	2	1.00	99.57	melpt	sat	BSAO	76MOU/WEI

Name: Sulfur fluoride (SF_6)
Formula: F_6S

CAS-RN: 2551-62-4
Group No.: 2-070
Molar Mass: 146.06

Table 2.70.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
38EUC/SCH	225.0–230.0	2	nosp	99.6	melpt	p	BSAO	38EUC/SCH
94OHT/YAM	226.0–249.6	9	nosp	99.99	melpt	sat	BSAO	87YAM/OGU

Table 2.70.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94OHT/YAM	226.0–249.6	9	0.15 #	0.345	7.81–3	0.05	6.28–5	2
Rejected data								
38EUC/SCH	(6.44–1,4.48,−6.44–1,−1)							

Table 2.70.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	11	9	0.463	1.05−2	0.07	6.28−5	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
226.0–249.6	5.23398+2	−6.40173+2	2.66578+2	−3.66717+1	II

Name: Germane
Formula: GeH_4

CAS-RN: 7782-65-2
Group No.: 2-072
Molar Mass: 76.64

Table 2.72.1. Experimental heat capacities

Reference	Temp. range K	No. pnts.	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
42CLU/FAB	112.7–165.4	8	nosp	not specified		*p*	BSIO	36CLU/GOL
78MOU/WEI	107.8–110.8	4	1.00	99.98	melpt	sat	BSAO	76MOU/WEI

Table 2.72.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
42CLU/FAB	112.7–165.4	8	1.50 #	0.738	8.14−2	1.11	−2.23−2	−2
78MOU/WEI	107.8–110.8	4	1.00	0.662	5.08−2	0.66	2.21−2	2

Table 2.72.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	12	12	0.824	8.39−2	1.13	−7.49−3	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
107.8–165.4	1.59426+1	−1.25867+1	4.55734	IV

Name: Ammonia
Formula: H_3N

CAS-RN: 7664-41-7
Group No.: 2-086
Molar Mass: 17.03

Table 2.86.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
18OSB/VAN	N	226.8–319.1	41	0.40	99.98	anal	sat	BSIO	18OSB/VAN
18OSB/VAN	N	234.2–308.9	9	0.40	99.98	anal	sat	BSIO	18OSB/VAN
24EUC/KAR		199.5–221.1	7	3.00	not specified		sat	BSIO	24EUC/KAR
26DAN/JEN		246.8–290.4	10	2.00	not specified		sat	BSIO	26DAN/JEN
37OVE/GIA		197.8–238.3	13	nosp	99.999	melpt	sat	BSIO	37GIA/EGA
71POP/MAN		199.2–200.8	2	1.00	99.99	anal	*p*	BSAO	68BAG/KUC

18OSB/VAN used method of measurements under saturation conditions
18OSB/VAN used method of measurements at constant pressure with full vessel of liquid

Table 2.86.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
18OSB/VAN	226.8–319.1	41	0.40	0.206	7.75–3	0.08	−6.65–4	−5
18OSB/VAN	234.2–308.9	9	0.40	0.202	7.60–3	0.08	2.62–3	2
37OVE/GIA	197.8–238.3	13	0.30 #	0.406	1.10–2	0.12	1.67–5	1
71POP/MAN	199.2–200.8	2	1.00	0.174	1.54–2	0.17	1.44–2	2
Rejected data								
24EUC/KAR	(3.38–1,3.66,3.15–1,7)		26DAN/JEN		(2.75–1,2.82,2.18–1,6)			

Table 2.86.3. Parameters of regression polynomial ±

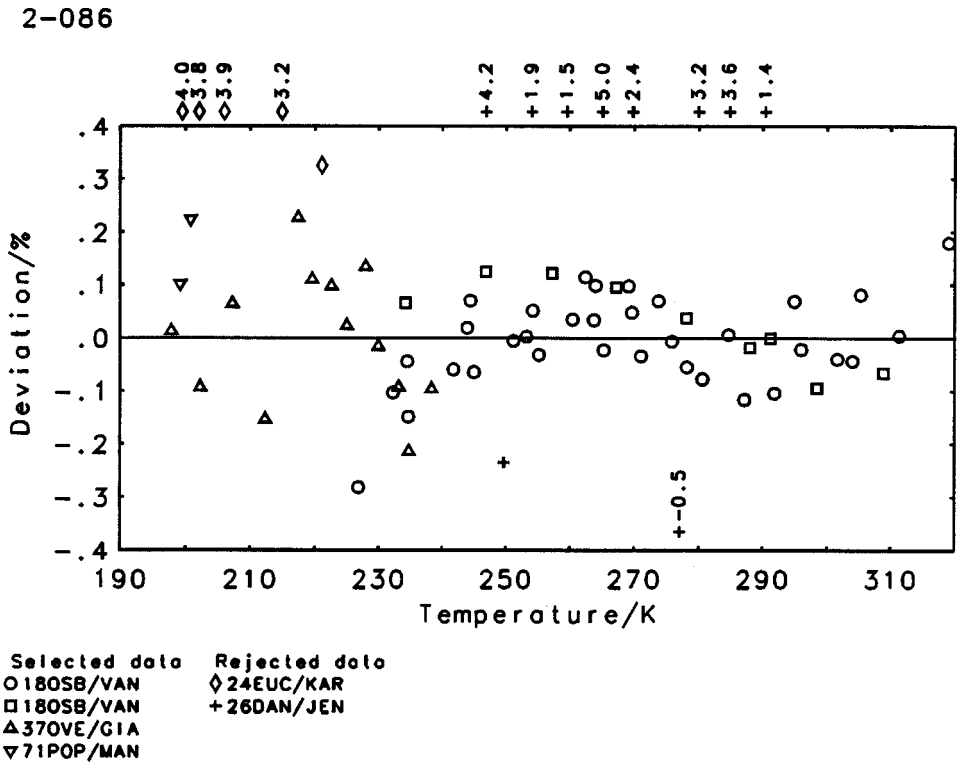
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	82	65	0.266	9.08–3	0.10	3.91–4	0
sat	82	65	0.258	8.60–3	0.09	2.94–4	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
197.8–319.1	−1.17631	1.20127+1	−4.94002	7.19471–1	III
197.8–319.1	6.00878–1	9.65070	−3.88986	5.62935–1	III

Table 2.86.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	82	65	0.409	1.30–2	0.14	8.66–4	3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
197.8–319.1	405.60	−3.40434–1	3.77221–1	7.86096	7.68086–2	IV



Name: Nitrogen oxide (N_2O)
Formula: N_2O

CAS-RN: 10024-97-2
Group No.: 2-099
Molar Mass: 44.01

Table 2.99.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
35BLU/GIA		183.6–187.1	5	nosp	99.999	estim	sat	BSIO	28GIA/WIE1
74ATA/CHI		183.1–184.4	6	nosp	99.999	melpt	sat	BSAO	74ATA/CHI
94HAA/TIL	N	295.2–309.5	11	nosp	not specified		sat	not specified	

94HAA/TIL calorimeter described in Tillmann W.: Dissertation, Aachen (1993)

Name: 2,2,4,4,6,6-Hexachloro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine
Formula: $Cl_6N_3P_3$

CAS-RN: 940-71-6
Group No.: 2-104
Molar Mass: 347.66

Table 2.104.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99LEB/KUL2	423.1–450.5	7	1.50	not specified		*p*	BDHT	69YAG

Table 2.104.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	7	7	0.573	3.09–1	0.86	3.81–3	5

Temp. range K	A_1	A_2	Level of uncertainty
423.1–450.5	2.37508+1	2.91470	V

Name: 2,2,4,4,6,6,8,8-Octachloro-2,2,4,4,6,6,8,8-octahydro-1,3,5,7,2,4,6,8-tetrazatetraphosphorine
Formula: $Cl_8N_4P_4$

CAS-RN: 2950-45-0
Group No.: 2-105
Molar Mass: 463.54

Table 2.105.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99LEB/KUL2	441.0–450.0	4	1.50	not specified		*p*	BDHT	69YAG

Table 2.105.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	4	4	0.088	6.22–2	0.13	1.23–4	−2

Temp. range K	A_1	Level of uncertainty
441.0–450.0	4.71189+1	V

Name: Tetrafluorosilane
Formula: F_4Si

CAS-RN: 7783-61-1
Group No.: 2-106
Molar Mass: 104.08

Table 2.106.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
58KOS/SAM	N	187.6–194.4	7	nosp	99.16	melpt	*p*	BSAO	54STR/ICK
63PAC/MOS		190.1–193.9	4	nosp	99.97	melpt	sat	BSAO	55PAC/PIE

58KOS/SAM data from a graph only

Table 2.106.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
58KOS/SAM	187.6–194.4	7	1.00 #	1.489	2.24–1	1.49	−1.56–1	−5
63PAC/MOS	190.1–193.9	4	0.60 #	1.761	1.65–1	1.06	1.06–1	2

Table 2.106.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	11	11	1.761	2.26–1	1.49	−6.09–2	−3

Temp. range K	A_1	A_2	Level of uncertainty
187.6–194.4	1.25573+1	1.46512	IV

Name: Selenium fluoride (SeF_6)
Formula: F_6Se

CAS-RN: 7783-79-1
Group No.: 2-107
Molar Mass: 192.95

Table 2.107.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96OHT/YAM	240.70	0.7845	0.10	99.99	melpt	sat	BSAO	87YAM/OGU

Name: Tungsten fluoride (WF_6)
Formula: F_6W

CAS-RN: 69175-55-9
Group No.: 2-108
Molar Mass: 297.83

Table 2.108.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96OHT/YAM	276.3–291.0	8	0.10	99.95	melpt	sat	BSAO	87YAM/OGU

Table 2.108.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	8	8	0.374	7.65–3	0.04	8.82–6	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
276.3–291.0	6.70136+1	−3.54279+1	6.70041	II

Name: Water-^{18}O
Formula: $H_2\,^{18}O$

CAS-RN: 14314-42-2
Group No.: 2-109
Molar Mass: 20.02

Table 2.109.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93NAG/MIY	N	275.5–300.5	11	0.30	99.9993	melpt	sat	BSAO	84OGA/KOB

93NAG/MIY the abundance of ^{18}O isotop is 96.2%

Table 2.109.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	11	11	0.123	3.41–3	0.04	1.91–6	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
275.5–300.5	1.79955+1	−5.89072	9.84278−1	II

Name: Ethane
Formula: C_2H_6

CAS-RN: 74-84-0
Group No.: 11-004
Molar Mass: 30.07

Table 11.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
28EUC/HAU		100.0–270.0	18 S	nosp	not specified		sat	BSIO	28EUC/HAU
30WIE/HUB	N	96.8–138.2	15	1.00	99.0	estim	sat	BSIO	30WIE/HUB
37WIT/KEM		91.6–180.9	29	0.40	99.5	melpt	*p*	BSIO	28GIA/WIE1
76ATA/CHI		91.0–102.4	11	nosp	99.999	melpt	*p*	BSAO	74ATA/CHI
76ROD1		92.2	1	nosp	not specified		*p*	BSAO	61GOO
76ROD2		93.7–301.5	106	0.50	99.98	chrom	sat	BSAO	61GOO
94HAA/TIL	N	295.4–305.1	9	nosp	not specified		sat	not specified	

30WIE/HUB error below and above n.b.t. 0.5% and 1.0%, respectively
94HAA/TIL calorimeter described in Tillmann W.: Dissertation, Aachen (1993)

Table 11.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
30WIE/HUB	96.8–138.2	15	1.00	0.428	3.56–2	0.43	1.63–3	−1
37WIT/KEM	91.6–180.9	29	0.40	1.001	3.39–2	0.40	2.20–4	7
76ATA/CHI	90.9–102.4	11	0.10 #	0.386	3.18–3	0.04	1.33–3	4
76ROD1	92.2	1	0.30 #	0.427	1.06–2	0.13	1.06–2	1
76ROD2	93.7–301.5	106	0.50	1.572	1.37–1	0.79	3.22–4	−21
94HAA/TIL	295.4–303.9	8	3.00 #	0.844	1.15	2.53	−6.92–1	−4
Rejected data								
28EUC/HAU	(1.70,15.54,1.63,18)							

Table 11.4.3. Parameters of cubic spline polynomials

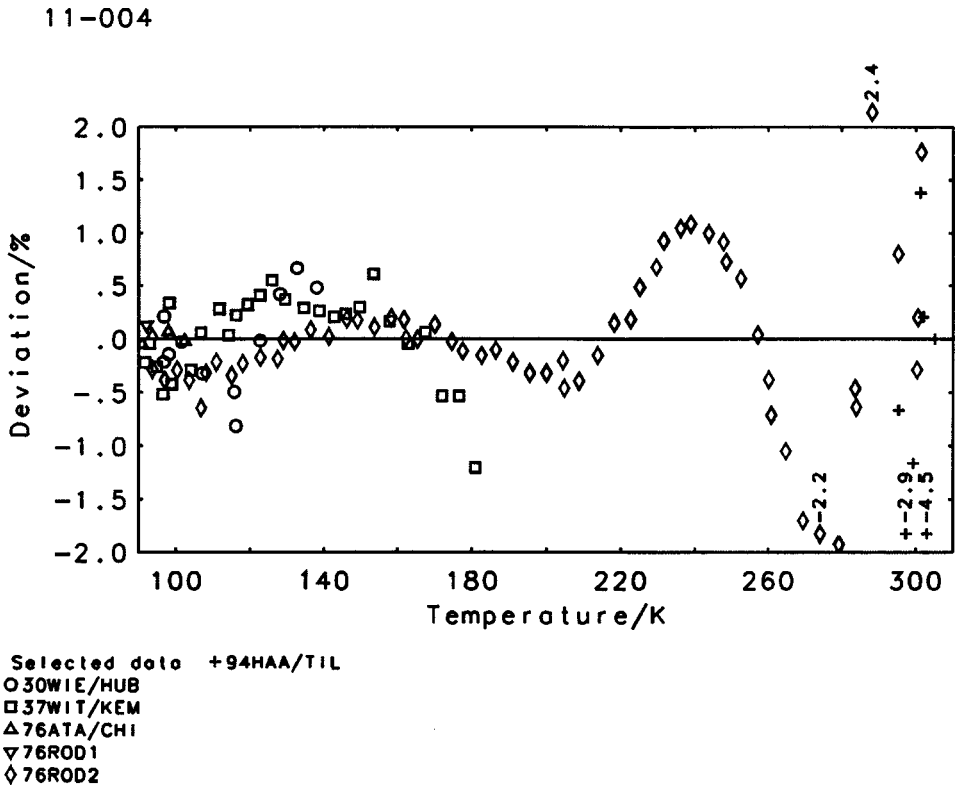
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	189	170	1.364	2.78–1	0.88	−3.20–2	−14
sat	189	170	1.023	1.54–1	0.67	−1.91–2	−13

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
91.0–150.0	6.09172	5.32742	−4.46188	1.29835	II
150.0–220.0	1.10928+1	−4.67472	2.20622	−1.83445–1	III
220.0–285.0	−1.43159+2	2.05669+2	−9.34047+1	1.43031+1	IV
285.0–300.0	−6.74890+4	7.10960+4	−2.49672+4	2.92352+3	V
300.0–303.9	−1.11741+7	1.11777+7	−3.72718+6	4.14281+5	V
91.0–150.0	6.47989	4.33507	−3.63542	1.07473	II
150.0–220.0	1.05600+1	−3.82507	1.80467	−1.34180–1	III
220.0–285.0	−9.10276+1	1.34703+2	−6.11628+1	9.40635	IV
285.0–300.0	−3.90170+4	4.11094+4	−1.44383+4	1.69094+3	V
300.0–303.9	−6.00983+6	6.01193+6	−2.00471+6	2.22832+5	V

Table 11.4.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	189	169	1.089	4.29–1	1.07	−6.48–2	−17

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
90.9–303.0	305.33	−2.09832	2.67682–1	7.93333	−2.03952	−3.39326	3.23774	IV



Name: Hexane
Formula: C_6H_{14}

CAS-RN: 110-54-3
Group No.: 11-013
Molar Mass: 86.18

Table 11.13.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
30PAR/HUF2		183.5–295.1	8	nosp	not specified		*p*	BSIO	25PAR
31HUF/PAR		188.8–293.5	5	1.00	not specified		*p*	BSIO	25PAR
37STU		180.0–320.0	15 S	nosp	not specified		*p*	BDHO	37STU
39PHI		300.6	1	nosp	not specified		*p*	BSIO	49WEI
46DOU/HUF2	N	180.4–301.0	24	0.10	99.992	melpt	*p*	BSAO	43RUE/HUF
51CON/SAG		299.8–366.5	13 S	0.70	not specified		*p*	BSAO	39SAG/EVA
69WIL/ROT		293.1	1	0.40	not specified		*p*	BDAO	65FIN/GRU
71AMI/ALI	N	343.1–506.1	19 S	2.00	not specified		*p*	not specified	
71REC/SAD		303.1	1	0.30	not specified		*p*	BSIO	70REC
74DIA/REN		298.2–324.7	14	0.30	not specified		*p*	BSAO	74DIA/REN
75GRI/RAS	N	304.5–463.1	9	1.00	not specified		*p*	BDAO	75RAS/GRI
76KAR/GRO		298.2	1	nosp	not specified		*p*	FSIT	71PIC/LED
80KAL/JED		180.6–301.4	33	0.20	99.95	chrom	*p*	BSAO	80KAL/JED
81GRO/ING		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
82WIL/ING		298.1	1	nosp	99.5	estim	*p*	FSIT	71PIC/LED
82ZAR		298.0–323.0	2	0.60	not specified		*p*	BDCT	82ZAR
84BEN/DAR		298.1	1	nosp	99.98	melpt	*p*	FSIT	71PIC/LED
84BRA/PIN		298.1	1	nosp	99.0	melpt	*p*	FSIT	71PIC/LED
85COS/PAT1		298.2	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
85COS/PAT8		298.1–313.1	2	nosp	99.	estim	*p*	FSIT	71PIC/LED
85CZA		299.9	1	nosp	not specified		*p*	BSIO	79CZA
86BEN/DAR1		298.1	1	nosp	99.88	anal	*p*	FSIT	71PIC/LED
86NAZ/BAS2		308.4–333.1	2	2.00	99.8	estim	*p*	BDHO	86NAZ/BAS1
88MEL/VER		183.1–473.1	11	2.50	not specified		sat	not specified	
88SAI/TAN		298.1	1	nosp	99.95	anal	*p*	FSIT	71PIC/LED
89OHN/FUJ		298.1	1	nosp	99.9	chrom	*p*	FSIO	85OGA/MUR
89VOG/SCH		333.1	1	nosp	not specified		*p*	BDHT	69PER/COM

Table 11.13.1. Experimental heat capacities—Continued

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91OGA/MIT		298.1	1	nosp	not specified		*p*	FSIO	85OGA/MUR
91PES/NIK	N	298.1	1	nosp	not specified		*p*	BSAO	83KUK/KOR
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
93CON/GIR1		298.0–333.0	eqn	5.00	not specified		sat	BDHT	93CON/GIR1

46DOU/HUF2 smoothed data in 67MES/GUT
71AMI/ALI calculated from C_v measured at the saturation line
75GRI/RAS all values (except the first one) at pressures above the vapor pressure
91PES/NIK water content below 0.05%

Name: Octane
Formula: C_8H_{18}

CAS-RN: 111-65-9
Group No.: 11-032
Molar Mass: 114.23

Table 11.32.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*98LOU	N	344.9	1	nosp	not specified		avg	DSIO	*98LOU
30PAR/HUF2		223.0–293.7	8	nosp	not specified		*p*	BSIO	25PAR
31HUF/PAR		227.0–298.3	5	nosp	not specified		*p*	BSIO	25PAR
47OSB/GIN		285.6–305.6	5 S	0.10	99.96	estim	sat	BSAO	47OSB/GIN
49TSC/WET		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
51CON/SAG		299.8–366.5	13 S	nosp	not specified		*p*	BSAO	39SAG/EVA
54FIN/GRO	N	222.6–297.6	18	0.20	99.94	melpt	sat	BSAO	43RUE/HUF
61ROU		283.1–312.3	15	nosp	99.83	anal	*p*	BSAO	61ROU
70AKH		293.1	1	nosp	not specified		*p*	BDHO	59ABA/MUS
71AMI/ALI	N	403.1–567.2	21 S	2.00	not specified		*p*	not specified	
75GRI/RAS	N	303.9–462.1	9	1.00	not specified		*p*	BDAO	75RAS/GRI
77NAZ/MUS		303.2–383.2	5	1.50	not specified		*p*	BSAO	77NAZ/MUS
80SHA/LYU		216.4–300.0	12 S	0.50	99.57	melpt	*p*	BSAO	80SHA/LYU
81GRO/ING		298.1	1	nosp	99.0	chrom	*p*	FSIT	71PIC/LED
82ZAR		298.0–363.0	3	0.60	not specified		*p*	BDCT	82ZAR
84GRI/AND	N	297.5–386.1	7	0.50	not specified		*p*	BSAO	67RAS/GAN
84ROU/GRO		298.1	1	0.30	99.	estim	*p*	FSIT	71PIC/LED
85COS/PAT2		298.2	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
85LAI/GRO		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
85LAI/ROD		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
86BEN/DAR1		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
91BAN/GAR		318.1–373.1	12	0.40	98.8	chrom	*p*	BDCT	91BAN/GAR
91OGA/MIT		298.1	1	nosp	not specified		*p*	FSIO	85OGA/MUR
91SOE/NAK		298.1	1	nosp	99.99	chrom	*p*	FSIO	85OGA/MUR
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
92LAI/ROD		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
93CZA1		298.8	1	2.00	not specified		*p*	BSIO	79CZA
99BUR/ZOC		298.1–323.1	2	2.00	not specified		*p*	FSIO	99BUR/ZOC
99TAM/OSA		298.1	1	nosp	99.99	anal	*p*	FSIO	85OGA/MUR

*98LOU average value in temperature range 294–396 K
54FIN/GRO smoothed data in 67MES/GUT
71AMI/ALI calculated from C_v measured at the saturation line
75GRI/RAS grade: pure; the last five values at pressures higher than vapor pressure
84GRI/AND grade: pure

Name: 2,2,4-Trimethylpentane
Formula: C_8H_{18}

CAS-RN: 540-84-1
Group No.: 11-034
Molar Mass: 114.23

Table 11.34.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
30PAR/HUF2		169.6–295.2	15	1.00	not specified		*p*	BSIO	25PAR
40PIT2		171.1–317.3	8	0.20	99.99	melpt	*p*	BSIO	28LAT/GRE
47OSB/GIN		285.6–305.6	5 S	0.10	99.96	melpt	sat	BSAO	47OSB/GIN
49TSC/WET		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
50AUE/SAG		299.8–366.5	13	1.00	99.9	melpt	*p*	BSAO	39SAG/EVA
61ROU		300.4–315.4	12	nosp	99.99	anal	*p*	BSAO	61ROU
73SUB/RAJ	N	298.1–323.1	3	0.30	not specified		*p*	BSIO	64MOE/THO
76FOR/BEN1		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
84FIL/LAU		293.0	1	2.00	not specified		*p*	BDHO	84FIL/LAU
87KAL/KOH		293.1–313.1	2	nosp	99.98	chrom	*p*	FSIT	71PIC/LED
88COS/VAN		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
88SHI/OGA1		298.1	1	nosp	99.9	chrom	*p*	FSIO	85OGA/MUR
94BEN/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
99PIN/BRA		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED

73SUB/RAJ same data in 74RAJ/SUB

Name: Nonane
Formula: C_9H_{20}

CAS-RN: 111-84-2
Group No.: 11-038
Molar Mass: 128.26

Table 11.38.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
30PAR/HUF2		224.5–299.1	8	1.00	not specified		*p*	BSIO	25PAR
31HUF/PAR		228.3–297.9	8	1.00	not specified		*p*	BSIO	25PAR
47OSB/GIN		283.1–313.1	4 S	0.10	99.96	estim	sat	BSAO	47OSB/GIN
54FIN/GRO	N	225.0–313.9	22	0.20	99.88	melpt	sat	BSAO	43RUE/HUF
58SWI/ZIE1	N	348.8	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
70AKH		293.1	1	nosp	not specified		*p*	BDHO	59ABA/MUS
76MUS		307.8–417.8	10	2.50	not specified		*p*	BDAO	71MUS
79GRO/HAM		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
82WIL/ING		298.1	1	nosp	99.0	estim	*p*	FSIT	71PIC/LED
82ZAR		323.0–363.0	2	0.60	not specified		*p*	BDCT	82ZAR
88AND/PAT		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
91BAN/GAR		318.1–373.1	12	0.40	99.8	chrom	*p*	BDCT	91BAN/GAR
91OGA/MIT		298.1	1	nosp	not specified		*p*	FSIO	85OGA/MUR
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
97TOV/CAR2		288.1–308.1	3	nosp	99.0	anal	*p*	BDCT	83ROU/ROU

54FIN/GRO smoothed data in 67MES/GUT
58SWI/ZIE1 average value in temperature range 295–402 K

Table 11.38.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
47OSB/GIN	283.1–313.1	4	0.10	1.666	5.69–2	0.17	2.63–3	0
54FIN/GRO	225.0–313.9	22	0.20	0.311	2.08–2	0.06	5.57–3	2
79GRO/HAM	298.1	1	0.50 #	0.283	4.83–2	0.14	−4.83–2	−1
82WIL/ING	298.1	1	0.50 #	0.495	8.44–2	0.25	−8.44–2	−1
82ZAR	323.0–363.0	2	0.60	0.844	1.87–1	0.51	−1.86–1	−2
88AND/PAT	298.1	1	0.50 #	0.224	3.83–2	0.11	3.83–2	1
91BAN/GAR	318.1–373.1	12	0.40 #	0.555	8.06–2	0.22	−3.49–2	−6
91TRE/COS	298.1	1	0.50 #	0.072	1.22–2	0.04	−1.22–2	−1
97TOV/CAR2	288.1–308.1	3	0.30 #	0.187	1.93–2	0.06	2.77–3	−1
Rejected data								
30PAR/HUF2	(4.25–1,1.29,−4.24–1,−7)		31HUF/PAR	(3.05–1,0.93,−2.99–1,−8)				
58SWI/ZIE1	(1.63,4.21,1.63,1)		70AKH	(5.78–1,1.67,5.78–1,1)				
76MUS	(9.01–1,2.44,−8.00–1,−6)		91OGA/MIT	(2.04–1,0.59,2.04–1,1)				

Table 11.38.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	76	47	0.670	6.59–2	0.18	−1.61–2	−9

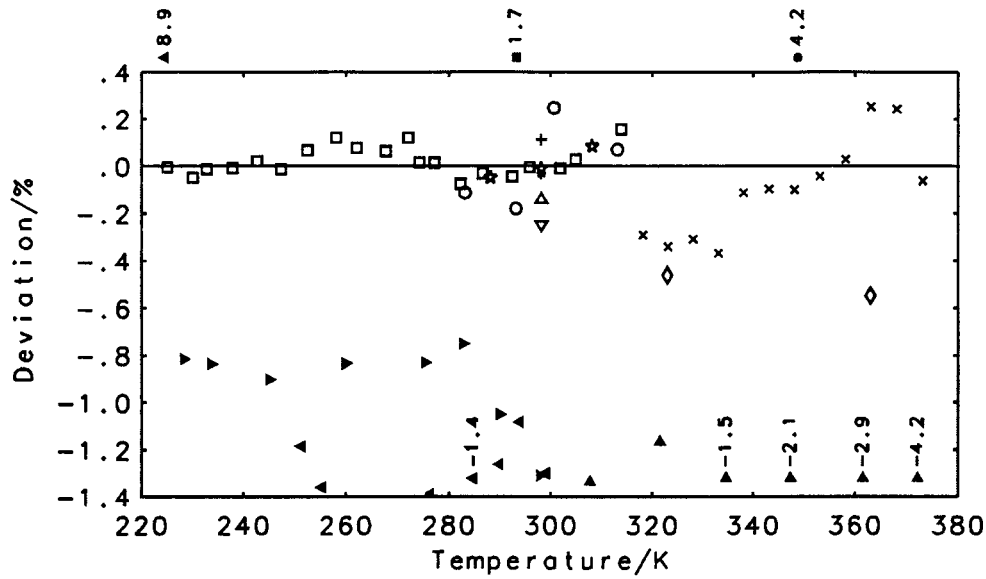
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
225.0–300.0	1.23776+2	−1.01511+2	3.61333+1	−4.07916	II
300.0–373.1	−8.31340+1	1.05399+2	−3.28368+1	3.58418	III

Table 11.38.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	76	47	1.899	1.20–1	0.35	5.16–3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
225.0–373.1	594.90	1.61014+1	1.36656+1	1.55105+1	4.74287	III

11-038



Selected data
○ 47OSB/GIN
□ 54FIN/GRO2
△ 79GRO/HAM
▽ 82WIL/ING
◊ 82ZAR
+ 88AND/PAT
× 91BAN/GAR
* 91TRE/COS
☆ 97TOV/CAR2

Rejected data
◄ 30PAR/HUF2
► 31HUF/PAR
● 58SWI/ZIE1
■ 70AKH
▲ 76MUS
▼ 91OGA/MIT

Name: Decane
Formula: $C_{10}H_{22}$

CAS-RN: 124-18-5
Group No.: 11-041
Molar Mass: 142.28

Table 11.41.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*98LOU	N	360.9	1	nosp	not specified		avg	DSIO	*98LOU
30PAR/HUF2		242.3–295.5	6	1.00	not specified		*p*	BSIO	25PAR
31HUF/PAR		251.2–297.7	6	1.00	not specified		*p*	BSIO	25PAR
47OSB/GIN		290.6–305.6	4 S	0.10	99.96	estim	sat	BSAO	47OSB/GIN
52SCH/SAG		299.8–366.5	13 S	1.00	99.7	estim	sat	BSAO	39SAG/EVA
54FIN/GRO	N	247.0–318.6	17	0.20	99.91	melpt	sat	BSAO	43RUE/HUF
70AKH		293.1	1	nosp	not specified		*p*	BDHO	59ABA/MUS
75GRI/RAS	N	303.3–462.4	9	1.00	not specified		*p*	BDAO	75RAS/GRI
79GRO/HAM		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
82PFE/KUC		298.1	1	nosp	not specified		*p*	BDCT	68WAD
82WIL/ING		298.1	1	nosp	99.0	estim	*p*	FSIT	71PIC/LED
82ZAR		298.0–363.0	3	0.60	not specified		*p*	BDCT	82ZAR
83SID/SVE		293.1	1	nosp	99.9	melpt	*p*	FSIT	71PIC/LED
84GRO/ING		298.1	1	nosp	99.0	melpt	*p*	FSIT	71PIC/LED
84ROU/GRO		298.1	1	nosp	98.0	estim	*p*	FSIT	71PIC/LED
85BAL/BRA		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
85COS/PAT3		298.2	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
85COS/PAT8		283.1–313.1	3	nosp	99.	estim	*p*	FSIT	71PIC/LED
85LAI/ROD		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
85LAI/WIL		298.1	1	0.30	99.	estim	*p*	FSIT	71PIC/LED
86GAT/WOO		298.1–368.1	4	nosp	99.	anal	*p*	BDCT	83ROU/ROU
87WIL/ING		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
88COS/VAN		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
88KUZ/KHA		293.8–335.2	15	nosp	99.8	chrom	*p*	FSIO	75SAF/GER
88KUZ/KHA		310.1–421.9	16	nosp	99.8	chrom	*p*	BSAO	67RAS/GAN
88PIN/BRA		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
91BAN/GAR		318.1–373.1	12	0.40	98.9	chrom	*p*	BDCT	91BAN/GAR
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
92LAI/ROD		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
93CZA2		298.9	1	2.00	not specified		*p*	BSIO	79CZA
94JIM/ROM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
96ROU/HER		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED

*98LOU average value in temperature range 295–427 K
54FIN/GRO smoothed data in 67MES/GUT
75GRI/RAS last two values at pressures above the vapor pressure

Table 11.41.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
				Selected data				
54FIN/GRO	247.0–318.6	17	0.20	0.179	1.34–2	0.04	2.28–3	0
75GRI/RAS	303.3–462.4	9	1.00	0.661	2.75–1	0.66	−7.23–2	−1
82ZAR	298.0–363.0	3	0.60	0.948	2.27–1	0.57	−2.12–1	−3
84GRO/ING	298.1	1	0.50 #	0.280	5.28–2	0.14	−5.28–2	−1
84ROU/GRO	298.1	1	0.50 #	0.101	1.91–2	0.05	−1.91–2	−1
86GAT/WOO	298.1–368.1	4	0.30 #	1.063	1.29–1	0.32	−1.27–1	−4
88KUZ/KHA	293.8–335.2	15	0.50 #	0.451	8.66–2	0.23	7.99–2	15
88KUZ/KHA	310.1–421.9	16	0.60 #	0.343	8.81–2	0.21	4.16–2	5
91BAN/GAR	318.1–373.1	12	0.40	0.340	5.73–2	0.14	2.46–2	3
93CZA2	298.9	1	2.00	0.043	3.22–2	0.09	−3.22–2	−1
94JIM/ROM	298.1	1	0.50 #	0.637	1.20–1	0.32	−1.20–1	−1
96ROU/HER	298.1	1	0.50 #	0.612	1.15–1	0.31	−1.15–1	−1
				Rejected data				
*98LOU	(4.04–1,0.96,4.04–1,1)			30PAR/HUF2	(6.58–1,1.85,−6.19–1,−5)			
31HUF/PAR	(3.08–1,0.85,−3.04–1,−6)			47OSB/GIN	(3.29–1,0.87,−2.14–2,0)			
52SCH/SAG	(3.97–1,1.02,−3.59–1,−11)			70AKH	(4.46–1,1.20,−4.46–1,−1)			
79GRO/HAM	(1.28–1,0.34,−1.28–1,−1)			82PFE/KUC	(2.64–1,0.70,−2.64–1,−1)			
82WIL/ING	(2.22–1,0.59,−2.22–1,−1)			83SID/SVE	(2.21–1,0.59,−2.21–1,−1)			
85BAL/BRA	(1.36–1,0.36,−1.36–1,−1)			85COS/PAT3	(1.28–1,0.34,1.28–1,1)			
85COS/PAT8	(1.58–1,0.41,4.81–2,1)			85LAI/ROD	(1.66–1,0.44,−1.66–1,−1)			
85LAI/WIL	(1.54–1,0.41,−1.54–1,−1)			87WIL/ING	(1.74–1,0.46,−1.74–1,−1)			
88COS/VAN	(1.14–1,0.30,1.14–1,1)			88PIN/BRA	(1.49–1,0.40,−1.49–1,−1)			
91TRE/COS	(1.31–1,0.35,1.31–1,1)			92LAI/ROD	(2.13–1,0.57,−2.13–1,−1)			

Table 11.41.3. Parameters of cubic spline polynomials

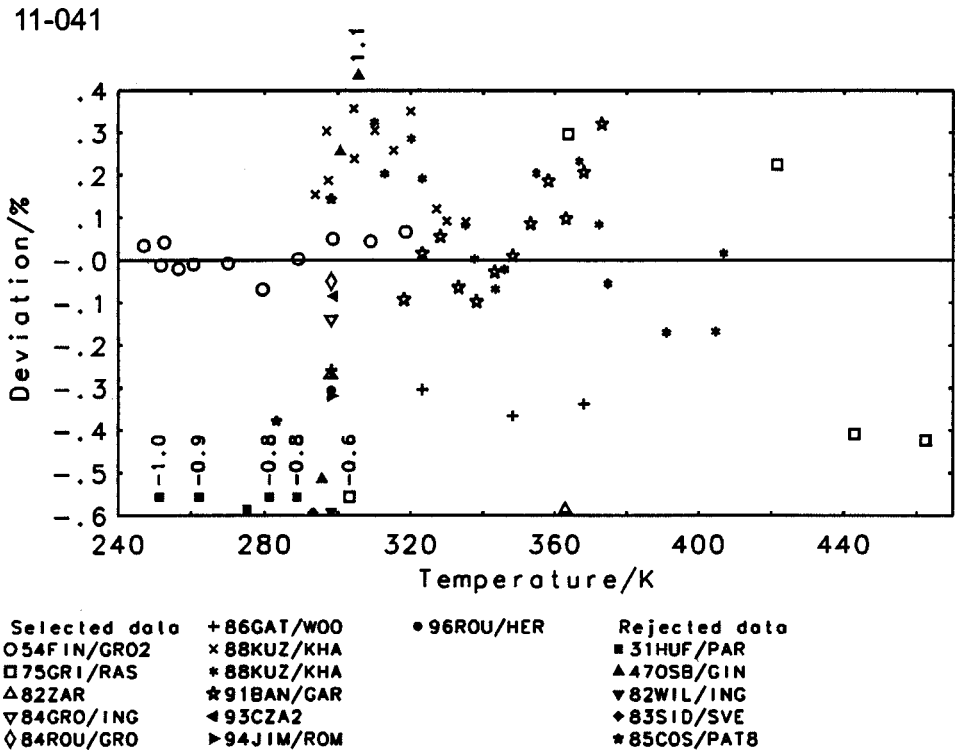
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	128	81	0.498	1.26–1	0.31	7.86–4	10
sat	128	81	0.499	1.26–1	0.31	8.16–4	10

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
247.0–314.0	8.23450+1	−5.00004+1	1.66449+1	−1.63834	II
314.0–462.4	3.62508+1	−5.96135	2.61979	−1.49470–1	III
247.0–314.0	8.19315+1	−4.95633+1	1.64917+1	−1.62051	II
314.0–462.4	3.74686+1	−7.08286	2.96287	−1.84328–1	III

Table 11.41.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	128	81	1.196	2.20–1	0.52	−6.42–3	2
p	128	81	1.196	2.20–1	0.52	−6.42–3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
247.0–462.4	617.65	−8.48603	2.02090	2.41615+1	8.90849	III
247.0–462.4	617.65	−8.48603	2.02090	2.41615+1	8.90849	III



Name: Dodecane
Formula: $C_{12}H_{26}$

CAS-RN: 112-40-3
Group No.: 11-049
Molar Mass: 170.34

Table 11.49.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
31HUF/PAR		275.1–297.7	4	1.00	not specified		*p*	BSIO	25PAR
54FIN/GRO	N	266.7–317.4	11	0.20	99.93	melpt	sat	BSAO	43RUE/HUF
71REC/SAD		303.1	1	0.30	not specified		*p*	BSIO	70REC
73KAL/WOY		303.1	1	0.20	99.5	chrom	*p*	BSIO	70REC
77NAZ/MUS		303.2–483.2	10	1.50	not specified		*p*	BSAO	77NAZ/MUS
81GRO/ING		298.1	1	nosp	99.0	chrom	*p*	FSIT	71PIC/LED
82ZAR		298.0–363.0	3	0.60	not specified		*p*	BDCT	82ZAR
84GRO/BEN		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
84KUM/BEN		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
84ROU/GRO		298.1	1	nosp	98.	estim	*p*	FSIT	71PIC/LED
85BEN/KUM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
85COS/PAT4		298.2	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
85COS/PAT8		283.1–313.1	3	nosp	99.0	estim	*p*	FSIT	71PIC/LED
85LAI/ROD		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
86BEN/DAR3		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
86WIL/LAI		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
88COS/VAN		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
89LAI/ROD		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
89VOG/SCH		333.1	1	nosp	not specified		*p*	BDHT	69PER/COM
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
92LAI/ROD		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
98SAL/FER		293.0–370.0	eqn	nosp	99.	chrom	*p*	BDHT	98SAL/FER
99BUR/ZOC		298.1–323.1	2	2.00	99.5	chrom	*p*	FSIO	99BUR/ZOC

54FIN/GRO smoothed data in 67MES/GUT

Name: Tetradecane
Formula: $C_{14}H_{30}$

CAS-RN: 629-59-4
Group No.: 11-052
Molar Mass: 198.39

Table 11.52.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
34PAR/LIG		280.6–290.6	4	1.00	not specified		*p*	BSIO	25PAR
54FIN/GRO	N	282.7–302.8	7	0.20	99.93	melpt	sat	BSAO	43RUE/HUF
76MUS		307.8–501.5	18	2.50	not specified		*p*	BDAO	71MUS
82ZAR		298.0–363.0	3	0.60	not specified		*p*	BDCT	82ZAR
84GRI/AND		296.2–433.3	8	0.80	not specified		*p*	BSAO	67RAS/GAN
84GRO/BEN		298.1	1	nosp	99.5	estim	*p*	FSIT	71PIC/LED
84GRO/ING		298.1	1	nosp	99.	estim	*p*	FSIT	71PIC/LED
84ROU/GRO		298.1	1	nosp	99.	estim	*p*	FSIT	71PIC/LED
85BAL/BRA		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
85LAI/WIL		298.1	1	0.30	99.5	estim	*p*	FSIT	71PIC/LED
86WIL/LAI		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
87WIL/ING		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
88COS/VAN		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
92LAI/ROD		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
96ROU/HER		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

54FIN/GRO smoothed data in 67MES/GUT

Name: 2,2,4,4,6,8,8-Heptamethylnonane
Formula: $C_{16}H_{34}$

CAS-RN: 4390-04-9
Group No.: 11-054
Molar Mass: 226.45

Table 11.54.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
88COS/VAN	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
99PIN/BRA	298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED

Table 11.54.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
88COS/VAN	298.1	1	0.50 #	1.140	3.14–1	0.57	3.14–1	1
99PIN/BRA	298.1	1	0.50 #	1.127	3.07–1	0.56	−3.07–1	−1

Table 11.54.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	1.603	4.40–1	0.80	3.53–3	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	5.48662+1	IV

Name: Hexadecane
Formula: $C_{16}H_{34}$

CAS-RN: 544-76-3
Group No.: 11-055
Molar Mass: 226.45

Table 11.55.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
49PAR/MOO		290.0–300.0	2 S	1.00	95.	estim	*p*	BSIO	25PAR
54FIN/GRO	N	295.4–320.3	9	0.20	99.88	melpt	sat	BSAO	43RUE/HUF
56SCH/GOT		292.1–294.6	4	2.00	not specified		*p*	BSAO	33SOU/BRI
62GOL/BEL		310.9–422.0	3	nosp	96.9	chrom	*p*	BDHT	63GUD/CAM
68REC1	N	298.0–313.0	eqn	nosp	not specified		*p*	BSAO	68REC1
70AKH		293.1	1	nosp	not specified		*p*	BDHO	59ABA/MUS
71REC/SAD		303.1	1	0.30	not specified		*p*	BSIO	70REC
72REC/SAD		298.1	1	0.30	not specified		*p*	BSIO	70REC
73KAL/WOY		303.1	1	0.20	99.5	chrom	*p*	BSIO	70REC
74DIA/REN		300.1–323.5	9	0.30	not specified		*p*	BSAO	74DIA/REN
74PET/TER		297.8–453.5	14	1.00	98.	melpt	*p*	BDCT	74PET/TER
81GRO/ING		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
82PFE/KUC		298.1	1	nosp	not specified		*p*	BDCT	68WAD
82ZAR		298.0–363.0	3	0.60	not specified		*p*	BDCT	82ZAR
85COS/PAT5		298.2	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
85LAI/ROU		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
86WIL/LAI		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
88COS/VAN		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
89LAI/ROD		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
91BAN/GAR		318.1–373.1	12	0.40	99.4	chrom	*p*	BDCT	91BAN/GAR
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
92LAI/ROD		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
94BEN/ROU		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED

54FIN/GRO smoothed data in 67MES/GUT
68REC1 same data in 68REC3

Name: Heptadecane
Formula: $C_{17}H_{36}$

CAS-RN: 629-78-7
Group No.: 11-056
Molar Mass: 240.47

Table 11.56.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
67MES/GUT	301.9–384.4	11	0.10	99.89	melpt	sat	BSAO	47HUF
70AKH	293.1	1	nosp	not specified		*p*	BDHO	59ABA/MUS
#00VAN	299.0–401.1	46	0.20	99.	anal	*p*	BSAO	98VAN/VAN

Table 11.56.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
67MES/GUT	301.9–384.4	11	0.10	2.823	1.98–1	0.28	−1.56–1	−9
#00VAN	299.0–401.1	46	0.20	1.193	1.67–1	0.24	1.51–1	45

Table 11.56.3. Parameters of regression polynomial

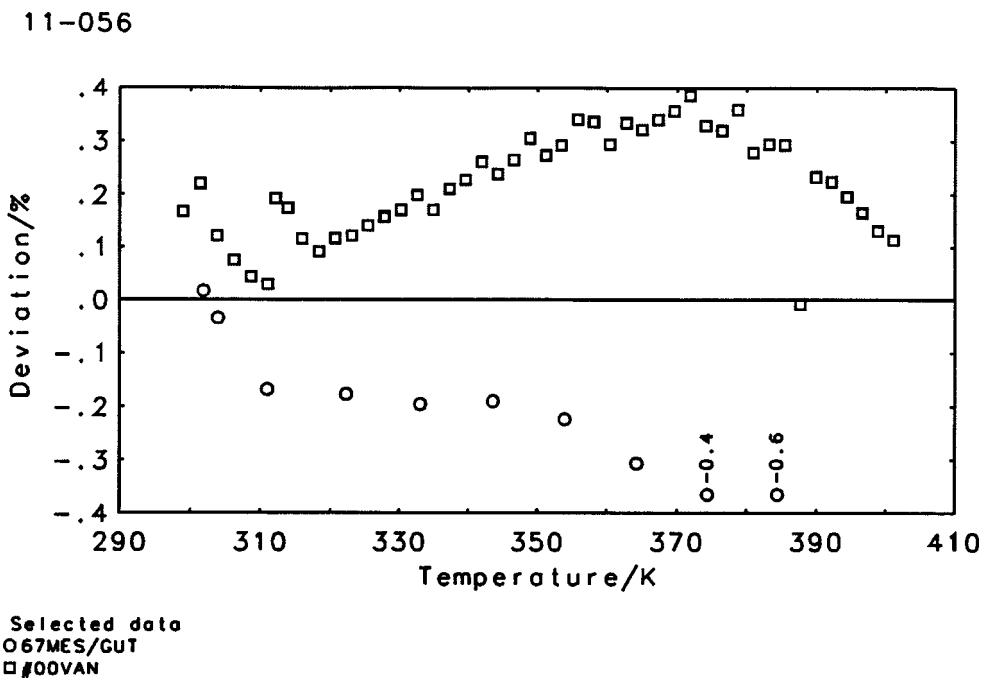
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	58	57	1.684	1.78–1	0.25	9.20–2	36

Temp. range K	A_1	A_2	A_3	Level of uncertainty
299.0–401.1	6.17907+1	−5.83983	2.22416	II

Table 11.56.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	58	57	1.881	1.48−1	0.21	2.00−3	18

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
299.0–401.1	735.00	−1.06915+1	1.34417+1	3.51130+1	2.12600	II



Name: Octadecane
Formula: $C_{18}H_{38}$

CAS-RN: 593-45-3
Group No.: 11-057
Molar Mass: 254.50

Table 11.57.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
49PAR/MOO		300.0	1	1.00	96.	estim	*p*	BSIO	25PAR
67MES/GUT		304.4–378.7	11	0.10	99.98	melpt	sat	BSAO	47HUF
81HOE		325.0–375.0	3 S	5.00	not specified		*p*	BDHT	69PER/COM
83MEY/MEY	N	303.0	1	nosp	99.5	melpt	*p*	BSIO	83MEY/MEY
86DJO/LAU	N	315.0	1	nosp	not specified		*p*	BDHT	69PER/COM
93DUR/AOU	N	373.0–473.0	51	nosp	not specified		*p*	BDCT	86MER/BEN
#00VAN		306.7–401.1	38	0.20	99.8	anal	*p*	BSAO	98VAN/VAN

83MEY/MEY in the article temperature unspecified; probably above melting temperature
86DJO/LAU very suspect value
93DUR/AOU an equation in 96DUR/AOU

Table 11.57.2. Correlated heat capacities

Reference	Temp. range K	No. Pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
				Selected data				
49PAR/MOO	300.0	1	1.00	0.370	2.51–1	0.37	−2.51–1	−1
67MES/GUT	304.4–378.7	11	0.10	2.481	1.84–1	0.25	−1.41–1	−11
83MEY/MEY	303.0	1	1.00 #	0.247	1.69–1	0.25	1.69–1	1
#00VAN	306.7–401.1	38	0.20	1.229	1.81–1	0.25	1.66–1	34
				Rejected data				
81HOE	(2.53,3.63,−2.52,−3)			86DJO/LAU	(1.04+1,13.03,1.04+1,1)			
93DUR/AOU	(1.22,1.54,1.21,5)							

Table 11.57.3. Parameters of regression polynomial

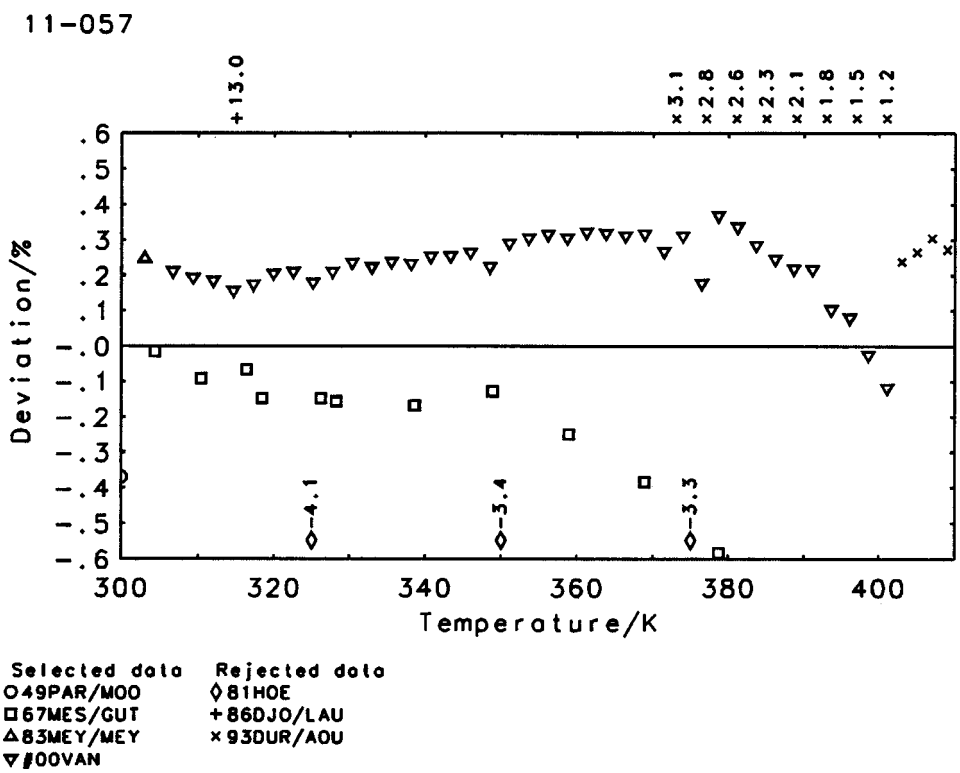
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	106	51	1.615	1.88–1	0.26	9.14–2	23

Temp. range K	A_1	A_2	A_3	Level of uncertainty
300.0–401.1	7.28757+1	−1.04237+1	2.94698	II

Table 11.57.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	106	51	1.837	1.61–1	0.22	−3.25–3	19

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–401.1	746.00	4.80074	2.37668+1	3.07599+1	2.42430–1	II



Name: Nonadecane
Formula: $C_{19}H_{40}$

CAS-RN: 629-92-5
Group No.: 11-058
Molar Mass: 268.53

Table 11.58.1. Experimental heat capacities

Reference		Temp. range	No.	Error	Purity		Type	Calorimeter	
%		K	pnts	%	method	Type	capac	Type	Reference
69ATK/LAR		305.0–453.0	eqn	nosp	99.9	chrom	*p*	BSAO	58WES/GIN
84GRI/AND		313.1–433.2	10	0.70	not specified		*p*	BSAO	67RAS/GAN
93DUR/AOU	N	373.0–473.0	51	nosp	not specified		*p*	BDCT	86MER/BEN
99VAN/OON		306.2–380.0	47	0.20	99.54	melpt	*p*	BSAO	87VAN/VAN

93DUR/AOU an equation in 96DUR/AOU

Table 11.58.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
69ATK/LAR	305.0–453.0	9	0.50 #	0.933	3.53–1	0.47	−2.85–1	−9
84GRI/AND	313.1–433.2	10	0.70	1.046	5.66–1	0.73	−5.28–1	−10
99VAN/OON	306.4–380.0	45	0.20	0.709	1.08–1	0.14	1.92–2	−1
Rejected data								
93DUR/AOU	(1.92,2.29,3.27–1,5)							

Table 11.58.3. Parameters of regression polynomial

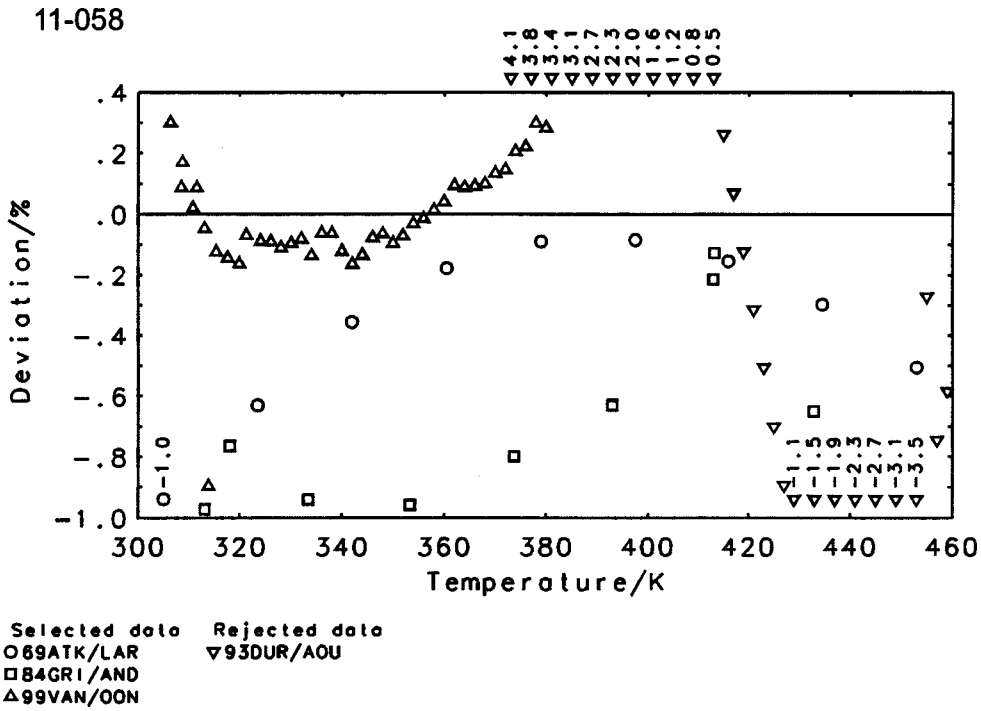
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	117	64	0.824	2.82–1	0.37	−1.09–1	−20

Temp. range K	A_1	A_2	A_3	Level of uncertainty
305.0–453.0	5.26380+1	3.62494	9.36989−1	III

Table 11.58.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	117	64	1.280	2.60–1	0.35	4.48–2	30

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
305.0–453.0	756.20	−7.05468	1.92176−1	4.20334+1	6.47435+1	IV



Name: Eicosane
Formula: $C_{20}H_{42}$

CAS-RN: 112-95-8
Group No.: 11-060
Molar Mass: 282.55

Table 11.60.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
81HOE	325.0–400.0	4 S	5.00	not specified		*p*	BDHT	69PER/COM
99VAN/OON	310.9–398.1	61	0.20	99.91	melpt	*p*	BSAO	87VAN/VAN

Table 11.60.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
99VAN/OON	310.9–398.1	61	0.20	0.218	3.53–2	0.04	3.19–5	−2
Rejected data								
81HOE	(1.34,1.59,1.23,3)							

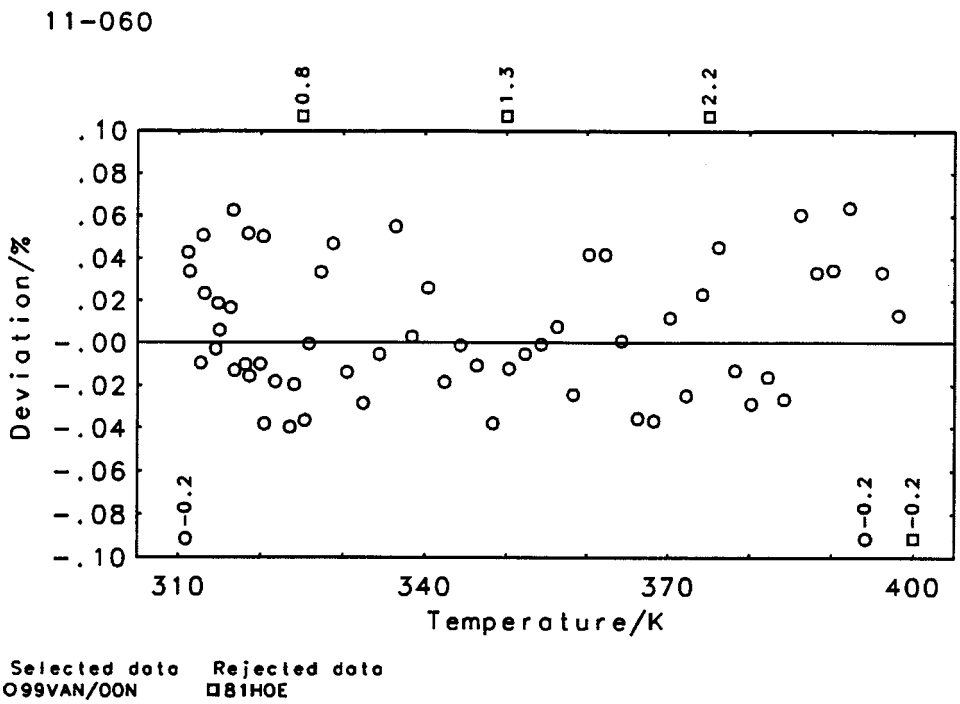
Table 11.60.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	65	61	0.225	3.66–2	0.05	3.19–5	−2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
310.9–398.1	1.72485+2	−9.24405+1	2.71671+1	−2.35443	II

Table 11.60.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	65	61	0.326	5.30−2	0.07	6.30−5	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
310.9–398.1	774.60	−1.16426+1	1.83175+1	3.95512+1	1.85001		III



Name: Hexatriacontane
Formula: $C_{36}H_{74}$

CAS-RN: 630-06-8
Group No.: 11-077
Molar Mass: 506.98

Table 11.77.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
48MAZ		350.1–359.1	2	nosp	not specified		p	BDHO	33STR/MAL
69ATK/LAR		349.0–453.0	eqn	nosp	not specified		p	BSAO	58WES/GIN
81HOE		375.0–500.0	6 S	5.00	not specified		p	BDHT	69PER/COM
91JIN/WUN		360.0–430.0	8	1.00	98.	anal	p	BDHT	90JIN/WUN
93DUR/AOU	N	373.0–473.0	51	nosp	not specified		p	BDCT	86MER/BEN
99WAN/TAN		350.2–370.0	9	0.50	99.45	melpt	p	BSAO	83TAN/ZHO

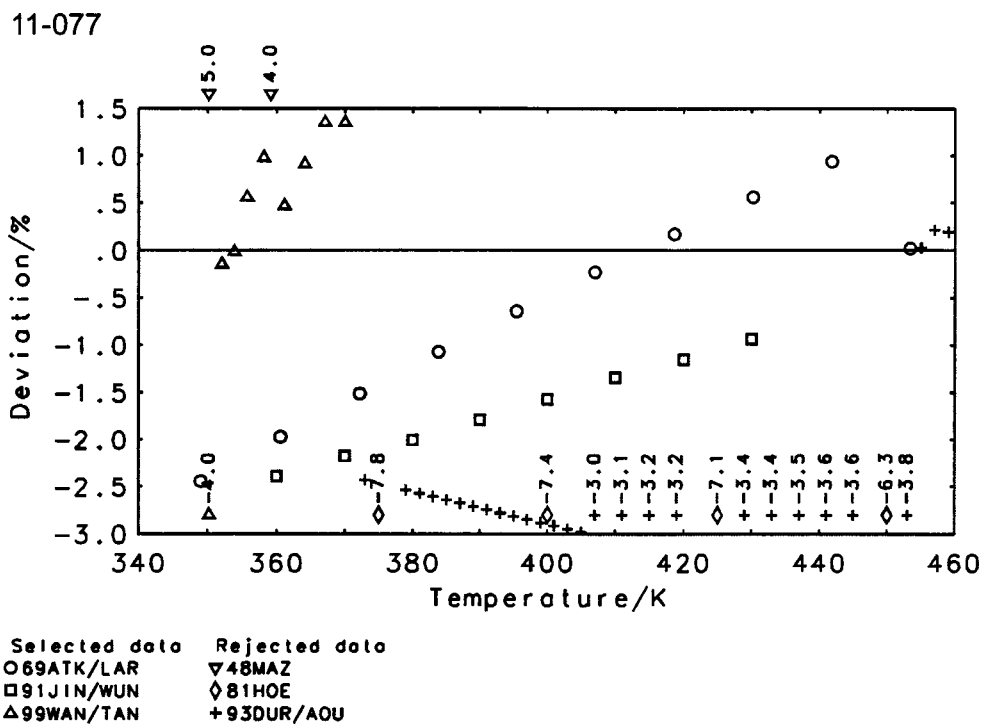
93DUR/AOU an equation in 96DUR/AOU

Table 11.77.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
69ATK/LAR	349.0–453.4	10	0.80 #	1.616	1.94	1.29	−6.79–1	−2
91JIN/WUN	360.0–430.0	8	1.00	1.739	2.62	1.74	−2.53	−8
99WAN/TAN	352.1–370.0	8	0.50	1.730	1.32	0.86	1.03	4
			Rejected data					
48MAZ	(7.05,4.53,7.01,2)		81HOE	(1.06+1,7.19,−1.05+1,−4)				
93DUR/AOU	(4.83,3.14,−4.78,−41)							

Table 11.77.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	86	26	1.759	2.10	1.40	−7.21–1	−6
Temp. range K		A_1	A_2				Level of uncertainty
349.0–453.4		9.14193+1	1.61279+1				V



Name: Cyclohexane
Formula: C_6H_{12}

CAS-RN: 110-82-7
Group No.: 12-007
Molar Mass: 84.16

Table 12.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
19DEJ		295.6–323.3	10	nosp	not specified		*p*	BSIO	19DEJ
30PAR/HUF2		283.1–298.9	5	0.30	not specified		*p*	BSIO	25PAR
39PHI		304.1	1	nosp	not specified		*p*	BSIO	49WEI
43AST/SZA		281.6–292.5	4	nosp	99.905	melpt	*p*	BSAO	39AST/EID1
43RUE/HUF		282.3–301.3	7	0.10	99.985	melpt	*p*	BSAO	43RUE/HUF
48TSC2		292.6	1	nosp	not specified		*p*	BSIO	48TSC1
48TSC6		293.6	1	nosp	not specified		*p*	BSIO	48TSC1
50AUE/SAG		299.8–366.5	13	nosp	99.9	melpt	*p*	BSAO	39SAG/EVA
60SWI/ZIE	N	311.6–322.2	2	nosp	not specified		avg	DSIO	58SWI/ZIE1
61ROU		300.4–315.8	7	nosp	99.94	anal	*p*	BSAO	61ROU
64MOE/THO		298.0–327.7	4	0.50	not specified		*p*	BSIO	64MOE/THO
66KLE		293.1–343.1	11 S	0.10	not specified		*p*	BSAO	66KLE
66NIK/RAB		283.1–333.1	11 S	0.30	not specified		*p*	BSAO	47SKU
68REC1	N	298.0–313.0	eqn	nosp	not specified		*p*	BSAO	68REC1
69WIL/SCH		293.1–313.1	3	0.40	not specified		*p*	BDAO	65FIN/GRU
73SUB/RAJ		298.1–323.1	3	0.30	not specified		*p*	BSIO	64MOE/THO
74WIL/ZET		283.1–323.1	5	nosp	not specified		*p*	BSAO	64ARN1
75JOL/BOI		298.1	1	0.30	99.9	melpt	*p*	FSIT	71PIC/LED
75SAN	N	398.1–523.2	9 S	1.00	not specified		*p*	FSIO	75SAN
78GRO/WIL		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
78SAF		299.1–311.7	7	0.30	not specified		*p*	BSAO	67RAS/GAN
78SAF		299.1–311.7	7	0.30	not specified		*p*	FSIO	75SAF/GER
78SAF		299.1–311.7	7	nosp	not specified		*p*	BSAO	67RAS/GAN
79FOR/DAR		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
79MAR/BRA		298.1	1	1.00	not specified		*p*	BDCT	70PAZ/PAZ
79WIL/GRO		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
82GRO/ING		298.1	1	0.30	99.5	melpt	*p*	FSIT	71PIC/LED
82TAN		293.1–303.1	3 S	0.30	99.99	chrom	*p*	FSIT	71PIC/LED
83SID/SVE		293.1	1	0.30	99.9	chrom	*p*	FSIT	71PIC/LED
85NKI/CHA		298.0	1	0.30	not specified		*p*	FSIT	71PIC/LED
85TAN/NAK		283.1–318.1	3	0.30	100.0	chrom	*p*	FSIT	71PIC/LED
86JIM/ROM		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
86ORT		298.1	1	1.00	99.5	anal	*p*	BDCT	70PAZ/PAZ
87KAL/KOH		293.1–313.1	2	nosp	not specified		*p*	FSIT	71PIC/LED
88SHI/OGA2		298.1	1	nosp	99.9	chrom	*p*	FSIO	85OGA/MUR
89JIM/ROU		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
89LAI/ROD		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
90JAL/ROB		293.0	1	5.00	99.	anal	*p*	BDHT	87PER/COM
91OGA/MIT		298.1	1	nosp	not specified		*p*	FSIO	85OGA/MUR
91TRE/COS		298.1	1	nosp	99.98	anal	*p*	FSIT	71PIC/LED
94BEN/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
94CON/GIA1		298.1	1	nosp	not specified		*p*	FSIT	88CON/GIA
94CON/GIA2		298.1	1	nosp	99.8	anal	*p*	FSIT	88CON/GIA
94LAI/WIL		298.1–298.1	2	nosp	99.5	anal	*p*	FSIT	71PIC/LED
95LOW/PEU		298.2	1	1.00	not specified		*p*	BDCO	95LOW/PEU
97CON/GIA		298.1	1	nosp	not specified		*p*	FSIT	88CON/GIA
97TOV/CAR1		288.1–308.1	3	nosp	99.9	anal	*p*	BDCT	83ROU/ROU
99BRO/CAL		298.1	1	nosp	99.9	chrom	*p*	FSIT	71PIC/LED

60SWI/ZIE average values in temperature ranges 294–329 K and 294–350 K
68REC1 same data in 68REC2
75SAN same data in 76SAN/MEL; C_p at the saturation pressure extrapolated from high pressure measurement

Name: Tetracyclo[3.2.0.0^{2,7}.0^{4,6}]heptane
Formula: C_7H_8

CAS-RN: 278-06-8
Group No.: 12-009
Molar Mass: 92.14

Table 12.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
73HAL/SMI		297.1	1	nosp	99.9	chrom	*p*	BDHT	71DU/COM
78STE	N	298.1	1	nosp	not specified		*p*	not specified	

78STE unspecified DSC instrument used for measurement

Table 12.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	± %
Selected data								
78STE	298.1	1	1.00 #	0.000	0.00	0.00	0.00	0

Table 12.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	± %
p	2	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	1.89548+1	V

Name: Methylcyclohexane
Formula: C_7H_{14}

CAS-RN: 108-87-2
Group No.: 12-019
Molar Mass: 98.19

Table 12.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
30PAR/HUF1	151.4–294.2	12	1.00	not specified		*p*	BSIO	25PAR
46DOU/HUF1	155.1–285.8	15	0.10	99.989	melpt	*p*	BSAO	43RUE/HUF
48TSC2	292.6	1	nosp	not specified		*p*	BSIO	48TSC1
48TSC6	293.6	1	nosp	not specified		*p*	BSIO	48TSC1
66HWA/ZIE	174.8–308.1	32	nosp	99.0	melpt	*p*	BSAO	45SCO/MEY
75HOL/ZIE	144.0–312.0	eqn	0.20	99.88	anal	*p*	BSAO	45SCO/MEY
79WIL/GRO	298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
82GRO/ING	298.1	1	0.30	99.5	estim	*p*	FSIT	71PIC/LED
83SID/SVE	293.1	1	0.30	99.9	chrom	*p*	FSIT	71PIC/LED
85TAN	298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
88SHI/OGA2	298.1	1	nosp	99.9	chrom	*p*	FSIO	85OGA/MUR
#00BEC/AUF	288.2–353.2	14	0.20	99.95	chrom	sat	BDCT	#00BEC/AUF

Table 12.19.2. Correlated heat capacities

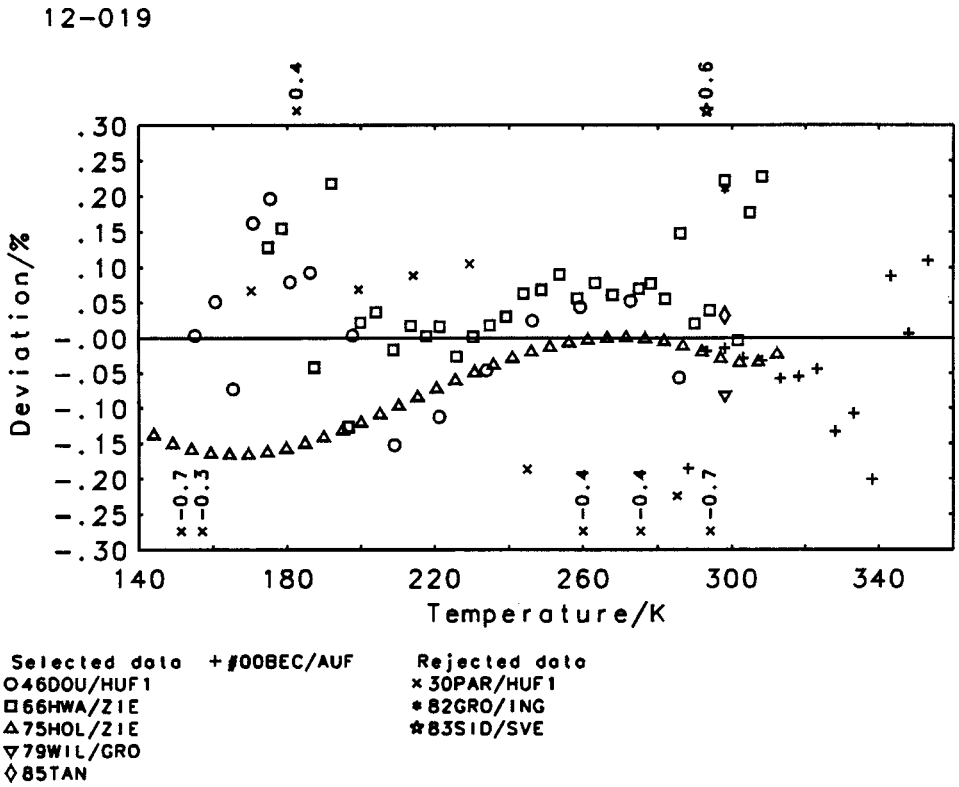
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
46DOU/HUF1	155.1–285.8	15	0.10	0.956	1.72–2	0.10	2.96–3	3
66HWA/ZIE	174.8–308.1	32	0.20 #	0.580	2.33–2	0.12	1.44–2	22
75HOL/ZIE	144.0–312.3	34	0.20	0.489	1.72–2	0.10	−1.34–2	−27
79WIL/GRO	298.1	1	0.30	0.223	1.48–2	0.07	−1.48–2	−1
85TAN	298.1	1	0.30	0.156	1.04–2	0.05	1.04–2	1
#00BEC/AUF	288.2–353.2	14	0.20	0.608	2.88–2	0.12	−1.24–2	−6
			Rejected data					
30PAR/HUF1	(7.04–2,0.36,−3.52–2,−2)		48TSC2	(6.83–2,0.31,−6.83–2,−1)				
48TSC6	(6.90–2,0.31,−6.90–2,−1)		82GRO/ING	(5.01–2,0.22,5.01–2,1)				
83SID/SVE	(1.34–1,0.60,1.34–1,1)		88SHI/OGA2	(5.93–2,0.27,−5.93–2,−1)				

Table 12.19.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	114	97	0.642	2.18–2	0.11	−1.34–3	−8
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
144.0–290.0		1.52819+1	−9.30055−2	6.91448−1	4.09100−2		II
290.0–353.2		2.90944+1	−1.43818+1	5.61863	−5.25433−1		II

Table 12.19.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	114	97	1.571	5.98–2	0.28	−6.32–3	−1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
144.0–353.2	572.20	−4.85992	3.99105	9.49688	1.47948		III



Name: 6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane
Formula: $C_{10}H_{16}$

CAS-RN: 127-91-3
Group No.: 12-045
Molar Mass: 136.24

Table 12.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81BER/OGI	243.1–303.1	3 S	nosp	not specified		avg	DSIO	*79BER
98SAM/NIE	313.1–403.1	19	1.50	98.84	chrom	*p*	BDCT	86MER/BEN

Table 12.45.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
98SAM/NIE	318.1–403.1	18	1.50	0.037	1.90–2	0.06	5.32–5	−1

Table 12.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	22	18	0.042	2.15–2	0.06	5.32–5	−1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
318.1–403.1		2.76642+2	−2.03575+2	5.48167+1	−4.73167		V

Name: 1,3-Dimethyltricyclo[3.3.1.1^{3,7}]decane
Formula: $C_{12}H_{20}$

CAS-RN: 702-79-4
Group No.: 12-063
Molar Mass: 164.29

Table 12.63.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
77STE/WAT	N	298.1	1	nosp	not specified		*p*	not specified	
96STE/CHI1		300.0–700.0	21 S	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

77STE/WAT unspecified DSC calorimeter was used

Table 12.63.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
96STE/CHI1	300.0–700.0	21	1.00	0.539	3.33–1	0.54	4.93–3	−1

Table 12.63.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	22	21	0.617	3.81–1	0.62	4.93–3	−1
sat	22	21	0.394	2.25–1	0.39	1.69–3	−3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–650.0	−2.77796+1	3.04061+1	−4.62286	3.16275−1	IV
650.0–700.0	−6.31253+4	2.91523+4	−4.48492+3	2.30075+2	IV
300.0–650.0	−2.26751+1	2.64800+1	−3.63254	2.34218−1	IV
650.0–700.0	−3.79884+4	1.75491+4	−2.69942+3	1.38480+2	IV

Table 12.63.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	22	21	0.193	1.00–1	0.19	4.50–4	−5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
300.0–700.0	708.00	−3.45464	3.36440−1	−1.45488+1	1.35298+2	−9.23507+1	2.26084+1	IV

Name: Tetradecahydrophenanthrene
Formula: $C_{14}H_{24}$

CAS-RN: 5743-97-5
Group No.: 12-080
Molar Mass: 192.34

Table 12.80.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	not specified		*p*	BDHT	63GUD/CAM
#00ROH/CEN	305.4–335.2	21	1.00	not specified		*p*	BDCT	91BAN/GAR

Table 12.80.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
63GUD/CAM	313.1–483.1	4	2.00 #	1.093	9.75–1	2.19	6.84–1	2
#00ROH/CEN	305.4–335.2	21	1.00	0.206	8.17–2	0.21	−3.01–2	−3

Table 12.80.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	25	25	0.496	4.14–1	0.93	8.41–2	−1

Temp. range K	A_1	A_2	Level of uncertainty
305.4–483.1	5.62985	1.04600+1	V

Name: Ethenylcyclohexane
Formula: C_8H_{14}

CAS-RN: 695-12-5
Group No.: 12-125
Molar Mass: 110.20

Table 12.125.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93LEB/SMI	146.5–400.0	8 S	0.20	99.13	melpt	p	BSAO	76LEB/LIT

Table 12.125.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	8	8	2.588	1.07–1	0.52	5.25–4	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
146.5–400.0	1.56136+1	1.12286	5.97453−1	IV

Table 12.125.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	8	8	3.528	1.46–1	0.71	1.33–3	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
146.5–400.0	607.00	−6.80584	1.33774	1.27684+1	8.65629	IV

Name: (3aα,4β,7β,7aα)-Octahydro-4,7-methano-1*H*-indene
Formula: $C_{10}H_{16}$

CAS-RN: 2825-82-3
Group No.: 12-126
Molar Mass: 136.24

Table 12.126.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78GOO/SCO	275.0–365.0	eqn	nosp	not specified		sat	BDHT	69PER/COM
78MOY/SAS	210.0–340.0	eqn	nosp	96.8	melpt	*p*	BDHT	69PER/COM
79SMI/GOO	298.1	1	nosp	not specified		*p*	BDHT	69PER/COM
80GOO/THO	260.0–465.0	eqn	nosp	99.98	chrom	sat	BDHT	69PER/COM

Table 12.126.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
78MOY/SAS	210.0–340.0	27	3.00 #	1.082	8.22–1	3.25	−6.47–1	−21
80GOO/THO	260.0–465.0	42	2.00 #	0.551	2.84–1	1.10	2.06–1	26
Rejected data								
78GOO/SCO	(3.32,10.93,3.31,19)		79SMI/GOO	(3.14,11.04,3.14,1)				

Table 12.126.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	89	69	0.820	5.72–1	2.26	−1.27–1	5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
210.0–465.0		6.03009	5.44583	3.42303−1			V

Name: Tricyclo[3.3.1.1^{3,7}]decane
Formula: $C_{10}H_{16}$

CAS-RN: 281-23-2
Group No.: 12-127
Molar Mass: 136.24

Table 12.127.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00KAB/BLO	543.2–600.0	7 S	nosp	99.98	chrom	*p*	BDHT	92KAB/KOZ

Table 12.127.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	7	7	0.102	9.68–2	0.20	2.06–4	1
Temp. range K		A_1	A_2				Level of uncertainty
543.2–600.0		4.14351−1	8.12859				V

Name: Octahydro-1,2,4-ethanylylidene-1*H*-cyclobuta[*cd*]pentalene
Formula: $C_{11}H_{14}$

CAS-RN: 4421-32-3
Group No.: 12-128
Molar Mass: 146.23

Table 12.128.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95KAB/KOZ	475.80	2.315	2.00	98.9	chrom	*p*	BDHT	92KAB/KOZ

Name: Dodecahydroacenaphtylene
Formula: $C_{12}H_{20}$

CAS-RN: 2146-36-3
Group No.: 12-129
Molar Mass: 164.29

Table 12.129.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00ROH/CEN	307.9–327.8	9	1.00	not specified		*p*	BDCT	91BAN/GAR

Table 12.129.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	9	9	0.125	4.44–2	0.13	8.73–5	1

Temp. range K	A_1	A_2	Level of uncertainty
307.9–327.8	9.96115	7.97931	IV

Name: (3aα,4β,7β,7aα)-Octahydrodimethyl-4,7-methano-1*H*-indene
Formula: $C_{12}H_{20}$

CAS-RN: 28014-61-1
Group No.: 12-130
Molar Mass: 164.29

Table 12.130.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78GOO/SCO	260.0–360.0	eqn	nosp	not specified		sat	BDHT	69PER/COM
79SMI/GOO	298.1	1	nosp	not specified		*p*	BDHT	69PER/COM

Table 12.130.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
Selected data								
78GOO/SCO	260.0–360.0	21	3.00 #	0.003	3.11–3	0.01	3.01–3	6
79SMI/GOO	298.1	1	2.00 #	0.038	2.79–2	0.08	−2.79–2	−1

Table 12.130.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	22	22	0.009	7.01−3	0.02	1.60−3	5
Temp. range K		A_1	A_2				Level of uncertainty
260.0–360.0		1.16673+1	8.32461				V

Name: Dodecahydro-1,3,4,6-ethanediylidenedicyclopenta[*cd*,*gh*]pentalene
Formula: $C_{14}H_{16}$

CAS-RN: 17872-39-8
Group No.: 12-131
Molar Mass: 184.28

Table 12.131.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94KAB/KOZ	440.0–500.0	7 S	2.00	99.8	chrom	*p*	BDHT	92KAB/KOZ

Table 12.131.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	7	7	0.000	2.41−6	0.00	−1.09−6	0
Temp. range K		A_1	A_2				Level of uncertainty
440.0–500.0		1.25697+1	6.59986				V

Name: Dodecahydro-4,7-methano-2,3,8-methenocyclopent[*a*]indene (stereoisomer HNN)
Formula: $C_{14}H_{18}$

CAS-RN: 66289-74-5
Group No.: 12-132
Molar Mass: 186.30

Table 12.132.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78MOY/SAS	292.0–339.0	eqn	nosp	98.5	melpt	*p*	BDHT	69PER/COM

Table 12.132.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	10	10	0.000	1.51−6	0.00	1.91−7	0
Temp. range K		A_1	A_2				Level of uncertainty
292.0–338.8		−2.32681	1.14372+1				V

Name: Dodecahydro-4,7-methano-2,3,8-methenocyclopent[*a*]indene (stereoisomer HXN)
Formula: $C_{14}H_{18}$

CAS-RN: 66289-73-4
Group No.: 12-133
Molar Mass: 186.30

Table 12.133.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78MOY/SAS	326.0–344.0	eqn	nosp	98.3	melpt	*p*	BDHT	69PER/COM

Table 12.133.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	8	8	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
326.0–344.2	2.92447	9.84351	V

Name: Dodecahydro-4,7-methano-2,3,8-methenocyclopent[*a*]indene (stereoisomer HXX)
Formula: $C_{14}H_{18}$

CAS-RN: 64162-49-8
Group No.: 12-134
Molar Mass: 186.30

Table 12.134.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78MOY/SAS	297.0–341.0	eqn	nosp	97.3	melpt	*p*	BDHT	69PER/COM

Table 12.134.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	15	15	0.000	2.24−6	0.00	−2.54−7	0

Temp. range K	A_1	A_2	Level of uncertainty
297.0–340.4	−3.70098	1.18122+1	V

Name: Dodecahydro-1,4:5,8-dimethanobiphenylene
Formula: $C_{14}H_{20}$

CAS-RN: 25079-41-8
Group No.: 12-135
Molar Mass: 188.31

Table 12.135.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78MOY/SAS	344.0–384.0	eqn	nosp	97.8	melpt	*p*	BDHT	69PER/COM

Table 12.135.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	8	8	0.000	3.12−6	0.00	1.91−6	0

Temp. range K	A_1	A_2	Level of uncertainty
344.0–383.9	−8.89704	1.33615+1	V

Name: Nonadecylcyclohexane
Formula: $C_{25}H_{50}$

CAS-RN: 22349-03-7
Group No.: 12-136
Molar Mass: 350.67

Table 12.136.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
83MEY/MEY	N	316.15	2.184	nosp	94.5	melpt	*p*	BSIO	83MEY/MEY

83MEY/MEY in the article temperature unspecified; probably above melting temperature of stabile modification

Name: (5α)-Cholestane
Formula: $C_{27}H_{48}$

CAS-RN: 481-21-0
Group No.: 12-137
Molar Mass: 372.68

Table 12.137.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00MOK/RUZ	357.6–486.7	30	1.00	97.8	chrom	*p*	BDCT	91BAN/GAR

Table 12.137.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	30	30	0.219	2.22−1	0.22	8.83−4	7

Temp. range K	A_1	A_2	A_3	Level of uncertainty
357.6–486.7	1.13527+1	2.45732+1	−7.57983−1	IV

Name: 1-Butene
Formula: C_4H_8

CAS-RN: 106-98-9
Group No.: 13-007
Molar Mass: 56.11

Table 13.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
36TOD/PAR		81.3–253.4	24	0.50	99.9	estim	*p*	BSIO	25PAR
46AST/FIN	N	89.8–258.5	18	0.30	99.54	melpt	*p*	BSIO	28GIA/WIE1
49SCH/SAG		310.9–366.5	11	1.50	not specified		*p*	BSAO	39SAG/EVA
91TAK/YAM		89.8–299.8	81	0.20	99.78	melpt	sat	BSAO	87YAM/OGU

46AST/FIN errors below and above 200 K 0.3% and 0.5%, respectively

Table 13.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
36TOD/PAR	81.3–253.4	24	0.50	0.636	4.19–2	0.32	−6.75–3	−7
46AST/FIN	89.8–258.5	18	0.30	1.349	5.27–2	0.40	−3.22–2	−9
49SCH/SAG	310.9–366.5	11	1.50	0.250	6.82–2	0.38	5.23–3	1
91TAK/YAM	89.8–299.8	81	0.20	0.420	1.11–2	0.08	3.57–3	30

Table 13.7.3. Parameters of cubic spline polynomials

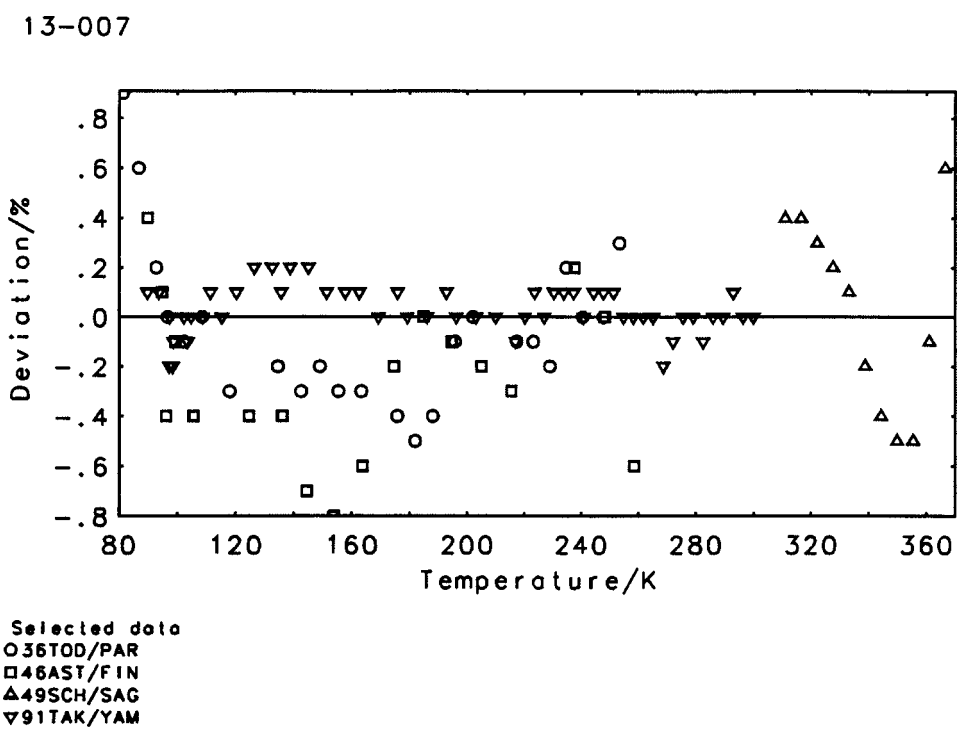
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	134	134	0.670	3.46–2	0.24	−2.95–3	15
sat	134	134	0.672	3.51–2	0.25	−3.64–3	13

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
81.3–200.0	1.63560+1	−5.93600	2.88498	−3.45255−1	II
200.0–310.0	1.28979+1	−7.48819−1	2.91400−1	8.70088−2	II
310.0–366.5	−2.57468+2	2.60896+2	−8.41101+1	9.16244	V
81.3–200.0	1.63527+1	−5.92847	2.87955	−3.43987−1	II
200.0–310.0	1.35057+1	−1.65800	7.44315−1	1.18853−2	II
310.0–366.5	−2.08986+2	2.13656+2	−6.87120+1	7.48030	V

Table 13.7.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	134	86	2.015	7.42–2	0.52	5.77–3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
141.9–366.5	419.95	−1.98272	5.98736−1	1.08233+1	−7.90902−2	3.82303−1	7.46031−2	V



Name: 1-Pentene
Formula: C_5H_{10}

CAS-RN: 109-67-1
Group No.: 13-021
Molar Mass: 70.13

Table 13.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
47TOD/OLI	125.7–295.3	24	0.20	not specified		sat	BSAO	47HUF
49SCH/SAG	310.9–366.5	11	1.50	not specified		*p*	BSAO	39SAG/EVA
90MES/TOD	111.0–308.4	25	0.10	99.913	melpt	sat	BSAO	47HUF
95TAK/YAM	108.8–303.5	65	0.10	99.1	melpt	sat	BSAO	82MOR/MAT

Table 13.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
				Selected data				
47TOD/OLI	125.7–295.3	24	0.20	0.614	1.99–2	0.12	3.60–3	3
49SCH/SAG	310.9–366.5	11	1.50	01.000	3.02–1	1.50	−2.77–1	−11
90MES/TOD	111.0–308.4	25	0.10	1.367	2.43–2	0.14	−8.45–3	3
95TAK/YAM	108.8–303.5	65	0.10	1.119	1.87–2	0.11	3.20–3	12

Table 13.21.3. Parameters of cubic spline polynomials

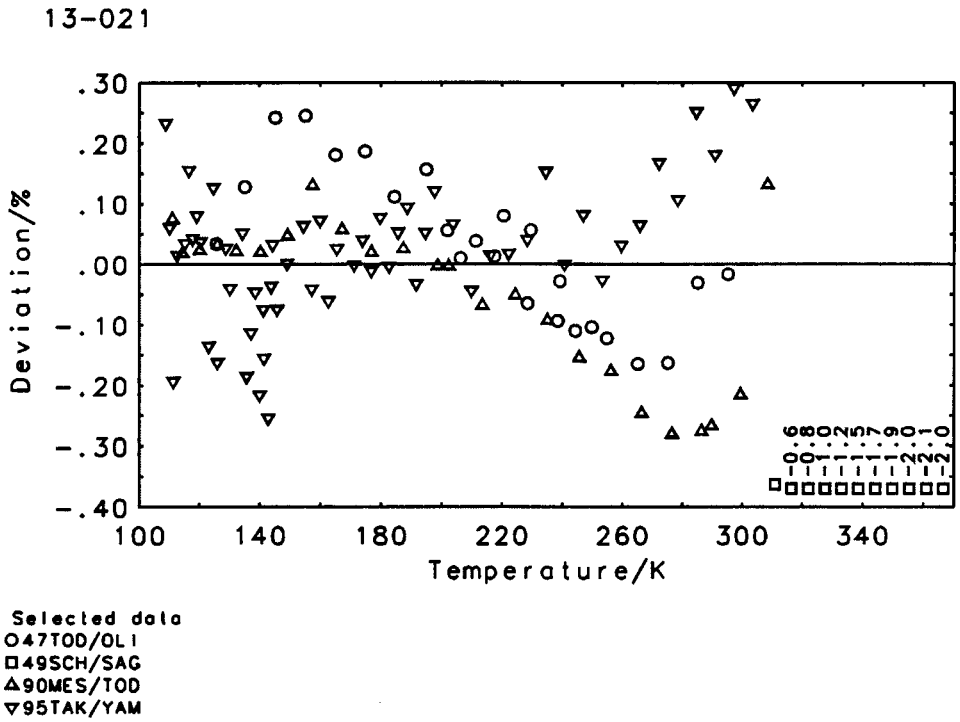
Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	125	125	1.111	9.35–2	0.47	−2.37–2	7
sat	125	125	1.110	9.07–2	0.46	−2.29–2	6

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
108.8–250.0	1.82932+1	−4.45103	1.90781	−1.22834−1	II
250.0–366.5	2.36815+1	−1.09170+1	4.49421	−4.67686−1	V
108.8–250.0	1.83222+1	−4.50466	1.93972	−1.28928−1	II
250.0–366.5	2.52519+1	−1.28203+1	5.26598	−5.72429−1	V

Table 13.21.4. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	125	125	2.663	5.12–2	0.30	6.60–3	−3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
108.8–366.5	464.78	6.74740+1	4.61088	1.03754+1	6.96221+1	−7.31450	8.70906+1	V



Name: 1-Heptene
Formula: C_7H_{14}

CAS-RN: 592-76-7
Group No.: 13-030
Molar Mass: 98.19

Table 13.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
36PAR/TOD2	151.1–295.1	21	0.50	99.85	melpt	*p*	BSIO	25PAR
57MCC/FIN1	157.1–299.6	22	0.10	99.86	melpt	sat	BSAO	47HUF
88GUS/MIR1	303.1–343.1	3	nosp	not specified		*p*	BDHT	84GUS/MIR1

Table 13.30.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
57MCC/FIN1	157.1–299.6	22	0.10	0.239	5.68–3	0.02	3.21–4	1
88GUS/MIR1	303.1–343.1	3	0.80 #	0.767	1.59–1	0.61	−1.48–1	−3
Rejected data								
36PAR/TOD2	(1.04–1,0.44,5.21–3,−2)							

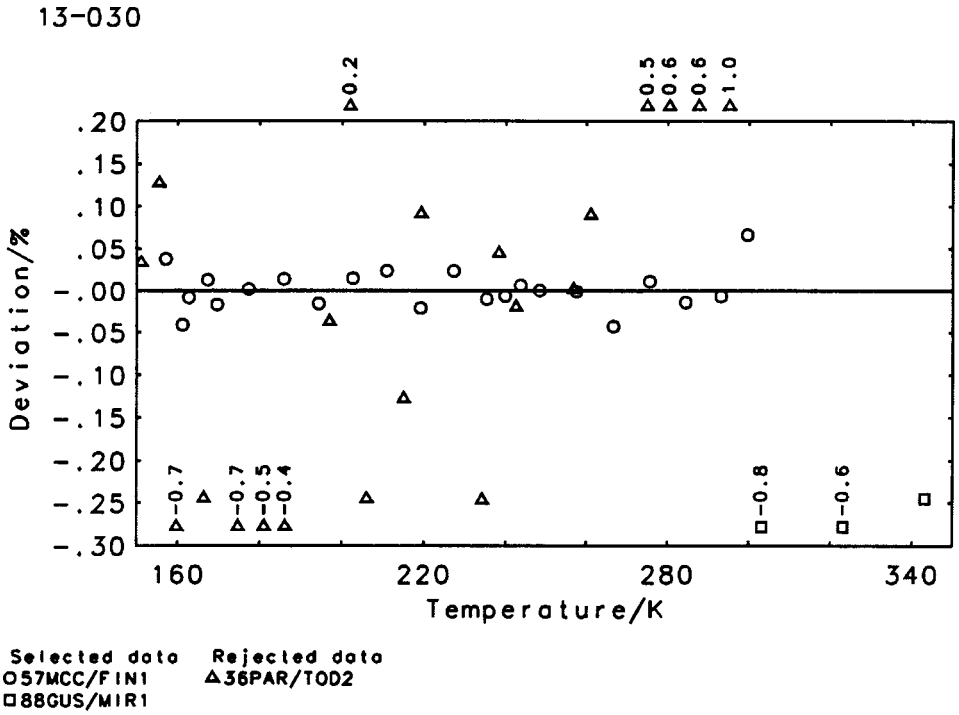
Table 13.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	46	25	0.379	6.04–2	0.23	−1.74–2	−2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
157.1–343.1		2.98111+1	−1.12277+1	4.61440	−4.48681−1		II

Table 13.30.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	46	25	0.798	8.58−2	0.32	3.10−3	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
157.1–343.1	537.30	5.70825+2	5.71077+1	−3.78482+1	5.48469+2	6.00042+1	4.34554+2	IV



Name: 1-Nonene
Formula: C_9H_{18}

CAS-RN: 124-11-8
Group No.: 13-034
Molar Mass: 126.24

Table 13.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
88GUS/MIR1	303.1–383.1	5	nosp	not specified		*p*	BDHT	84GUS/MIR
90MES/TOD	199.4–380.3	25	0.10	99.979	melpt	sat	BSAO	47HUF

Name: 1-Decene
Formula: $C_{10}H_{20}$

CAS-RN: 872-05-9
Group No.: 13-035
Molar Mass: 140.27

Table 13.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
57MCC/FIN1	211.4–355.8	19	0.10	99.9	melpt	sat	BSAO	47HUF
88GUS/MIR1	303.1–423.1	7	nosp	not specified		*p*	BDHT	84GUS/MIR1

Name: Ethyne
Formula: C_2H_2

CAS-RN: 74-86-2
Group No.: 13-039
Molar Mass: 26.04

Table 13.39.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
07MCI	N	200.90	4.400	nosp	not specified		*p*	BSIO	07MCI

07MCI pressure of liquid Ethyne corresponded to this temperature is about 160 kPa

Name: 4-Methyl-1-pentene
Formula: C_6H_{12}

CAS-RN: 691-37-2
Group No.: 13-040
Molar Mass: 84.16

Table 13.40.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94LEB/SMI2	N	118.9–327.0	45 S	0.20	96.02	melpt	*p*	BSAO	76LEB/LIT
97STE/CHI1		290.0–460.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

94LEB/SMI2 only a graph given in the paper; smoothed values provided by the author

Table 13.40.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94LEB/SMI2	118.9–300.0	39	0.60 #	0.896	1.16–1	0.54	−3.76–2	−3
97STE/CHI1	290.0–460.0	35	1.00	1.227	3.03–1	1.23	1.27–1	5

Table 13.40.3. Parameters of cubic spline polynomials

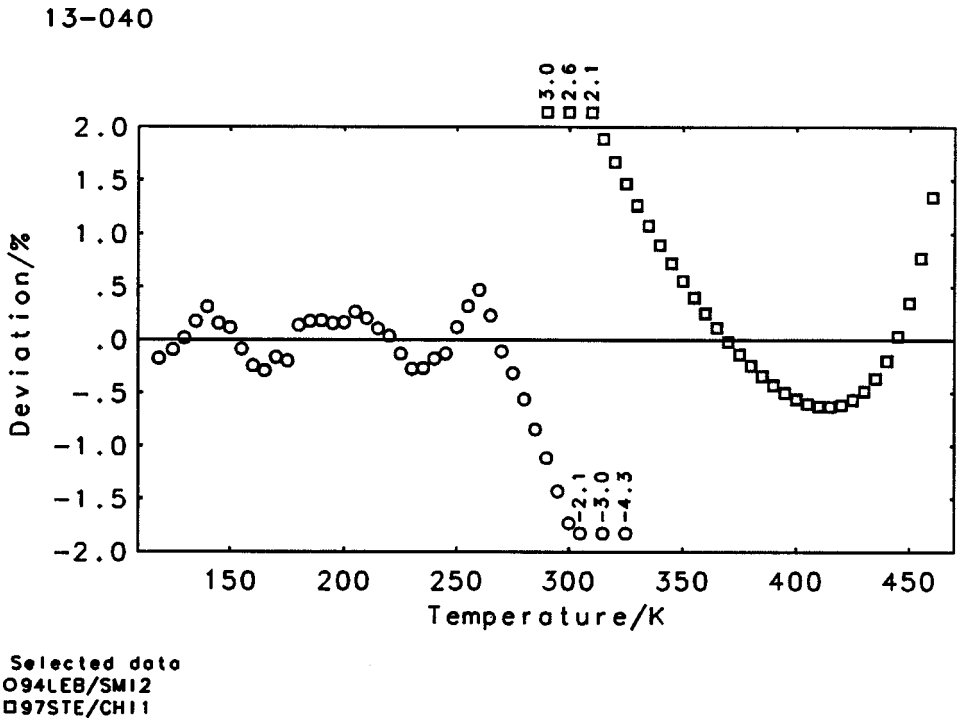
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	80	74	1.103	2.32–1	0.96	4.05–2	2
sat	80	74	1.062	2.13–1	0.92	3.84–2	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
118.9–300.0	1.69996+1	5.58370−1	−4.39679−1	2.83278−1	IV
300.0–460.0	2.24431+1	−4.88515	1.37483	8.16664−2	IV
118.9–300.0	1.67502+1	9.43967−1	−6.26921−1	3.11907−1	IV
300.0–460.0	3.32602+1	−1.55660+1	4.87640	−2.99573−1	IV

Table 13.40.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	80	74	1.136	2.21–1	0.92	1.18–2	−3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
118.9–460.0	495.00	4.71336−1	6.87283−4	1.72768+1	6.34515−1	−3.54662	2.92533+1	IV



Name: Benzene
Formula: C_6H_6

CAS-RN: 71-43-2
Group No: 14-003
Molar Mass: 78.11

Table 14.3.1 Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
19DEJ		297.6–323.1	16	nosp	not specified		*p*	BSIO	19DEJ
21TRE		289.4–331.3	12	nosp	not specified		*p*	BSIO	49WEI
24WIL/DAN		305.0–335.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
25WIL/DAN		293.1–333.1	5 S	nosp	not specified		*p*	BSAO	24WIL/DAN
26AND/LYN		293.0–383.0	eqn	nosp	not specified		*p*	DSIO	26AND/LYN
30HUF/PAR1		281.1–300.0	6	1.00	not specified		*p*	BSIO	25PAR
31FIO/GIN	N	328.1–378.1	6 S	0.10	not specified		sat	BSIO	31FIO/GIN
33KOL/UDO	N	287.9	1	nosp	not specified		*p*	BSIT	34KOL/UDO
37COH/BUI		283.1–295.1	7	nosp	not specified		*p*	BSAO	20COH/MOE
39PHI		301.4	1	nosp	not specified		*p*	BSIO	49WEI
41ZHD		281.4–318.8	3	nosp	not specified		*p*	BSIT	34KOL/UDO
42ZIE/AND		283.5–322.6	9	2.00	99.99	melpt	*p*	BDHO	37STU
47KUR		290.0–321.8	5	nosp	not specified		avg	DSIO	47KUR
48OLI/EAT		286.9–336.9	9	0.20	99.967	melpt	sat	BSAO	43RUE/HUF
48TSC1		295.1	1	nosp	not specified		*p*	BSIO	48TSC1
48TSC5		295.1	1	nosp	not specified		*p*	BSIO	48TSC1
51SIE/CRU	N	293.1	1	nosp	not specified		*p*	not specified	
55STA/TUP		288.4–346.9	13	0.20	not specified		*p*	BSAO	55STA/TUP
56DUF/EVE	N	303.1–353.1	6 S	0.50	not specified		*p*	not specified	
60SWI/ZIE	N	316.3–322.1	2	nosp	not specified		avg	DSIO	58SWI/ZIE1
62RAB/NIK		283.1–303.1	5 S	0.30	not specified		*p*	BSAO	47SKU
65FIN/GRU		300.0	1	0.40	not specified		*p*	BDAO	65FIN/GRU
65KAU/BIT		293.1–349.1	8	1.00	not specified		*p*	FSIO	65KAU/BIT
67PAC		298.1	1	nosp	not specified		*p*	BDHT	79DU/COM
67RAS/GAN		293.1–353.1	4 S	0.50	not specified		*p*	BSAO	67RAS/GAN
68REC1	N	298.0–313.0	eqn	nosp	not specified		*p*	BSAO	68REC1
71DES/BHA		298.1–318.1	3 S	1.00	not specified		*p*	BSIO	58MUR/VAN
71KHA/SUB	N	298.1–313.1	2	nosp	not specified		*p*	BSIO	64MOE/THO
74RAJ/SUB		298.1–323.1	3	0.30	not specified		*p*	BSIO	64MOE/THO
75RAS/GRI	N	305.1–463.1	9	nosp	not specified		*p*	BDAO	75RAS/GRI
75SAN	N	433.1–493.1	6 S	1.00	not specified		*p*	FSIO	75SAN

Table 14.3.1 Experimental heat capacities—Continued

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
76FOR/BEN2		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
77BEL/BUB		298.1	1	nosp	not specified		*p*	BDCT	68WAD
77WIL/GRO		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
78GRO/WIL		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
81ATA/ELS		293.1	1	2.50	not specified		*p*	BDHO	81ATA/ELS
82GOR/SIM2		279.0–353.0	eqn	nosp	99.9	anal	*p*	FSIO	83GOR/SIM
82GRO/ING		298.1	1	nosp	98.5	melpt	*p*	FSIT	71PIC/LED
82TAN		293.1–303.1	3 S	0.30	99.99	melpt	*p*	FSIT	71PIC/LED
82WIL/FAR		298.1	1	nosp	98.5	melpt	*p*	FSIT	71PIC/LED
83GOR/SIM	N	283.8–348.5	12	0.25	99.9	anal	*p*	FSIO	83GOR/SIM
85OGA/MUR		298.1	1	0.10	not specified		*p*	FSIO	85OGA/MUR
85TAN		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
86NAZ/BAS1		322.0–351.1	2	2.00	not specified		*p*	BDHO	86NAZ/BAS1
87GRO/ROU		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
87KAL/KOH		293.1–313.1	2	nosp	not specified		*p*	FSIT	71PIC/LED
87TAN		293.1–303.1	3	nosp	not specified		*p*	FSIT	71PIC/LED
88SHI/OGA1		298.1	1	nosp	99.9	chrom	*p*	FSIO	85OGA/MUR
89LAI/ROD		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
89PFE/SCH		313.1	1	nosp	not specified		*p*	BDCT	68WAD
89PRA/RAJ		318.1–333.1	4	3.00	not specified		*p*	BDHT	89PRA/RAJ
90YAM/OGA		298.1	1	nosp	99.97	chrom	*p*	FSIO	85OGA/MUR
91CZA		298.5	1	2.00	not specified		*p*	BSIO	79CZA
91GRO/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
91TAN/ADA		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91WIL/JIM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
92MIY/TAM1		298.1	1	nosp	99.99	chrom	*p*	FSIO	85OGA/MUR
92MIY/TAM2		298.1	1	nosp	99.9	chrom	*p*	FSIO	85OGA/MUR
93DUR/AOU		303.0–347.0	23	nosp	not specified		*p*	BDCT	86MER/BEN
93GRO/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
94CHI/STE		300.0–540.0	13 S	1.00	99.9	chrom	sat	BDHT	89KNI/ARC
95DUR/AOU		303.0–347.0	eqn	2.00	99.99	anal	*p*	BDCT	86MER/BEN
95FUJ/TAM2		298.1	1	nosp	99.95	chrom	*p*	FSIO	85OGA/MUR
97HU/TAM1		298.1	1	nosp	99.96	chrom	*p*	FSIO	85OGA/MUR
97TAN/NAK		298.1–303.1	2	nosp	100.0	chrom	*p*	FSIT	71PIC/LED
97TAN/TOY		298.1	1	0.15	99.95	chrom	*p*	FSIT	71PIC/LED

31FIO/GIN	water content below 0.01%; data calculated using procedure by 85WIL/CHA
33KOL/UDO	same datum in 34KOL/UDO
51SIE/CRU	heat of mixing calorimeter used
56DUF/EVE	measured by a non-calorimetric method (piezo-thermometric)
60SWI/ZIE	average values in temperature ranges 294–339 K and 294–350 K
68REC1	same data in 68REC2
71KHA/SUB	reproducibility given as 0.3%
75RAS/GRI	data above 343 K measured at superambient pressures up to 1.33 MPa
75SAN	same data in 76SAN/MEL; C_p at saturation curve extrapolated from high pressure measurements
83GOR/SIM	same data in 82GOR/GRI

Table 14.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
48OLI/EAT	286.9–336.9	9	0.20	0.366	1.20–2	0.07	1.03–2	8
56DUF/EVE	303.1–353.1	6	0.50	0.593	5.03–2	0.30	1.36–2	2
65FIN/GRU	300.0	1	0.40	0.191	1.25–2	0.08	1.25–2	1
71KHA/SUB	298.1–313.1	2	0.50 #	0.387	3.23–2	0.19	−2.24–2	−1
75RAS/GRI	305.1–463.1	9	0.80 #	0.876	1.42–1	0.70	−6.45–2	−3
75SAN	433.1–493.1	6	1.00	1.828	4.42–1	1.83	3.26–1	4
76FOR/BEN2	298.1	1	0.30	0.326	1.60–2	0.10	−1.60–2	−1
77WIL/GRO	298.1	1	0.30	0.720	3.52–2	0.22	−3.52–2	−1
78GRO/WIL	298.1	1	0.30	0.696	3.40–2	0.21	−3.40–2	−1
82GOR/SIM2	279.0–353.1	4	1.00 #	0.464	7.94–2	0.46	7.86–2	4
82GRO/ING	298.1	1	0.50 #	0.255	2.08–2	0.13	−2.08–2	−1
82TAN	293.1–303.1	3	0.30	0.424	2.08–2	0.13	−2.05–2	−3
85OGA/MUR	298.1	1	0.10	1.228	2.01–2	0.12	2.01–2	1
85TAN	298.1	1	0.30	0.425	2.08–2	0.13	−2.08–2	−1
87GRO/ROU	298.1	1	0.50 #	0.211	1.72–2	0.11	−1.72–2	−1
87TAN	293.1–303.1	3	0.50 #	0.315	2.58–2	0.16	−2.55–2	−3
89LAI/ROD	298.1	1	0.50 #	0.403	3.28–2	0.20	−3.28–2	−1
91CZA	298.5	1	2.00	0.019	6.14–3	0.04	−6.14–3	−1
91GRO/ROU	298.1	1	0.50 #	0.373	3.04–2	0.19	−3.04–2	−1
91TAN/ADA	298.1	1	0.50 #	0.314	2.56–2	0.16	−2.56–2	−1
92MIY/TAM1	298.1	1	0.50 #	0.069	5.66–3	0.03	5.66–3	1
92MIY/TAM2	298.1	1	0.50 #	0.025	2.05–3	0.01	2.05–3	1
93GRO/ROU	298.1	1	0.50 #	0.299	2.44–2	0.15	−2.44–2	−1
94CHI/STE	300.0–540.0	13	1.00	0.842	2.05–1	0.84	−1.25–1	−7
95FUJ/TAM2	298.1	1	0.50 #	0.196	1.60–2	0.10	−1.60–2	−1
97HU/TAM1	298.1	1	0.50 #	0.069	5.66–3	0.03	5.66–3	1
97TAN/NAK	298.1–303.1	2	0.50 #	0.313	2.57–2	0.16	−2.56–2	−2
97TAN/TOY	298.1	1	0.15	0.997	2.44–2	0.15	−2.44–2	−1

Rejected data

19DEJ	(2.75–1,1.61,2.49–1,16)	21TRE	(1.64–1,0.97,4.66–2,4)
24WIL/DAN	(3.10–1,1.80,4.42–2,0)	25WIL/DAN	(3.44–1,1.97,6.48–3,−1)
26AND/LYN	(3.46–1,2.08,−4.66–2,1)	30HUF/PAR1	(1.02–1,0.64,−9.93–2,−6)
31FIO/GIN	(1.30–1,0.73,1.22–1,6)	33KOL/UDO	(2.90–1,1.83,−2.90–1,−1)
37COH/BUI	(2.23–1,1.40,−2.22–1,−7)	39PHI	(7.61–2,0.47,−7.61–2,−1)
41ZHD	(3.64–2,0.22,6.96–3,0)	42ZIE/AND	(1.57–1,0.94,−7.00–2,−7)
47KUR	(2.67–1,1.68,−1.76–1,−3)	48TSC1	(2.29–1,1.43,−2.29–1,−1)
48TSC5	(1.50–1,0.93,−1.50–1,−1)	51SIE/CRU	(2.03–1,1.27,−2.03–1,−1)
55STA/TUP	(1.23–1,0.73,−1.11–1,−13)	60SWI/ZIE	(5.22–1,3.20,−3.15–1,0)
62RAB/NIK	(1.04–1,0.64,−1.03–1,−5)	65KAU/BIT	(3.62–1,2.04,1.14–1,0)
67PAC	(6.21–1,3.95,−6.21–1,−1)	67RAS/GAN	(8.31–2,0.47,6.21–2,2)
68REC1	(6.13–2,0.37,−6.11–2,−3)	71DES/BHA	(1.95–1,1.19,−1.95–1,−3)
74RAJ/SUB	(6.49–2,0.39,−5.82–2,−3)	77BEL/BUB	(7.22–2,0.44,−7.22–2,−1)
81ATA/ELS	(1.51–1,0.94,−1.51–1,−1)	82WIL/FAR	(3.52–2,0.22,−3.52–2,−1)
83GOR/SIM	(9.01–2,0.53,7.97–2,12)	86NAZ/BAS1	(1.78–1,1.02,1.26–3,0)
87KAL/KOH	(5.34–2,0.32,−4.85–2,−2)	88SHI/OGA1	(1.52–1,0.94,−1.52–1,−1)
89PFE/SCH	(2.81–1,1.65,2.81–1,1)	89PRA/RAJ	(4.47–1,2.67,−4.29–1,−4)
90YAM/OGA	(8.21–2,0.51,−8.21–2,−1)	91WIL/JIM	(3.52–2,0.22,−3.52–2,−1)
93DUR/AOU	(2.85–1,1.65,2.84–1,23)	95DUR/AOU	(2.75–1,1.60,2.72–1,4)

Table 14.3.3. Parameters of cubic spline polynomials

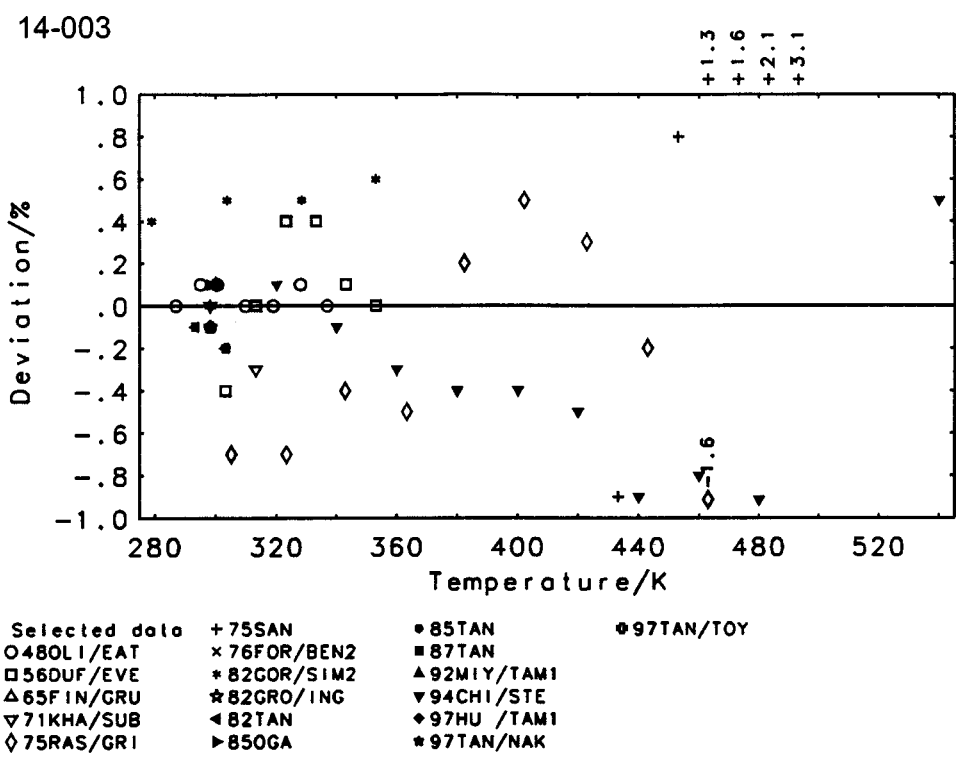
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	252	75	0.818	1.68−1	0.72	−3.46−3	−9
sat	252	75	0.833	1.68−1	0.74	−3.11−3	−8

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
279.0–380.0	2.18305+1	−8.42889	2.92873	−2.41104−1	II
380.0–490.0	−4.33672+1	4.30429+1	−1.06165+1	9.47073−1	IV
490.0–540.0	−2.78251+3	1.72007+3	−3.52866+2	2.42294+1	IV
279.0–380.0	2.05209+1	−7.34142	2.64185	−2.17800−1	II
380.0–490.0	−2.50391+1	2.86271+1	−6.82355	6.12497−1	IV
490.0–540.0	−1.30420+3	8.11788+2	−1.66652+2	1.14852+1	IV

Table 14.3.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	252	75	0.843	1.66−1	0.72	−1.94−2	−24

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
279.0–540.0	562.16	−2.70938	2.02562−1	9.06286	9.05991	IV



Name: Cyclohexene
Formula: C_6H_{10}

CAS-RN: 110-83-8
Group No.: 14-006
Molar Mass: 82.15

Table 14.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
30PAR/HUF1		175.2–293.2	12	1.00	not specified		*p*	BSIO	25PAR
48HUF/EAT		178.8–300.6	19	0.10	99.997	melpt	sat	BSAO	43RUE/HUF
77HAI/SUG1		171.2–293.4	42	nosp	99.96	melpt	sat	BSAO	65SUG/SEK
88KAL/WOY		183.0–298.1	26	nosp	not specified		*p*	BSAO	80KAL/JED
93STE/CHI2	N	298.1	1	1.00	99.95	chrom	*p*	BDHT	89KNI/ARC

93STE/CHI2 same datum in 96STE/CHI2

Name: Bicyclo[2.2.1]hepta-2,5-diene
Formula: C_7H_8

CAS-RN: 121-46-0
Group No.: 14-009
Molar Mass: 92.14

Table 14.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
73HAL/SMI		297.1	1	nosp	99.9	chrom	*p*	BDHT	71DU/COM
78STE	N	298.1	1	nosp	not specified		*p*	not specified	

78STE unspecified DSC instrument used for measurement

Table 14.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
78STE	298.1	1	1.00 #	0.000	0.00	0.00	0.00	0

Table 14.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	2	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	1.93878+1	IV

Name: Methylbenzene
Formula: C_7H_8

CAS-RN: 108-88-3
Group No.: 14-011
Molar Mass: 92.14

Table 14.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		304.8–341.3	7 S	nosp	not specified		avg	DSIO	*81VON
*86SCH		309.3–329.0	11 S	nosp	not specified		avg	DSIO	*86SCH
07BAT	N	181.1–248.1	6	nosp	not specified		*p*	BSIO	07BAT
24WIL/DAN		305.0–348.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
25WIL/DAN		293.1–333.1	5 S	nosp	not specified		*p*	BSAO	24WIL/DAN
29KEL5	N	183.8–284.4	11	nosp	not specified		*p*	BSIO	29KEL1
30SOU/AND	N	183.8–244.8	7	0.50	not specified		*p*	BSAO	30SOU/AND
31SMI/AND1		184.4–298.5	9	nosp	not specified		*p*	DSIO	26AND/LYN
35AOY/KAN		195.2–227.8	2	nosp	not specified		*p*	BSAO	35AOY/KAN
37VOL		298.1	1	nosp	not specified		*p*	BSIO	37VOL
41ZHD		278.5–320.4	3	nosp	not specified		*p*	BSIT	34KOL/UDO
47KUR		241.9–310.5	4	nosp	not specified		avg	DSIO	47KUR
48TSC1		295.1	1	nosp	not specified		*p*	BSIO	48TSC1
48TSC5		295.1	1	nosp	not specified		*p*	BSIO	48TSC1
56SCH/GOT		270.0–292.5	10	2.00	not specified		*p*	BSAO	33SOU/BRI
58SWI/ZIE2	N	323.9–333.2	2	nosp	not specified		avg	DSIO	58SWI/ZIE1
62SCO/GUT		183.2–371.0	23	0.20	99.999	melpt	sat	BSAO	47HUF
66HWA/ZIE		180.9–304.4	34	nosp	99.99	melpt	*p*	BSAO	45SCO/MEY
67RAS/GAN		293.1–373.1	5 S	0.50	not specified		*p*	BSAO	67RAS/GAN
71DES/BHA		298.1–318.1	3 S	1.00	not specified		*p*	BSIO	58MUR/VAN
73AKH/EKS		298.1	1	0.20	not specified		*p*	FSIO	59RIB/EGO
74RAJ/SUB		298.1–323.1	3	0.30	not specified		*p*	BSIO	64MOE/THO
75HOL/ZIE		162.0–312.0	eqn	0.20	not specified		*p*	BSAO	45SCO/MEY
75PED/KAY		300.6–347.3	19	nosp	not specified		*p*	BSIO	75PED/KAY
75RAS/GRI	N	303.0–462.7	9	1.00	not specified		*p*	BDAO	75RAS/GRI
76FOR/BEN1		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
76SAN/MEL	N	393.1–503.1	8 S	1.00	not specified		*p*	FSIO	75SAN
77BEL/BUB		298.1	1	nosp	not specified		*p*	BDCT	68WAD
77FOR/BEN		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
77WIL/GRO		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
79AND/GRI	N	293.1–373.3	9	0.50	not specified		*p*	BSAO	67RAS/GAN
80NEF/FIL		300.0–520.0	12 S	nosp	not specified		sat	BDHO	84FIL/LAU
81ATA/ELS		293.1	1	2.50	not specified		*p*	BDHO	81ATA/ELS
82GRO/ING		298.1	1	0.30	99.5	estim	*p*	FSIT	71PIC/LED
82WIL/FAR		298.1	1	0.30	99.5	estim	*p*	FSIT	71PIC/LED
84STE/OLS		266.1–318.1	11 S	nosp	99.5	melpt	*p*	BDHT	69PER/COM
85COS/PAT6		298.2	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
86ROU/GRO		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
87OKH/RAZ		181.4–380.4	15	0.30	not specified		sat	BDAO	87OKH/RAZ
88SHI/OGA1		298.1	1	nosp	99.9	chrom	*p*	FSIO	85OGA/MUR
88STE/CHI		300.0–580.0	29 S	nosp	not specified		sat	BDHT	89KNI/ARC
89PRA/RAJ		318.1–333.1	4	3.00	not specified		*p*	BDHT	89PRA/RAJ
90RAO/RAJ		318.1–333.1	4	4.00	not specified		*p*	BDHT	89PRA/RAJ
91COB/GAR		298.1–368.1	4	nosp	not specified		*p*	BDCT	83ROU/ROU
91TAN/ADA		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91WIL/JIM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
93CON/GIR1		298.0–359.0	eqn	5.00	not specified		sat	BDHT	93CON/GIR1
93GRO/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
94CHI/STE		300.0–570.0	15 S	1.00	99.9	chrom	sat	BDHT	89KNI/ARC
94GRO/ROU		298.1	1	nosp	99.0	chrom	*p*	FSIT	71PIC/LED
94JIM/ROM		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
94PRA/RAJ		293.1–323.1	4	nosp	not specified		*p*	BDHT	89PRA/RAJ
95FUJ/TAM2		298.1	1	nosp	99.95	chrom	*p*	FSIO	85OGA/MUR
97TAN/NAK		298.1–303.1	2	nosp	100.0	chrom	*p*	FSIT	71PIC/LED
97TAN/TOY		298.1	1	0.15	99.95	chrom	*p*	FSIT	71PIC/LED
99BRO/CAL		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
#00BEC/AUF	N	302.0–337.0	8	0.30	99.95	chrom	sat	BDCT	#00BEC/AUF
#00BEC/AUF	N	288.1–353.2	14	0.20	99.95	chrom	sat	BDCT	#00BEC/AUF

Table 14.11.1. Experimental heat capacities—Continued

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
07BAT	same data in 08BAT							
29KEL5	high sample purity							
30SOU/AND	high sample purity							
58SWI/ZIE2	average values in temperature ranges 294–354 K and 294–372 K							
75RAS/GRI	data above 364 K measured at superambient pressures up to 0.72 MPa							
76SAN/MEL	C_p at saturation curve extrapolated from high pressure measurements							
79AND/GRI	grade: pure							
#00BEC/AUF	"step by step" method was used							
#00BEC/AUF	"three-step" method was used							

Table 14.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
			Selected data					
62SCO/GUT	183.2–371.0	23	0.20	0.483	1.98–2	0.10	−4.97–3	−1
66HWA/ZIE	180.9–304.5	34	0.20 #	0.451	1.59–2	0.09	1.15–3	−6
75HOL/ZIE	162.0–312.0	31	0.20	0.383	1.44–2	0.08	−8.09–3	−16
76FOR/BEN1	298.1	1	0.30	0.361	2.04–2	0.11	−2.04–2	−1
77FOR/BEN	298.1	1	0.50 #	0.146	1.38–2	0.07	−1.38–2	−1
77WIL/GRO	298.1	1	0.30	0.544	3.08–2	0.16	−3.08–2	−1
79AND/GRI	293.1–373.3	9	0.50	0.663	6.51–2	0.33	5.68–2	9
82GRO/ING	298.1	1	0.30	0.395	2.24–2	0.12	−2.24–2	−1
82WIL/FAR	298.1	1	0.30	0.097	5.52–3	0.03	−5.52–3	−1
86ROU/GRO	298.1	1	0.50 #	0.148	1.39–2	0.07	−1.39–2	−1
91COB/GAR	298.1–368.1	4	0.50 #	0.367	3.63–2	0.18	−3.40–2	−4
91TAN/ADA	298.1	1	0.50 #	0.262	2.48–2	0.13	−2.48–2	−1
91WIL/JIM	298.1	1	0.50 #	0.199	1.88–2	0.10	−1.88–2	−1
94CHI/STE	300.0–570.0	15	1.00	0.514	1.72–1	0.51	2.90–2	6
94GRO/ROU	298.1	1	0.50 #	0.081	7.71–3	0.04	7.71–3	1
94JIM/ROM	298.1	1	0.50 #	0.335	3.18–2	0.17	3.18–2	1
95FUJ/TAM2	298.1	1	0.30 #	0.199	1.13–2	0.06	1.13–2	1
97TAN/NAK	298.1–303.1	2	0.50 #	0.381	3.62–2	0.19	−3.55–2	−2
97TAN/TOY	298.1	1	0.15	0.955	2.70–2	0.14	−2.70–2	−1
99BRO/CAL	298.1	1	0.50 #	0.084	7.93–3	0.04	−7.93–3	−1
#00BEC/AUF	302.0–337.0	8	0.30	0.663	3.88–2	0.20	−1.65–2	−4
#00BEC/AUF	288.1–353.2	14	0.20	0.868	3.43–2	0.17	2.93–2	13
			Rejected data					
35AOY/KAN	(1.55–1,0.91,1.28–1,2)		75PED/KAY	(9.90–2,0.50,3.55–2,1)				
75RAS/GRI	(9.39–2,0.44,2.58–2,3)		76SAN/MEL	(7.80–1,2.73,6.07–1,8)				
77BEL/BUB	(6.70–2,0.36,−6.70–2,−1)		84STE/OLS	(1.58–1,0.82,1.48–1,11)				
87OKH/RAZ	(1.41–1,0.71,9.30–2,10)		88SHI/OGA1	(1.49–1,0.79,−1.49–1,−1)				
88STE/CHI	(5.22–1,1.86,4.62–1,26)		94PRA/RAJ	(3.65–1,1.88,3.29–1,4)				

Table 14.11.3. Parameters of cubic spline polynomials

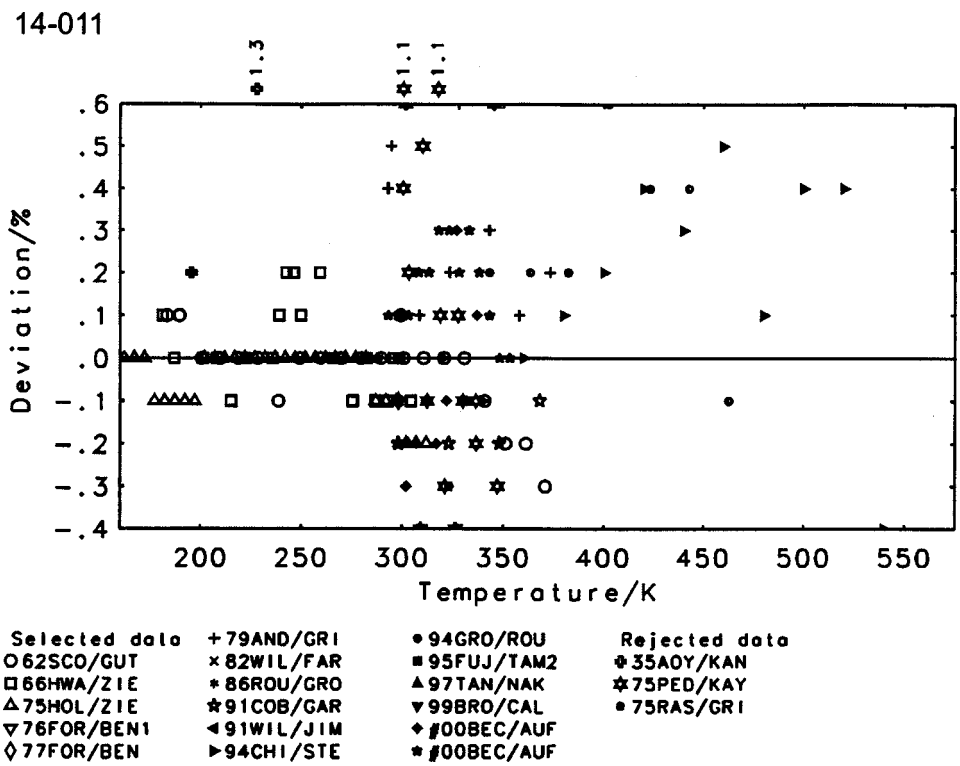
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	252	153	0.531	6.12−2	0.21	3.63−3	−12
sat	252	153	0.530	4.78−2	0.19	3.59−3	−15

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
162.0–350.0	2.16638+1	−7.51813	2.97181	−2.55049−1	II
350.0–500.0	2.78361	8.66490	−1.65192	1.85306−1	III
500.0–570.0	−1.69932+3	1.02992+3	−2.05904+2	1.38021+1	IV
162.0–350.0	2.17474+1	−7.62609	3.01725	−2.61290−1	II
350.0–500.0	6.44050	5.49414	−7.31388−1	9.57235−2	III
500.0–570.0	−8.78996+2	5.36756+2	−1.06984+2	7.17922	IV

Table 14.11.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	252	153	3.102	1.64−1	0.77	2.81−2	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
162.0–570.0	591.79	−3.12743	8.57315−2	1.37282+1	1.28971	6.42297	4.10989	V



Name: 1,2-Dimethylbenzene
Formula: C_8H_{10}

CAS-RN: 95-47-6
Group No.: 14-018
Molar Mass: 106.17

Table 14.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
24WIL/DAN		303.0–348.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
30HUF/PAR1		253.3–295.1	8	1.00	not specified		*p*	BSIO	25PAR
43PIT/SCO		251.6–301.9	9	0.20	99.88	melpt	*p*	BSIO	28LAT/GRE
47KUR		308.8–346.6	3	nosp	not specified		avg	DSIO	47KUR
48TSC3		293.1	1	nosp	not specified		*p*	BSIO	48TSC1
48TSC6		294.1	1	nosp	not specified		*p*	BSIO	48TSC1
58SWI/ZIE2	N	347.3	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
75RAS/GRI	N	303.2–463.1	10	1.00	not specified		*p*	BDAO	75RAS/GRI
77FOR/BEN		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
79FOR/BEN		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
91TAN/ADA		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
92JAI/CHA		303.6–321.6	7	nosp	98.	anal	*p*	BDCT	91BAN/GAR
93GAR/BAN		318.1–373.1	12	nosp	99.6	chrom	*p*	BDCT	91BAN/GAR
97CHI/KNI1		252.0–413.2	17	0.10	99.93	melpt	sat	BSAO	88STE/ARC
97CHI/KNI1		420.0–550.0	8 S	1.00	99.93	melpt	sat	BDHT	89KNI/ARC
97TAN/TOY		298.1	1	0.15	99.95	chrom	*p*	FSIT	71PIC/LED

58SWI/ZIE2 average value in temperature range 333–373 K
75RAS/GRI data above 348 K measured at superambient pressures up to 0.51 MPa

Table 14.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
43PIT/SCO	251.6–301.9	9	0.20	1.157	5.16–2	0.23	2.27–2	4
75RAS/GRI	303.2–463.1	10	1.00	0.826	2.04–1	0.83	−1.05–1	−6
77FOR/BEN	298.1	1	0.50 #	0.211	2.38–2	0.11	−2.38–2	−1
79FOR/BEN	298.1	1	0.30	0.230	1.55–2	0.07	−1.55–2	−1
91TAN/ADA	298.1	1	0.50 #	0.226	2.55–2	0.11	−2.55–2	−1
92JAI/CHA	303.6–321.6	7	0.30 #	0.357	2.49–2	0.11	−2.06–2	−6
97CHI/KNI1	252.0–413.2	17	0.10	0.187	4.69–3	0.02	−4.45–4	−1
97CHI/KNI1	420.0–550.0	8	1.00	0.166	5.60–2	0.17	−1.33–2	−4
97TAN/TOY	298.1	1	0.15	0.740	2.50–2	0.11	−2.50–2	−1
Rejected data								
24WIL/DAN	(8.21–1,3.60,−8.21–1,−5)			30HUF/PAR1	(2.30–1,1.06,−2.20–1,−8)			
47KUR	(2.86–1,1.24,−2.68–1,−3)			48TSC3	(4.91–1,2.24,−4.91–1,−1)			
48TSC6	(5.28–1,2.41,−5.28–1,−1)			58SWI/ZIE2	(2.53–1,1.02,2.53–1,1)			
93GAR/BAN	(1.94–1,0.80,−1.93–1,−12)							

Table 14.18.3. Parameters of cubic spline polynomials

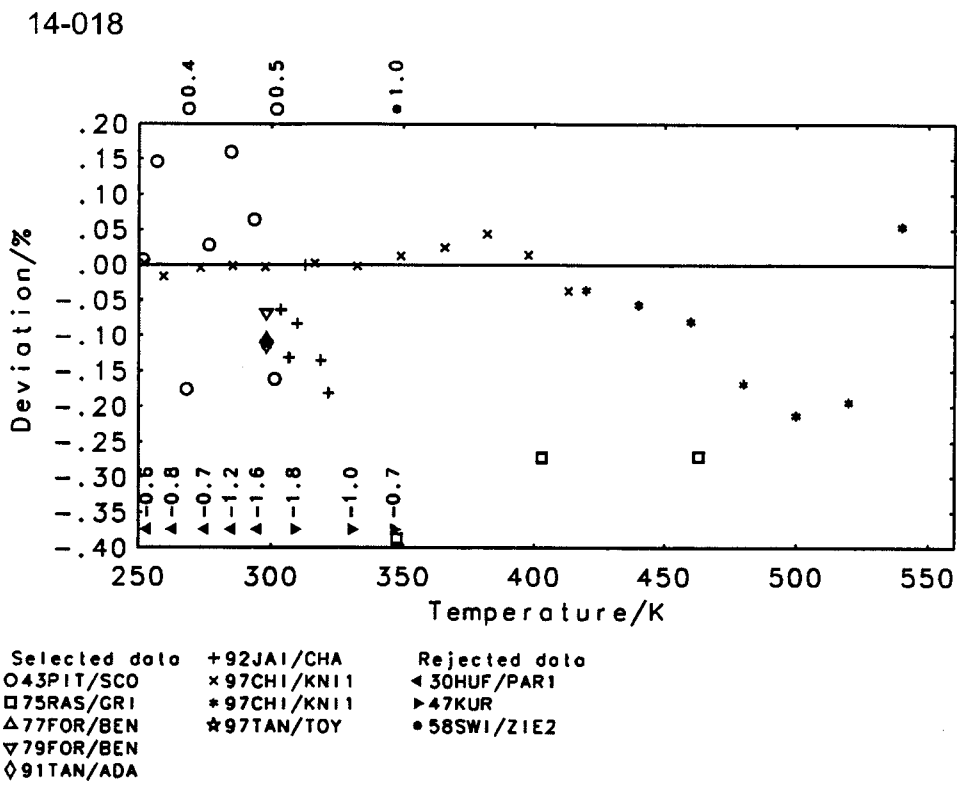
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	86	55	0.652	9.71–2	0.39	−2.18–2	−17
sat	86	55	0.649	9.51–2	0.39	−1.97–2	−17

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
251.6–350.0	2.27698+1	−5.97535	2.66140	−2.27424−1	II
350.0–550.0	7.49507	7.11732	−1.07936	1.28839−1	IV
251.6–350.0	2.27487+1	−5.96269	2.66041	−2.27713−1	II
350.0–550.0	1.01285+1	4.85463	−4.30255−1	6.66358−2	IV

Table 14.18.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	86	55	1.653	1.24−1	0.45	−1.75−2	9

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
251.6–550.0	630.30	2.75413	2.81260−2	1.65019+1	7.32563	1.36401+1	1.15983+1	IV



Name: 1,3-Dimethylbenzene
Formula: C_8H_{10}

CAS-RN: 108-38-3
Group No.: 14-019
Molar Mass: 106.17

Table 14.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH		308.9–334.8	11 S	nosp	not specified		avg	DSIO	*86SCH
24WIL/DAN		303.0–348.0	eqn	nosp	not specified		p	BSAO	24WIL/DAN
30HUF/PAR1	N	217.0–275.3	6	1.00	not specified		p	BSIO	25PAR
43PIT/SCO	N	231.4–318.2	11	0.20	97.66	melpt	p	BSIO	28LAT/GRE
47KUR		309.8–347.7	3	nosp	not specified		avg	DSIO	47KUR
48TSC3		293.1	1	nosp	not specified		p	BSIO	48TSC1
48TSC6		294.1	1	nosp	not specified		p	BSIO	48TSC1
58SWI/ZIE2	N	336.8	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
75RAS/GRI	N	302.9–462.5	9	1.00	not specified		p	BDAO	75RAS/GRI
75SAN	N	411.1–540.2	8 S	1.00	not specified		p	FSIO	75SAN
77FOR/BEN		298.1	1	nosp	not specified		p	FSIT	71PIC/LED
79FOR/BEN		298.1	1	0.30	not specified		p	FSIT	71PIC/LED
91TAN/ADA		298.1	1	nosp	not specified		p	FSIT	71PIC/LED
92JAI/CHA		303.6–321.6	7	nosp	98.	anal	p	BDCT	91BAN/GAR

Table 14.19.1. Experimental heat capacities—Continued

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93GAR/BAN	318.1–373.1	12	nosp	99.3	chrom	*p*	BDCT	91BAN/GAR
93GRO/ROU	298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED
97CHI/KNI2	232.3–423.4	17	0.10	99.9	melpt	sat	BSAO	88STE/ARC
97CHI/KNI2	440.0–550.0	7 S	1.00	99.9	melpt	sat	BDHT	89KNI/ARC

30HUF/PAR1	low sample purity
43PIT/SCO	corrected for content of 1,4-Dimethylbenzene
58SWI/ZIE2	average value in temperature range 333–373 K
75RAS/GRI	data above 384 K measured at superambient pressures up to 0.45 MPa
75SAN	same data in 76SAN/MEL; C_p at saturation line extrapolated from high pressure measurement

Table 14.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
75RAS/GRI	324.1–462.5	8	1.00	0.407	1.08–1	0.41	8.19–3	2
75SAN	411.1–523.2	7	1.00	0.658	1.92–1	0.66	1.33–1	3
77FOR/BEN	298.1	1	0.50 #	0.122	1.33–2	0.06	−1.33–2	−1
79FOR/BEN	298.1	1	0.30	0.079	5.15–3	0.02	−5.15–3	−1
92JAI/CHA	303.6–321.6	7	0.50 #	0.426	4.79–2	0.21	−4.53–2	−7
93GAR/BAN	318.1–373.1	12	0.50 #	0.874	1.05–1	0.44	−1.01–1	−12
97CHI/KNI2	232.3–423.4	17	0.10	0.345	7.76–3	0.03	3.23–3	4
97CHI/KNI2	440.0–550.0	7	1.00	0.266	8.94–2	0.27	−2.77–2	−4
Rejected data								
*86SCH	(3.97–1,1.68,3.74–1,11)		24WIL/DAN	(6.20–1,2.77,−6.20–1,−5)				
30HUF/PAR1	(1.77–1,0.84,1.74–1,2)		43PIT/SCO	(1.69–1,0.80,1.62–1,10)				
47KUR	(8.43–1,3.46,8.15–1,3)		48TSC3	(4.27–3,0.02,−4.27–3,−1)				
48TSC6	(2.77–1,1.26,2.77–1,1)		58SWI/ZIE2	(4.52–1,1.89,4.52–1,1)				
91TAN/ADA	(3.04–2,0.14,−3.04–2,−1)		93GRO/ROU	(3.65–1,1.64,3.65–1,1)				

Table 14.19.3. Parameters of cubic spline polynomials

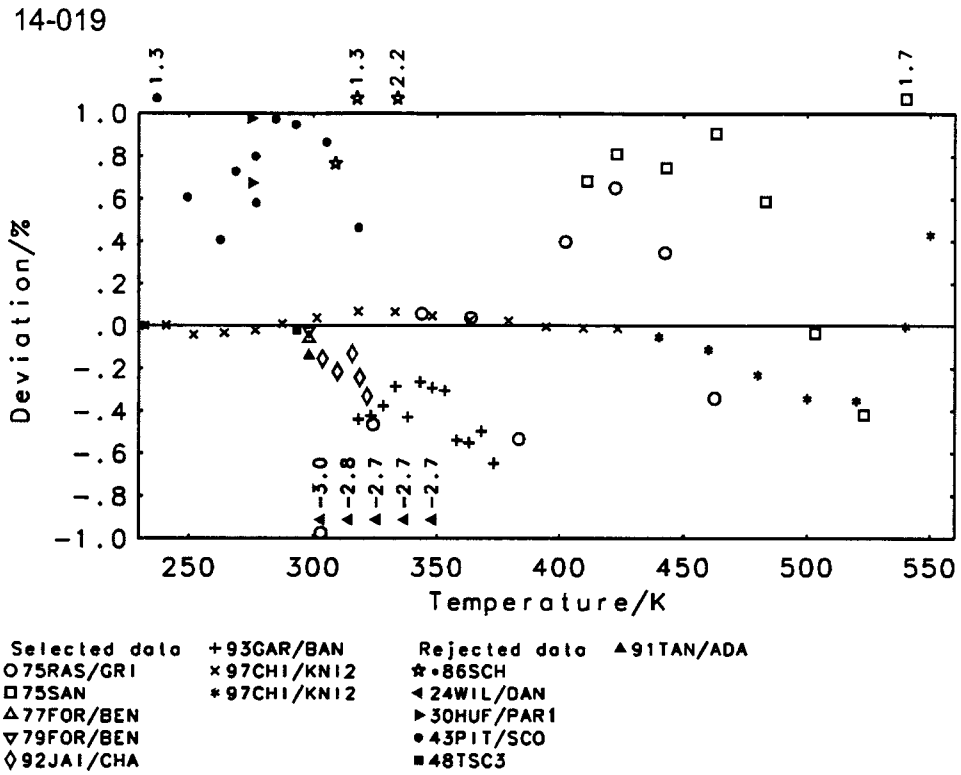
Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	103	60	0.561	1.01–1	0.37	−1.15–2	−16
sat	103	60	0.556	9.77–2	0.36	−9.15–3	−15

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
232.3–400.0	2.04036+1	−4.53989	2.18373	−1.67503−1	II
400.0–550.0	−1.93184+1	2.52516+1	−5.26415	4.53154−1	IV
232.3–400.0	2.06739+1	−4.83253	2.28833	−1.79839−1	II
400.0–550.0	−1.01961+1	1.83199+1	−3.49978	3.02503−1	IV

Table 14.19.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	103	60	10.960	2.50–1	1.18	1.10–1	26

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
232.3–550.0	617.05	−2.35405	5.81487−2	8.42181	2.38248+1	V



Name: 1,4-Dimethylbenzene
Formula: C_8H_{10}

CAS-RN: 106-42-3
Group No.: 14-020
Molar Mass: 106.17

Table 14.20.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH		312.2–335.7	6 S	nosp	not specified		avg	DSIO	*86SCH
24WIL/DAN		303.0–348.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
30HUF/PAR1		290.7–299.4	5	1.00	not specified		*p*	BSIO	25PAR
43PIT/SCO		292.0–354.6	10	0.20	99.98	melpt	*p*	BSIO	28LAT/GRE
47COR/GIN		293.1–573.2	15 S	0.20	99.9	melpt	sat	DSTO	50GIN/DOU
47KUR		309.3–349.1	3	nosp	not specified		avg	DSIO	47KUR
48TSC3		293.1	1	nosp	not specified		*p*	BSIO	48TSC1
48TSC6		294.1	1	nosp	not specified		*p*	BSIO	48TSC1
58SWI/ZIE2	N	336.6–347.0	2	nosp	not specified		avg	DSIO	58SWI/ZIE1
61ROU		298.0–315.9	20	nosp	not specified		*p*	BSAO	61ROU
71KHA/SUB	N	298.1–313.1	2	nosp	not specified		*p*	BSIO	64MOE/THO
75RAS/GRI	N	303.6–462.9	9	1.00	not specified		*p*	BDAO	75RAS/GRI
77BEL/BUB		298.1	1	nosp	not specified		*p*	BDCT	68WAD
77FOR/BEN		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
77WIL/GRO		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
79FOR/BEN		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
79OTT/GOA		288.1–328.1	9 S	0.30	99.9	melpt	*p*	FSIT	71PIC/LED
85COS/PAT7		298.2	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
88MES/FIN		295.4–373.4	11	0.10	99.996	melpt	sat	BSAO	47HUF
89PFE/SCH	N	313.1	1	nosp	not specified		*p*	BDCT	68WAD
89PRA/RAJ		318.1–333.1	4	3.00	not specified		*p*	BDHT	89PRA/RAJ
91TAN/ADA		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91WIL/JIM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
92JAI/CHA		303.6–321.6	7	nosp	98.	anal	*p*	BDCT	91BAN/GAR
93GAR/BAN		318.1–373.1	12	nosp	99.7	chrom	*p*	BDCT	91BAN/GAR

58SWI/ZIE2 average values in temperature ranges 294–379 K and 295–399 K
71KHA/SUB reproducibility given as 0.3%
75RAS/GRI data above 386 K measured at superambient pressures up to 0.49 MPa
89PFE/SCH the publish value at 298.15 K the same as 77BEL/BUB

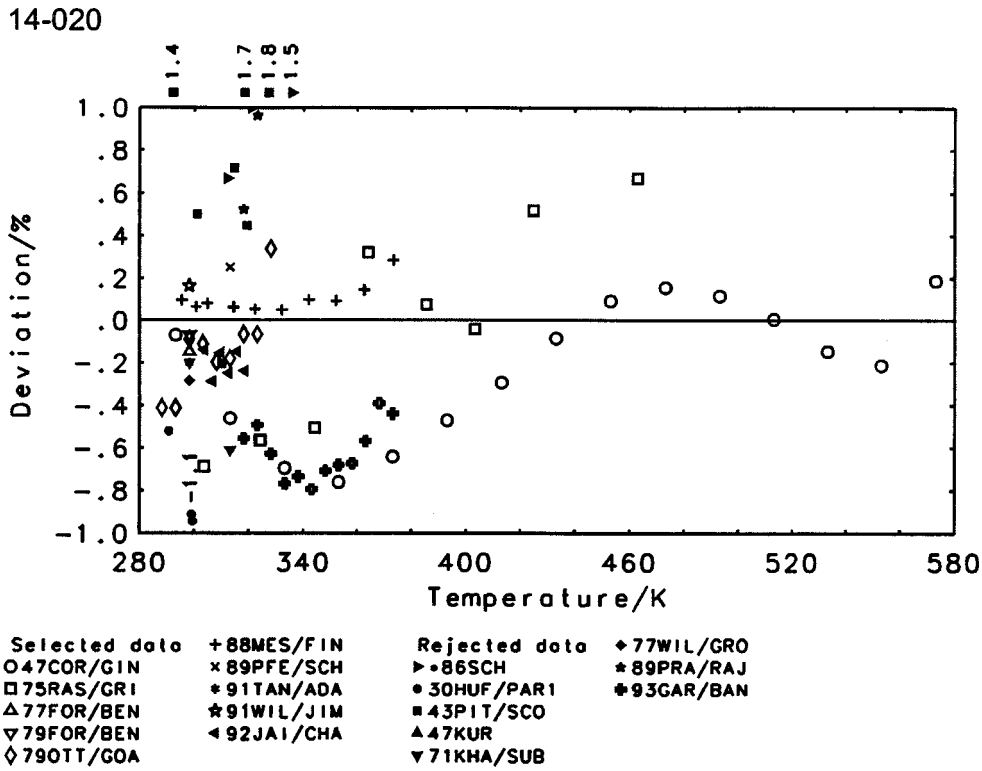
Table 14.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
					%			
			Selected data					
47COR/GIN	293.1–573.2	15	0.20	1.896	9.53–2	0.38	−5.29–2	−6
75RAS/GRI	303.6–462.9	9	1.00	0.572	1.53–1	0.57	3.63–2	1
77FOR/BEN	298.1	1	0.50 #	0.298	3.26–2	0.15	−3.26–2	−1
79FOR/BEN	298.1	1	0.30	0.234	1.54–2	0.07	−1.54–2	−1
79OTT/GOA	288.1–328.1	9	0.30	0.829	5.48–2	0.25	−2.87–2	−7
88MES/FIN	295.4–373.4	11	0.10	1.197	2.92–2	0.12	2.40–2	11
89PFE/SCH	313.1	1	0.50 #	0.503	5.68–2	0.25	5.68–2	1
91TAN/ADA	298.1	1	0.50 #	0.401	4.39–2	0.20	−4.39–2	−1
91WIL/JIM	298.1	1	0.50 #	0.324	3.55–2	0.16	3.55–2	1
92JAI/CHA	303.6–321.6	7	0.30 #	0.689	4.64–2	0.21	−4.48–2	−7
			Rejected data					
*86SCH	(2.61–1,1.11,2.47–1,6)		24WIL/DAN	(7.38–1,3.34,−7.32–1,−5)				
30HUF/PAR1	(2.16–1,1.00,−2.09–1,−5)		43PIT/SCO	(4.40–1,1.86,1.65–1,6)				
47KUR	(8.61–1,3.52,8.19–1,3)		48TSC3	(3.20–1,1.50,−3.20–1,−1)				
48TSC6	(3.08–1,1.44,−3.08–1,−1)		58SWI/ZIE2	(3.07–1,1.28,3.06–1,2)				
61ROU	(8.09–1,3.50,8.05–1,20)		71KHA/SUB	(1.02–1,0.45,−9.04–2,−2)				
77BEL/BUB	(3.31–1,1.53,−3.31–1,−1)		77WIL/GRO	(6.19–2,0.28,−6.19–2,−1)				
85COS/PAT7	(1.89–1,0.85,1.89–1,1)		89PRA/RAJ	(3.12–1,1.32,2.87–1,4)				
93GAR/BAN	(1.50–1,0.63,−1.47–1,−12)							

Table 14.20.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	130	56	1.274	8.91–2	0.35	−1.38–2	−9
sat	130	56	1.256	8.42–2	0.34	−1.53–2	−9

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
288.1–420.0	1.64349+1	−1.61036	1.52541	−1.24370−1	II
420.0–573.2	−7.50004+1	6.37006+1	−1.40248+1	1.10978	IV
288.1–420.0	1.23631+1	1.78263	5.97989−1	−4.14533–2	II
420.0–573.2	−3.77237+1	3.75589+1	−7.92017	6.34591−1	IV



Name: Ethylbenzene
Formula: C_8H_{10}

CAS-RN: 100-41-4
Group No.: 14-021
Molar Mass: 106.17

Table 14.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		304.8–362.1	8 S	nosp	not specified		avg	DSIO	*81VON
*86SCH		309.0–335.7	11 S	nosp	not specified		avg	DSIO	*86SCH
24WIL/DAN		303.0–343.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
30HUF/PAR1		185.0–304.9	16	1.00	not specified		*p*	BSIO	25PAR
31BLA/LEI		286.1–368.1	25	3.00	not specified		sat	BSIO	31BLA/LEI
31SMI/ANDI		184.4–298.5	9	nosp	99.9	estim	*p*	DSIO	26AND/LYN
34KOL/UDO	N	302.7	1	nosp	not specified		*p*	BSIT	34KOL/UDO
44GUT/SPI		181.5–305.4	16	0.10	99.93	melpt	*p*	BSAO	43RUE/HUF
45SCO/BRI		178.2–300.0	27 S	0.10	99.993	melpt	sat	BSAO	33SOU/BRI
47KUR		308.8–372.8	4	nosp	not specified		avg	DSIO	47KUR
48TSCI		295.1	1	nosp	not specified		*p*	BSIO	48TSCI
48TSC5		295.1	1	nosp	not specified		*p*	BSIO	48TSCI
76FOR/BEN2		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
77FOR/BEN		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
79AND/GRI	N	293.3–393.0	10	0.50	not specified		sat	BSAO	67RAS/GAN
79FOR/BEN		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
83GRO/FARI		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91TAN/ADA		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91WIL/JIM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
92JAI/CHA		303.6–321.6	7	nosp	98.	anal	*p*	BDCT	91BAN/GAR
93GAR/BAN		318.1–373.1	12	nosp	99.5	chrom	*p*	BDCT	91BAN/GAR
95FUJ/TAM1		298.1	1	nosp	99.95	chrom	*p*	FSIO	85OGA/MUR
97CHI/KNI3		183.4–412.4	18	0.10	99.99	melpt	sat	BSAO	88STE/ARC
97CHI/KNI3		420.0–550.0	8 S	1.00	99.99	melpt	sat	BDHT	89KNI/ARC

34KOL/UDO same datum in 34KOL/UDO1
79AND/GRI error 0.5% below 373 K and 0.8% at 433 K

Table 14.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
44GUT/SPI	181.5–305.4	16	0.20 #	0.267	1.14–2	0.05	−6.08–3	−5
45SCO/BRI	178.1–300.0	27	0.10	0.412	8.57–3	0.04	6.68–3	22
76FOR/BEN2	298.1	1	0.30	0.264	1.77–2	0.08	−1.77–2	−1
77FOR/BEN	298.1	1	0.50 #	0.397	4.43–2	0.20	−4.43–2	−1
79AND/GRI	293.3–393.0	10	0.50	1.084	1.38–1	0.54	−1.00–1	−6
79FOR/BEN	298.1	1	0.50 #	0.383	4.27–2	0.19	−4.27–2	−1
83GRO/FAR1	298.1	1	0.50 #	0.180	2.01–2	0.09	−2.01–2	−1
91TAN/ADA	298.1	1	0.50 #	0.353	3.94–2	0.18	−3.94–2	−1
91WIL/JIM	298.1	1	0.50 #	0.148	1.65–2	0.07	−1.65–2	−1
92JAI/CHA	303.6–321.6	7	1.00 #	0.214	4.95–2	0.21	4.54–2	7
97CHI/KNI3	183.4–412.4	18	0.10	0.626	1.36–2	0.06	−5.93–3	−10
97CHI/KNI3	420.0–550.0	8	1.00	0.433	1.45–1	0.43	−3.36–2	–3
			Rejected data					
*81VON	(3.42–1,1.41,−4.57–2,0)		*86SCH	(3.23–1,1.35,3.07–1,11)				
24WIL/DAN	(6.35–1,2.81,−6.31–1,−4)		30HUF/PAR1	(3.00–1,1.39,−2.55–1,−16)				
31BLA/LEI	(8.70–1,3.42,4.33–1,15)		31SMI/AND1	(4.48–1,2.33,−4.23–1,−9)				
34KOL/UDO	(1.04,4.86,−1.04,−1)		47KUR	(7.75–1,2.98,6.70–1,4)				
48TSC1	(3.74–2,0.17,3.74–2,1)		48TSC5	(1.44–1,0.64,1.44–1,1)				
93GAR/BAN	(1.57–1,0.66,−1.45–1,−12)		95FUJ/TAM1	(1.54–1,0.69,−1.54–1,−1)				

Table 14.21.3. Parameters of cubic spline polynomials

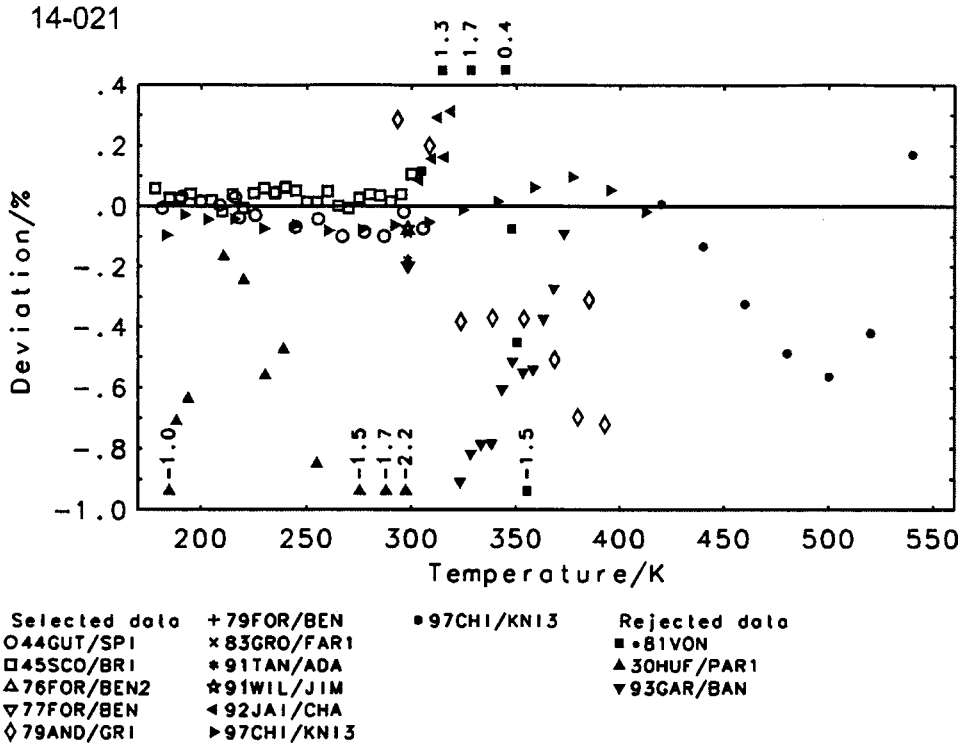
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	185	92	0.556	6.69–2	0.24	−1.26–2	−1
sat	185	92	0.546	5.75–2	0.22	−1.18–2	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
178.2–320.0	2.43915+1	−8.47695	3.64407	−3.45198−1	I
320.0–550.0	1.13184+1	3.77907	−1.85942−1	5.37611−2	IV
178.2–320.0	2.43241+1	−8.39297	3.60991	−3.40664−1	I
320.0–550.0	1.33155+1	1.92754	3.84754−1	−4.71070−3	IV

Table 14.21.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	185	92	2.908	2.79−1	0.84	6.30−2	10

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
178.1–550.0	617.24	1.28213+1	4.02331−1	1.60550+1	1.53738+1	1.82459+1	2.00389+1	V



Name: (1-Methylethenyl)benzene
Formula: C_9H_{10}

CAS-RN: 98-83-9
Group No.: 14-027
Molar Mass: 118.18

Table 14.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
67LEB/RAB1	N	250.8–300.0	6 S	0.50	99.5	melpt	p	BSAO	66NIK/LEB
97STE/CHI3		300.0–620.0	17	1.00	99.95	chrom	sat	BDHT	89KNI/ARC
99VER5		298.1	1	nosp	100.0	chrom	p	BDHT	69PER/COM

67LEB/RAB1 same data in 71LEB/RAB2

Table 14.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
67LEB/RAB1	250.8–300.0	6	0.50	0.725	8.56−2	0.36	−4.11−2	−1
97STE/CHI3	300.0–620.0	17	1.00	1.091	3.85−1	1.09	6.77−2	3
Rejected data								
99VER5	(4.69,23.89,−4.69,−1)							

Table 14.27.3. Parameters of cubic spline polynomials

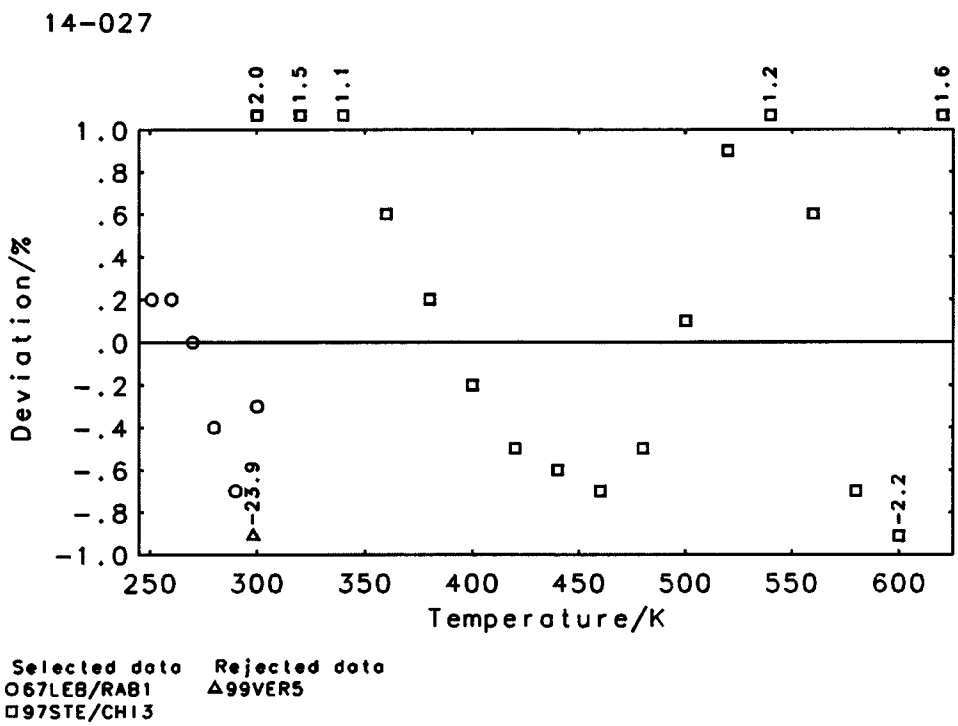
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	24	23	1.140	3.77–1	1.08	3.94–2	2
sat	24	23	0.984	2.82–1	0.90	3.79–2	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
250.8–500.0	3.12275+1	−1.36766+1	5.19242	−4.64379−1	IV
500.0–620.0	−7.76948+2	4.71229+2	−9.17886+1	6.00102	IV
250.8–500.0	3.00599+1	−1.26930+1	4.92945	−4.42476−1	IV
500.0–620.0	−5.32911+2	3.25090+2	−6.26271+1	4.06129	IV

Table 14.27.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	24	23	1.573	3.85–1	1.15	6.67–2	7

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
250.8–620.0	645.00	−2.62522	2.25884−1	4.87272	4.94109+1	−2.69630+1	5.31247	V



Name: (1-Methylethyl)benzene
Formula: C_9H_{12}

CAS-RN: 98-82-8
Group No.: 14-028
Molar Mass: 120.19

Table 14.28.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
34KOL/UDO	N	302.0	1	nosp	not specified		*p*	BSIT	34KOL/UDO
47KUR		308.8–359.6	4	nosp	not specified		avg	DSIO	47KUR
52SCH/SAG		299.8–366.5	13 S	1.00	99.8	estim	*p*	BSAO	39SAG/EVA
73KIS/SUG		179.9–313.1	45	nosp	99.93	melpt	sat	BSAO	65SUG/SEK
79AND/GRI	N	296.0–412.8	7	0.50	not specified		sat	BSAO	67RAS/GAN
95FUJ/TAM1		298.1	1	nosp	99.95	chrom	*p*	FSIO	85OGA/MUR

34KOL/UDO same datum in 34KOL/UDO
79AND/GRI error 0.5% below 373 K and 0.8% at 433 K

Name: Propylbenzene
Formula: C_9H_{12}

CAS-RN: 103-65-1
Group No.: 14-029
Molar Mass: 120.19

Table 14.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH	308.6–346.9	9 S	nosp	not specified		avg	DSIO	*86SCH
48TSC1	295.1	1	nosp	not specified		*p*	BSIO	48TSC1
48TSC5	294.1	1	nosp	not specified		*p*	BSIO	48TSC1
65MES/TOD2	180.9–370.5	23	0.10	99.97	melpt	sat	BSAO	47HUF
83GRO/FAR2	298.1	1	nosp	99.0	estim	*p*	FSIT	71PIC/LED
95FUJ/TAM1	298.1	1	nosp	99.95	chrom	*p*	FSIO	85OGA/MUR

Name: 1,3,5-Trimethylbenzene
Formula: C_9H_{12}

CAS-RN: 108-67-8
Group No.: 14-032
Molar Mass: 120.19

Table 14.32.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		303.9–348.8	4 S	nosp	not specified		avg	DSIO	*81VON
*86SCH		320.5–349.4	8 S	nosp	not specified		avg	DSIO	*86SCH
47KUR		309.9–359.3	5	nosp	not specified		avg	DSIO	47KUR
55HEL/HEI		294.3–377.6	16 S	nosp	99.78	melpt	*p*	BSAO	39SAG/EVA
55TAY/KIL		230.0–304.5	20	0.30	99.95	melpt	*p*	BSIO	55TAY/JOH
65ZIE	N	315.6–366.3	3	nosp	not specified		avg	DSIO	58SWI/ZIEI
68REC1	N	298.0–313.0	eqn	nosp	not specified		*p*	BSAO	68REC1
77FOR/BEN		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
79AND/GRI	N	295.0–423.6	8	0.50	not specified		sat	BSAO	67RAS/GAN
79WIL/FAR		298.1	1	0.30	99.0	estim	*p*	FSIT	71PIC/LED
93GRO/ROU		298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED

65ZIE average values in temperature ranges 295–438 K and 294–338 K
68REC1 same data in 68REC2
79AND/GRI error 0.5% below 373 K and 0.8% at 433 K

Name: Naphthalene
Formula: $C_{10}H_8$

CAS-RN: 91-20-3
Group No.: 14-033
Molar Mass: 128.17

Table 14.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*90PIC		353.0–372.0	2	4.00	not specified		*p*	BDHO	*90PIC
26AND/LYN	N	354.0–473.0	eqn	nosp	not specified		*p*	DSIO	26AND/LYN
31BLA/LEI		382.0–465.8	17	3.00	not specified		sat	BSIO	31BLA/LEI
32SPA/THO		363.1–463.1	11 S	1.00	not specified		*p*	BDHO	31THO/PAR
41SCH		353.0–473.0	eqn	nosp	not specified		*p*	not specified	
44EIB		353.0–473.0	eqn	nosp	not specified		*p*	not specified	
57MCC/FIN2		357.0–370.8	6	0.20	99.985	melpt	sat	BSAO	47HUF
64RAS/BAS		359.1	1	1.50	not specified		*p*	BSIO	64RAS/BAS
93CHI/KNI2		357.9–440.3	13	0.10	99.93	melpt	sat	BSAO	88STE/ARC
93CHI/KNI2		460.0–700.0	13	1.00	99.93	melpt	sat	BDHT	89KNI/ARC
93DUR/AOU		373.0–473.0	102	nosp	not specified		*p*	BDCT	86MER/BEN
95DUR/AOU		373.0–473.0	eqn	2.00	99.	anal	*p*	BDCT	86MER/BEN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

Table 14.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
57MCC/FIN2	357.0–370.8	6	0.20	0.557	2.98–2	0.11	−2.79–2	−6
93CHI/KNI2	357.9–440.3	13	0.10	0.205	5.53–3	0.02	3.13–3	5
93CHI/KNI2	460.0–700.0	13	1.00	0.253	1.01–1	0.25	1.02–2	2
Rejected data								
*90PIC	(4.08,13.11,4.08,1)		26AND/LYN	(1.16,3.66,1.09,7)				
31BLA/LEI	(5.81,16.30,5.74,17)		32SPA/THO	(8.56–1,2.86,8.53–1,11)				
41SCH	(2.55–1,0.82,1.36–1,3)		44EIB	(3.36–1,1.23,−2.46–1,−5)				
64RAS/BAS	(2.40,8.33,2.40,1)		93DUR/AOU	(9.44–1,3.10,7.52–1,102)				
95DUR/AOU	(2.24–1,0.79,1.90–1,10)							

Table 14.33.3. Parameters of cubic spline polynomials

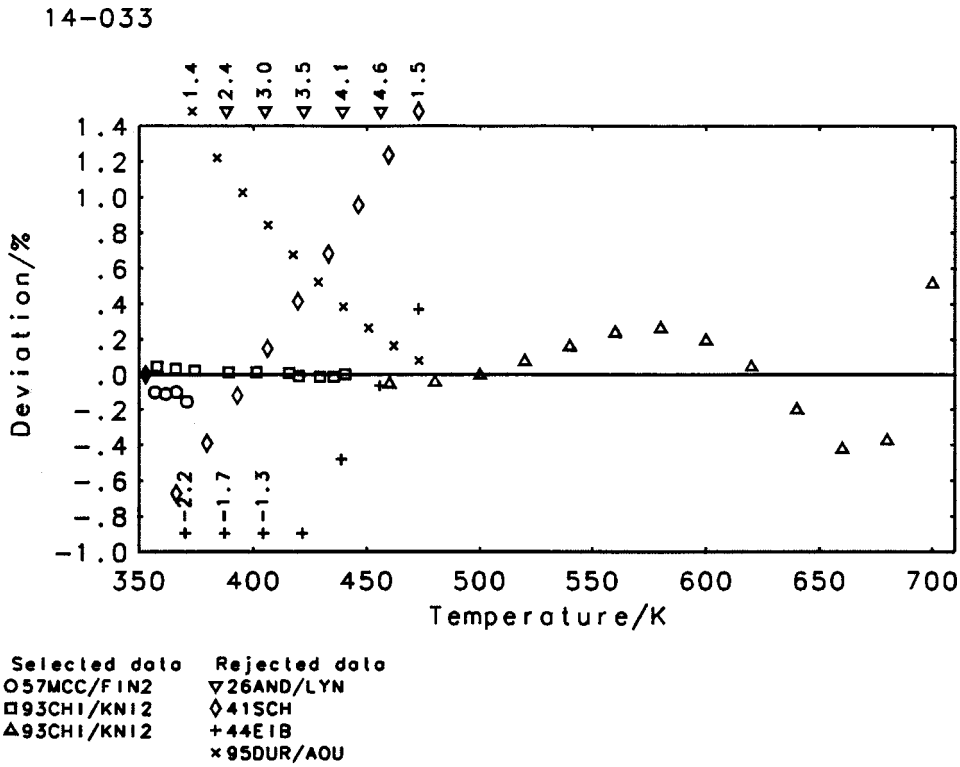
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	201	32	0.346	7.15–2	0.18	2.09–4	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
357.0–520.0	1.27115+1	1.99429	7.60133−1	−7.02083−2	III
520.0–700.0	−4.76592+1	3.68236+1	−5.93780	3.59147−1	V

Table 14.33.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	201	32	0.507	5.70–2	0.15	4.57–3	7

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
357.0–700.0	748.40	−1.74338	4.84034−2	4.59781	5.32247+1	−2.32848+1	3.48887	V



Name: 1,2,3,4-Tetrahydronaphthalene
Formula: $C_{10}H_{12}$

CAS-RN: 119-64-2
Group No.: 14-035
Molar Mass: 132.21

Table 14.35.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
22HER/SCH		289.6	1	nosp	not specified		*p*	DSIO	22HER/SCH
57MCC/FIN2		248.4–318.5	11	0.20	99.97	melpt	sat	BSAO	47HUF
88STE/CHI	N	300.0–720.0	43 S	nosp	not specified		sat	BDHT	89KNI/ARC
98RUZ/MOK		307.7–396.8	27	1.00	99.9	chrom	sat	BDCT	91BAN/GAR

88STE/CHI last two points at 710 K and 720 K are extraplated values

Table 14.35.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
				Selected data				
57MCC/FIN2	248.4–318.5	11	0.20	0.225	1.11–2	0.04	3.41–3	0
88STE/CHI	300.0–710.0	42	1.00 #	0.876	4.73–1	0.88	2.11–2	6
98RUZ/MOK	307.7–396.9	27	1.00	0.491	1.39–1	0.49	−5.11–2	−12
				Rejected data				
22HER/SCH	(1.15,4.29,1.15,1)							

Table 14.35.3. Parameters of cubic spline polynomials

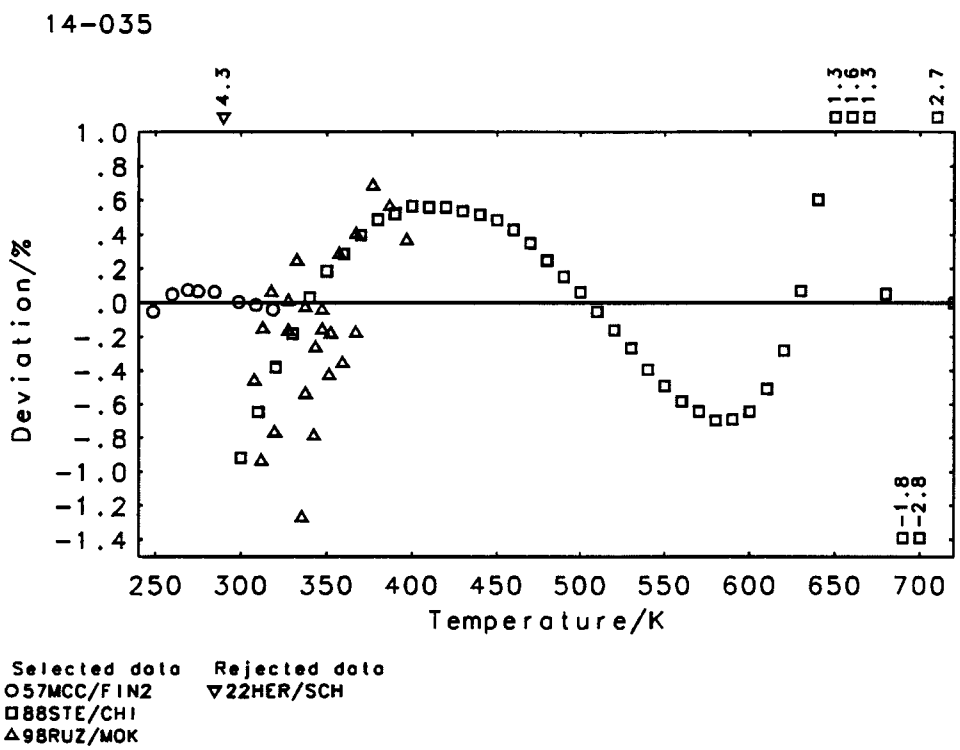
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	82	80	0.729	3.66−1	0.72	−5.71−3	−6
sat	82	80	0.527	2.12−1	0.52	−9.70−3	−6

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
248.4–320.0	3.76177+1	−2.22115+1	9.08395	−9.80732−1	II
320.0–640.0	3.06225	1.01843+1	−1.03973	7.38174−2	IV
640.0–710.0	−1.31743+4	6.18709+3	−9.66181+2	5.03416+1	V
248.4–320.0	3.59220+1	−2.04591+1	8.48467	−9.12926−1	II
320.0–640.0	4.75060	8.76414	−6.47589−1	3.83514−2	IV
640.0–710.0	−7.73784+3	3.63811+3	−5.67732+2	2.95740+1	IV

Table 14.35.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	82	80	0.903	2.81−1	0.80	9.62−2	23

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
248.4–710.0	721.00	−3.39311	2.48434−1	6.37947	5.20169+1	−2.47725+1	4.22034	V



Name: 1-Methyl-4-(1-methylethenyl)cyclohexene
Formula: $C_{10}H_{16}$

CAS-RN: 138-86-3
Group No.: 14-043
Molar Mass: 136.24

Table 14.43.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
33KOL/UDO	N	293.4	1	nosp	not specified		*p*	BSIT	34KOL/UDO
98SAM/NIE		318.1–403.1	18	1.50	99.96	chrom	*p*	BDCT	86MER/BEN

33KOL/UDO same datum in 34KOL/UDO

Table 14.43.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
			Selected data					
33KOL/UDO	293.4	1	3.00 #	0.208	1.87–1	0.62	−1.87–1	−1
98SAM/NIE	318.1–403.1	18	1.50	0.203	1.07–1	0.30	3.27–3	−2

Table 14.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	19	19	0.221	1.23–1	0.36	−6.74–3	−3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
293.4–403.1	2.27187+1	−3.14553−1	9.75296−1	V

Name: 1,1′-Biphenyl
Formula: $C_{12}H_{10}$

CAS-RN: 92-52-4
Group No.: 14-052
Molar Mass: 154.21

Table 14.52.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
31FOR/BRU		350.8–469.6	22	2.00	not specified		*p*	BSIO	31FOR/BRU
31FOR/BRU		420.8–620.2	8	2.00	not specified		*p*	FSIO	31FOR/BRU
31NEW/KAU	N	344.0–573.0	eqn	1.00	not specified		*p*	not specified	
32SPA/THO		353.1–373.1	3 S	nosp	not specified		*p*	BDHO	31THO/PAR
41SCH		342.0–473.0	eqn	nosp	not specified		*p*	not specified	
50KUR		386.4–492.8	10	nosp	not specified		avg	DSIO	47KUR
56MCE/MAL		422.0–588.7	4 S	nosp	not specified		*p*	not specified	
58WAL/BRO		429.8–533.3	3	2.00	not specified		*p*	DSIO	56WAL/GRA
83ORO/MRA		350.0–480.0	24 S	1.50	99.9	chrom	*p*	BDHT	69PER/COM
89CHI/KNI		349.1–440.3	11	0.10	99.983	melpt	sat	BSAO	47HUF
89CHI/KNI		360.0–700.0	18	1.00	99.983	melpt	sat	BDHT	89KNI/ARC
93DUR/AOU		373.0–473.0	51	nosp	not specified		*p*	BDCT	86MER/BEN
95DUR/AOU		373.0–473.0	eqn	2.00	99.	anal	*p*	BDCT	86MER/BEN

31NEW/KAU four different calorimeters used

Name: 2,7-Dimethylnaphthalene
Formula: $C_{12}H_{12}$

CAS-RN: 582-16-1
Group No.: 14-056
Molar Mass: 156.23

Table 14.56.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
77FIN/MES		372.6–391.0	6	0.20	99.95	melpt	sat	BSAO	47HUF
93CHI/KNI2	N	372.6–434.0	13	0.10	99.95	melpt	sat	BSAO	88STE/ARC
93CHI/KNI2		460.0–700.0	13	1.00	99.95	melpt	sat	BDHT	89KNI/ARC

93CHI/KNI2 the first 6 data points originally published in 77FIN/MES converted to the temperature scale ITS-90 by authors

Table 14.56.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93CHI/KNI2	372.6–434.0	13	0.10	0.848	3.02–2	0.08	−5.40–4	−3
93CHI/KNI2	460.0–700.0	13	1.00	0.271	1.25–1	0.27	5.99–2	7
Rejected data								
77FIN/MES	(3.18–2,0.09,−9.67–3,−2)							

Table 14.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
sat	32	26	0.669	9.71–2	0.21	2.97–2	4

Temp. range K	A_1	A_2	A_3	Level of uncertainty
372.6–700.0	1.33259+1	5.70950	−9.23097−3	III

Table 14.56.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
sat	32	26	0.667	9.12–2	0.20	3.19–2	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
372.6–700.0	775.00	1.68789−1	1.61721−4	1.34072+1	4.40417+1	III

Name: 9*H*-Fluorene
Formula: $C_{13}H_{10}$

CAS-RN: 86-73-7
Group No.: 14-061
Molar Mass: 166.22

Table 14.61.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
44EIB	387.0–473.0	eqn	nosp	not specified		*p*	not specified	
77FIN/MES	392.6–426.7	8	0.20	99.992	melpt	sat	BSAO	47HUF
95FUJ/FUJ	391.9–419.1	10	0.30	99.71	melpt	sat	BSAO	93FUJ/OGU1

Table 14.61.2. Correlated heat capacities

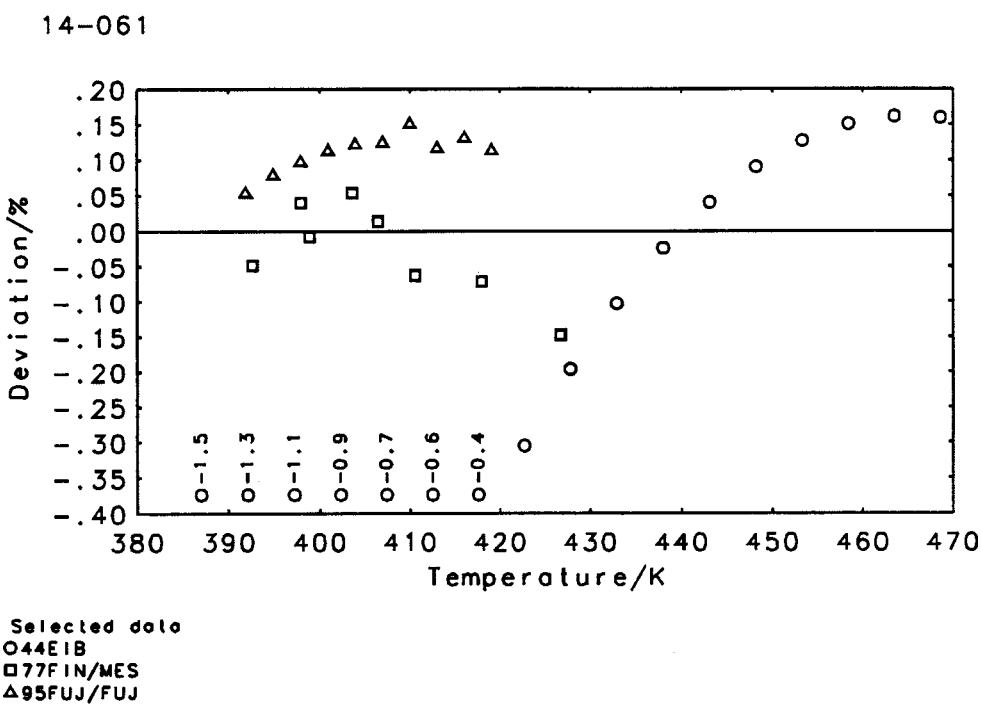
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
44EIB	387.0–473.7	18	1.00 #	0.640	2.27–1	0.64	−1.23–1	−4
77FIN/MES	392.6–426.7	8	0.20	0.345	2.56–2	0.07	−1.08–2	−1
95FUJ/FUJ	391.9–419.1	10	0.30	0.377	4.13–2	0.11	4.01–2	10

Table 14.61.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	36	36	0.543	1.70–1	0.48	−5.30–2	5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
387.0–473.7		2.83115+1	−1.91187	9.63811−1			III

Table 14.61.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	36	36	1.008	1.44–1	0.40	8.78–3	9
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
387.0–473.7	825.00	−1.30843+1	3.09162	1.45798+1	1.38439+1		III



Name: Anthracene
Formula: $C_{14}H_{10}$

CAS-RN: 120-12-7
Group No.: 14-066
Molar Mass: 178.23

Table 14.66.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
17HIL/DUS	N	526.2–541.2	2	nosp	not specified		avg	DSIO	11LEW/RAN
70GOU/GIR	N	496.7–511.3	5	0.10	99.99	melpt	sat	BSAO	53WES/HAT
93DUR/AOU		492.0–592.0	51	nosp	not specified		*p*	BDCT	86MER/BEN
95DUR/AOU		492.0–592.0	eqn	2.00	99.9	anal	*p*	BDCT	86MER/BEN

17HIL/DUS average values in temperature ranges 489–563 K and 489–593 K
70GOU/GIR smoothed value at 500 K in 68GOU/GIR

Name: Phenanthrene
Formula: $C_{14}H_{10}$

CAS-RN: 85-01-8
Group No.: 14-068
Molar Mass: 178.23

Table 14.68.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
41SCH	371.0–473.0	eqn	nosp	not specified		*p*	not specified	
44EIB	371.0–473.0	eqn	nosp	not specified		*p*	not specified	
64RAS/BAS	379.1	1	1.50	not specified		*p*	BSIO	64RAS/BAS
77FIN/MES	383.3–408.6	4	0.20	99.987	melpt	sat	BSAO	47HUF
93DUR/AOU	392.0–492.0	51	nosp	not specified		*p*	BDCT	86MER/BEN
95DUR/AOU	392.0–492.0	eqn	2.00	98.0	anal	*p*	BDCT	86MER/BEN

Name: 1,1′-Ethenylidenebisbenzene
Formula: $C_{14}H_{12}$

CAS-RN: 530-48-3
Group No.: 14-071
Molar Mass: 180.25

Table 14.71.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
31SMI/AND1	286.0–298.5	2	nosp	99.3	melpt	*p*	DSIO	26AND/LYN
99VER/EBE	298.1	1	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 1,1′-Ethylidenebisbenzene
Formula: $C_{14}H_{14}$

CAS-RN: 612-00-0
Group No.: 14-073
Molar Mass: 182.27

Table 14.73.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
31SMI/AND1	259.8–298.5	4	nosp	not specified		*p*	DSIO	26AND/LYN
99VER1	298.1	1	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: Fluoranthene
Formula: $C_{16}H_{10}$

CAS-RN: 206-44-0
Group No.: 14-078
Molar Mass: 202.26

Table 14.78.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
71WON/WES	393.7–422.6	5	0.10	99.936	melpt	sat	BSAO	68WES/WES
71WON/WES	386.4–451.7	10	0.10	99.61	melpt	sat	BSAO	68WES/WES
93DUR/AOU	492.0–592.0	51	nosp	not specified		*p*	BDCT	86MER/BEN
95DUR/AOU	492.0–592.0	eqn	2.00	98.	anal	*p*	BDCT	86MER/BEN

Name: Pyrene
Formula: $C_{16}H_{10}$

CAS-RN: 129-00-0
Group No.: 14-079
Molar Mass: 202.26

Table 14.79.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
71WON/WES	430.6–478.8	7	0.10	99.97	melpt	sat	BSAO	68WES/WES
93DUR/AOU	492.0–592.0	51	nosp	not specified		*p*	BDCT	86MER/BEN
95DUR/AOU	492.0–592.0	eqn	2.00	99.0	anal	*p*	BDCT	86MER/BEN

Name: 1,1′:4′,1″-Terphenyl
Formula: $C_{18}H_{14}$

CAS-RN: 92-94-4
Group No.: 14-083
Molar Mass: 230.31

Table 14.83.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
83CHA	487.0–580.0	6 S	0.50	99.9	chrom	*p*	BDHT	69PER/COM
93DUR/AOU	492.0–592.0	102	nosp	not specified		*p*	BDCT	86MER/BEN
95DUR/AOU	492.0–592.0	eqn	2.00	99.0	anal	*p*	BDCT	86MER/BEN

Name: Perylene
Formula: $C_{20}H_{12}$

CAS-RN: 198-55-0
Group No.: 14-087
Molar Mass: 252.32

Table 14.87.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
80WON/WES	554.4–573.0	5	0.10	99.97	melpt	*p*	BSAO	68WES/WES
93DUR/AOU	552.0–652.0	51	nosp	not specified		*p*	BDCT	86MER/BEN
95DUR/AOU	552.0–652.0	eqn	2.00	99.0	anal	*p*	BDCT	86MER/BEN

Name: Pentacene
Formula: $C_{22}H_{14}$

CAS-RN: 135-48-8
Group No.: 14-090
Molar Mass: 278.35

Table 14.90.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93DUR/AOU	546.0–594.0	25	nosp	not specified		*p*	BDCT	86MER/BEN
95DUR/AOU	546.0–594.0	eqn	2.00	not specified		*p*	BDCT	86MER/BEN

Name: 9,10-Diphenylanthracene
Formula: $C_{26}H_{18}$

CAS-RN: 1499-10-1
Group No.: 14-095
Molar Mass: 330.43

Table 14.95.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93DUR/AOU	522.0–622.0	51	nosp	not specified		*p*	BDCT	86MER/BEN
95DUR/AOU	522.0–620.0	eqn	2.00	99.	anal	*p*	BDCT	86MER/BEN

Name: 1,3-Cyclopentadiene
Formula: C_5H_6

CAS-RN: 542-92-7
Group No.: 14-098
Molar Mass: 66.10

Table 14.98.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
77LEB/LIT2	N	181.1–244.2	12	0.20	97.6	melpt	*p*	BSAO	76LEB/LIT
77LEB/LIT2	data from a graph only; above 230 K begin a dimerization								

Table 14.98.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	12	12	1.021	6.36–2	0.51	5.53–4	0

Temp. range K	A_1	A_2	Level of uncertainty
181.1–244.2	9.40931	1.42944	III

Name: Bicyclo[2.2.1]hept-2-ene
Formula: C_7H_{10}

CAS-RN: 498-66-8
Group No.: 14-099
Molar Mass: 94.16

Table 14.99.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92LEB/SMI	320.8–329.5	4	0.20	99.16	melpt	*p*	BSAO	76LEB/LIT
96STE/CHI3	340.0–580.0	13 S	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 14.99.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
Selected data								
92LEB/SMI	320.8–329.5	4	0.50 #	0.120	1.19–2	0.06	−4.07–4	−1
96STE/CHI2	340.0–580.0	13	1.00	1.185	4.56–1	1.18	1.67–2	1

Table 14.99.3. Parameters of cubic spline polynomials

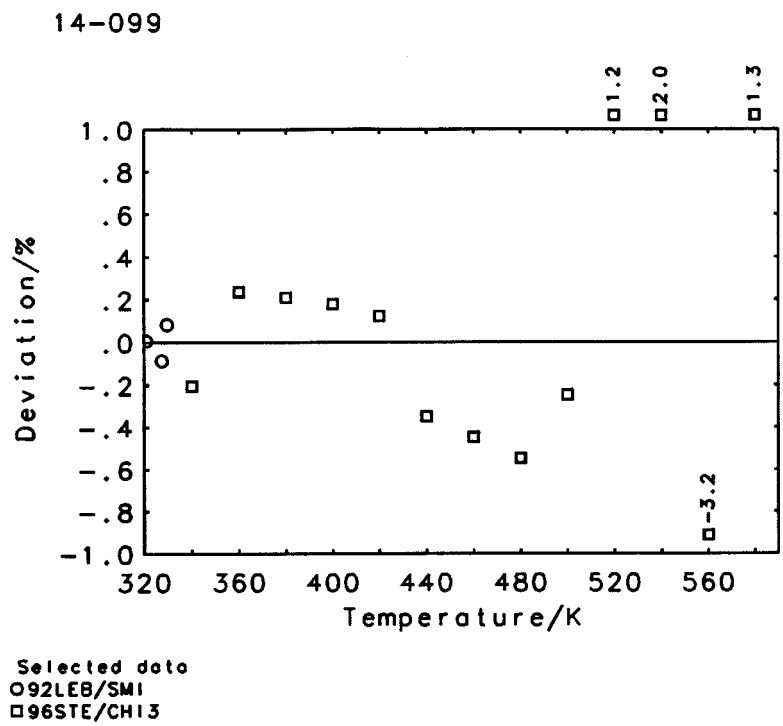
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	17	17	1.235	4.75–1	1.23	1.26–2	0
sat	17	17	0.786	2.74–1	0.78	3.60–3	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
320.8–520.0	−6.04209	1.19280+1	−1.78313	1.66625−1	IV
520.0–580.0	−1.27981+4	7.39194+3	−1.42102+3	9.11431+1	V
320.8–520.0	−6.71452	1.19450+1	−1.62478	1.35841−1	IV
520.0–580.0	−7.98697+3	4.61594+3	−8.87008+2	5.68912+1	V

Table 14.99.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	17	17	0.193	5.25–2	0.18	−1.37–3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
320.8–580.0	590.00	−2.25197	3.72027−1	−8.66639	6.88171+1	−4.70249+1	1.19851+1	IV



Name: Ethenyl-d_3-benzene-d_5
Formula: C_8D_8

CAS-RN: 19361-62-7
Group No.: 14-100
Molar Mass: 112.20

Table 14.100.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
85LEB/LEB	N	240.5–328.8	17	0.20	99.35	melpt	*p*	BSAO	76LEB/LIT

85LEB/LEB data from a graph only

Table 14.100.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	17	17	0.748	3.46−2	0.15	8.77−5	0

Temp. range K	A_1	A_2	Level of uncertainty
240.5–328.8	1.36534+1	3.47456	III

Name: 5-Ethenylbicyclo[2.2.1]hept-2-ene
Formula: C_9H_{12}

CAS-RN: 3048-64-4
Group No.: 14-101
Molar Mass: 120.19

Table 14.101.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96STE/CHI3	315.0–415.0	6	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 14.101.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	6	6	0.143	4.37−2	0.14	6.71−5	1
sat	6	6	0.142	4.32−2	0.14	6.71−5	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
315.0–415.0	1.62014+1	1.26484−1	8.92547−1	V
315.0–415.0	1.57512+1	3.99457−1	8.51252−1	V

Name: (*Z*)-5-Ethylidenebicyclo[2.2.1]hept-2-ene
Formula: C_9H_{12}

CAS-RN: 28304-66-7
Group No.: 14-102
Molar Mass: 120.19

Table 14.102.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI1	290.0–440.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 14.102.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	16	16	0.008	2.09−3	0.01	0.00	−1
sat	16	16	0.000	1.18−6	0.00	−1.19−7	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
290.0–440.0	5.78025	6.04643	1.32937−2	IV
290.0–440.0	5.39998	6.28001	−2.23518−2	IV

Table 14.102.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
total	used						
p	16	16	0.007	1.85−3	0.01	−1.55−6	−2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
290.0–440.0	629.00	−1.89211−1	2.34408−4	5.70533	3.81821+1	IV

Name: 1-Methylenepropylbenzene
Formula: $C_{10}H_{12}$

CAS-RN: 2039-93-2
Group No.: 14-103
Molar Mass: 132.21

Table 14.103.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER/EBE	298.15	1.310	nosp	99.99	chrom	p	BDHT	69PER/COM

Name: (3aα,4α,7α,7aα)-3a,4,7,7a-Tetrahydro-4,7-methano-1*H*-indene
Formula: $C_{10}H_{12}$

CAS-RN: 1755-01-7
Group No.: 14-104
Molar Mass: 132.21

Table 14.104.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
77LEB/LIT2	N	303.5–331.3	2 S	0.20	99.	melpt	p	BSAO	76LEB/LIT
77LEB/LIT2	data from a graph only								

Table 14.104.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Leve of uncertainty
303.5–331.3	4.18630	6.83559	III

Name: (*R*)-1-Methyl-4-(1-methylethenyl)cyclohexene
Formula: $C_{10}H_{16}$

CAS-RN: 5989-27-5
Group No.: 14-105
Molar Mass: 136.24

Table 14.105.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96GAL/VAN1	202.0–250.1	24	0.20	99.31	melpt	p	BSAO	87VAN/VAN

Table 14.105.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	24	24	0.206	1.08−2	0.04	6.99−6	−2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
202.0–220.0	−8.49715+2	1.21115+3	−5.59014+2	8.61210+1	II
220.0–250.1	2.00414+2	−2.20843+2	9.18923+1	−1.25012+1	II

Name: 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene
Formula: $C_{10}H_{16}$

CAS-RN: 80-56-8
Group No.: 14-106
Molar Mass: 136.24

Table 14.106.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98SAM/NIE	313.1–403.1	19	1.50	99.56	chrom	*p*	BDCT	86MER/BEN

Table 14.106.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	19	19	0.199	9.51−2	0.30	4.34−4	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
313.1–403.1	2.33551+2	−1.68608+2	4.50789+1	−3.80816	V

Name: (2-Methyl-1-methylenepropyl)benzene
Formula: $C_{11}H_{14}$

CAS-RN: 17498-71-4
Group No.: 14-107
Molar Mass: 146.23

Table 14.107.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER/EBE	298.15	1.720	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: (2,2-Dimethyl-1-methylenepropyl)benzene
Formula: $C_{12}H_{16}$

CAS-RN: 5676-29-9
Group No.: 14-108
Molar Mass: 160.26

Table 14.108.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER/EBE	298.15	1.600	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 1,3-Bis(1-methylethyl)benzene
Formula: $C_{12}H_{18}$

CAS-RN: 99-62-7
Group No.: 14-109
Molar Mass: 162.27

Table 14.109.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98VER2	298.15	1.480	nosp	99.30	chrom	*p*	BDHT	69PER/COM

Name: 1,4-Bis(1-methylethyl)benzene
Formula: $C_{12}H_{18}$

CAS-RN: 100-18-5
Group No.: 14-110
Molar Mass: 162.27

Table 14.110.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98VER2	298.15	1.300	nosp	99.92	chrom	*p*	BDHT	69PER/COM

Name: 1,3,5-Triethylbenzene
Formula: $C_{12}H_{18}$

CAS-RN: 102-25-0
Group No.: 14-111
Molar Mass: 162.27

Table 14.111.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI3	300.0–660.0	19	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 14.111.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	19	19	0.503	3.20–1	0.50	2.93–3	1
sat	19	19	0.318	1.93–1	0.32	1.07–3	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–580.0	1.67825+1	5.05053	5.40640−1	−4.24952−2	IV
580.0–660.0	−4.65613+3	2.42208+3	−4.16188+2	2.39074+1	IV
300.0–580.0	1.74528+1	4.35538	7.68465−1	−6.63189−2	IV
580.0–660.0	−2.92089+3	1.52419+3	−2.61272+2	1.49935+1	IV

Table 14.111.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	19	19	0.401	2.14–1	0.40	1.84–3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
300.0–660.0	679.00	−3.48736	3.37789−1	2.22386	9.18798+1	−5.70646+1	1.28197+1	IV

Name: 9,10-Dihydroanthracene
Formula: $C_{14}H_{12}$

CAS-RN: 613-31-0
Group No.: 14-112
Molar Mass: 180.25

Table 14.112.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
87CHI/HOS1	387.6–440.2	8	0.10	99.72	melpt	sat	BSAO	43RUE/HUF

Table 14.112.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	8	8	0.089	3.64–3	0.01	2.86–6	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
387.5–440.2	6.33712	1.03905+1	−4.89641−1	II

Name: 2,2′-Dimethyl-1,1′-biphenyl
Formula: $C_{14}H_{14}$

CAS-RN: 605-39-0
Group No.: 14-113
Molar Mass: 182.27

Table 14.113.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
87CHI/HOS2	N	272.6–398.4	26	0.10	99.969	melpt	sat	BSAO	43RUE/HUF
87CHI/HOS2	low temperature limit is below n.m.t.(293.1 K); undercooled liquid								

Table 14.113.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	26	26	0.195	7.42–3	0.02	3.23–6	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
272.6–398.4	3.50429+1	−8.64834	4.06938	−3.61494−1	II

Name: 2-Ethyl-1,1′-biphenyl
Formula: $C_{14}H_{14}$

CAS-RN: 1812-51-7
Group No.: 14-114
Molar Mass: 182.27

Table 14.114.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
87CHI/HOS2	274.6–440.4	19	0.10	99.84	melpt	sat	BSAO	43RUE/HUF

Table 14.114.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	19	19	0.122	4.74−3	0.01	1.20−6	2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
274.6–440.4		3.03193+1	−4.33476	2.89671	−2.53954−1		II

Name: 1-Methyl-2-(phenylmethyl)benzene
Formula: $C_{14}H_{14}$

CAS-RN: 713-36-0
Group No.: 14-115
Molar Mass: 182.27

Table 14.115.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
87CHI/HOS1	N	268.1–378.4	44	0.10	99.61	melpt	sat	BSAO	43RUE/HUF
87CHI/HOS1	low temperature limit is below n.m.t.(279.8 K); undercooled liquid								

Table 14.115.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	44	44	0.709	2.72−2	0.07	3.59−5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
268.1–378.4		2.18722+1	2.78081	6.20570−1			II

Name: 1,2,3,4-Tetrahydroanthracene
Formula: $C_{14}H_{14}$

CAS-RN: 2141-42-6
Group No.: 14-116
Molar Mass: 182.27

Table 14.116.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
87CHI/HOS1	380.5–438.4	10	0.10	99.98	melpt	sat	BSAO	43RUE/HUF

Table 14.116.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	10	10	0.164	6.90−3	0.02	2.67−6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
380.5–438.4		9.56036	9.09631	−2.74384−1			II

Name: 1,2,3,4-Tetrahydrophenanthrene
Formula: $C_{14}H_{14}$

CAS-RN: 1013-08-7
Group No.: 14-117
Molar Mass: 182.27

Table 14.117.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94CHI/GAM	N	307.7–431.3	19	0.10	99.945	melpt	sat	BSAO	88STE/ARC
94CHI/GAM	preliminary data in 87CHI/HOS								

Table 14.117.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	19	19	0.156	5.72–3	0.02	2.01–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
307.7–431.3		2.11243+1	−1.51663	2.63644	−2.48262−1		II

Name: 1,1′-(1,3-Propanediyl)bisbenzene
Formula: $C_{15}H_{16}$

CAS-RN: 1081-75-0
Group No.: 14-118
Molar Mass: 196.29

Table 14.118.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95FUJ/TAM2	298.15	1.665	nosp	99.8	chrom	*p*	FSIO	85OGA/MUR

Name: 1,3,5-Tris(1-methylethyl)benzene
Formula: $C_{15}H_{24}$

CAS-RN: 717-74-8
Group No.: 14-119
Molar Mass: 204.36

Table 14.119.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98VER2	298.15	0.9600	nosp	99.89	chrom	*p*	BDHT	69PER/COM

Name: 4,5,9,10-Tetrahydropyrene
Formula: $C_{16}H_{14}$

CAS-RN: 781-17-9
Group No.: 14-120
Molar Mass: 206.29

Table 14.120.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93CHI/KNI1	418.4–518.5	11	0.10	99.982	melpt	sat	BSAO	88STE/ARC
93CHI/KNI1	420.0–700.0	15	1.00	99.982	melpt	sat	BDHT	89KNI/ARC

Table 14.120.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93CHI/KNI1	418.4–518.5	11	0.10	0.103	5.21–3	0.01	4.10–4	1
93CHI/KNI1	420.0–700.0	15	1.00	0.241	1.13–1	0.24	−2.93–2	−2

Table 14.120.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	26	26	0.207	9.14−2	0.19	−1.68−2	−1
sat	26	26	0.210	9.26−2	0.20	−1.72−2	−2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
418.4−700.0	3.68228	1.25378+1	−5.45308−1	IV
418.4−700.0	3.35770	1.26786+1	−5.60495−1	IV

Table 14.120.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	26	26	0.796	1.20−1	0.23	1.96−2	5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
418.4−700.0	900.00	−8.59436−1	8.54448−1	−1.17289+1	1.81115+2	−1.52830+2	4.90632+1	IV

Name: 1,2,3,6,7,8-Hexahydropyrene
Formula: $C_{16}H_{16}$

CAS-RN: 1732-13-4
Group No.: 14-121
Molar Mass: 208.30

Table 14.121.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93CHI/KNI1	412.7−441.3	10	0.10	99.984	melpt	sat	BSAO	88STE/ARC
93CHI/KNI1	420.0−700.0	15	1.00	99.984	melpt	sat	BDHT	89KNI/ARC

Table 14.121.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93CHI/KNI1	412.8−441.3	10	0.10	0.204	9.66−3	0.02	3.36−5	−1
93CHI/KNI1	420.0−700.0	15	1.00	0.050	2.84−2	0.05	−2.13−3	−2

Table 14.121.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	25	25	0.147	2.49−2	0.04	−1.27−3	−3
sat	25	25	0.147	2.43−2	0.04	−1.44−3	−3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
412.8−700.0	−9.98795	2.02755+1	−1.94754	8.79145−2	IV
412.8−700.0	−9.13253	1.97180+1	−1.82719	7.93183−2	IV

Table 14.121.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	25	25	0.154	2.23−2	0.04	1.69−4	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
412.8–700.0	920.00	−3.08927	4.82780−1	−6.77064	1.60239+2	−1.19600+2	3.25447+1	IV

Name: 1,1′-(2-Methylpropylidene)bisbenzene
Formula: $C_{16}H_{18}$

CAS-RN: 1634-11-3
Group No.: 14-122
Molar Mass: 210.32

Table 14.122.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER1	298.15	2.000	nosp	99.99	chrom	p	BDHT	69PER/COM

Name: Dodecylbenzene
Formula: $C_{18}H_{30}$

CAS-RN: 123-01-3
Group No.: 14-123
Molar Mass: 246.44

Table 14.123.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00MOK/RUZ	307.8–446.6	41	1.00	99.90	chrom	p	BDCT	91BAN/GAR

Table 14.123.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	41	41	0.323	2.19−1	0.32	1.31−3	6

Temp. range K	A_1	A_2	A_3	Level of uncertainty
307.8–446.6	3.53061+1	6.02669	5.50021−1	IV

Table 14.123.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	41	41	0.320	2.16−1	0.32	1.28−3	5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
307.8–446.6	501.60	−1.39847	1.09279−2	3.02296+1	4.47415+1	IV

Name: Benzo[*a*]pyrene
Formula: $C_{20}H_{12}$

CAS-RN: 50-32-8
Group No.: 14-124
Molar Mass: 252.32

Table 14.124.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98RUZ/MOK	457.2–496.4	15	1.00	99.5	chrom	sat	BDCT	91BAN/GAR

Table 14.124.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	15	15	0.176	9.98–2	0.18	3.13–4	4

Temp. range K	A_1	A_2	Level of uncertainty
457.2–496.4	2.55746+1	6.53727	IV

Name: Nonadecylbenzene
Formula: $C_{25}H_{44}$

CAS-RN: 29136-19-4
Group No.: 14-125
Molar Mass: 344.62

Table 14.125.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
83MEY/MEY	N	303.15	2.117	nosp	99.7	melpt	*p*	BSIO	83MEY/MEY

83MEY/MEY in the article temperature unspecified; probably above melting temperature of stabile modification

Name: Tetrafluoromethane
Formula: CF_4

CAS-RN: 75-73-0
Group No.: 21-001
Molar Mass: 88.00

Table 21.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
38EUC/SCH		100.0–145.0	6 S	nosp	99.9	estim	*p*	BSAO	38EUC/SCH
58KOS/SAM	N	90.0–94.8	14	nosp	99.92	melpt	*p*	BSAO	54STR/ICK
69ENO/SHI2		90.4–91.7	2	nosp	99.985	melpt	*p*	BSAO	66SHI/ATA
69SMI/PAC		92.0–139.9	21	nosp	99.985	melpt	sat	BSAO	55PAC/PIE
72COP/REA		121.6–141.4	6	nosp	99.9	estim	*p*	BSAO	68WES/FUR

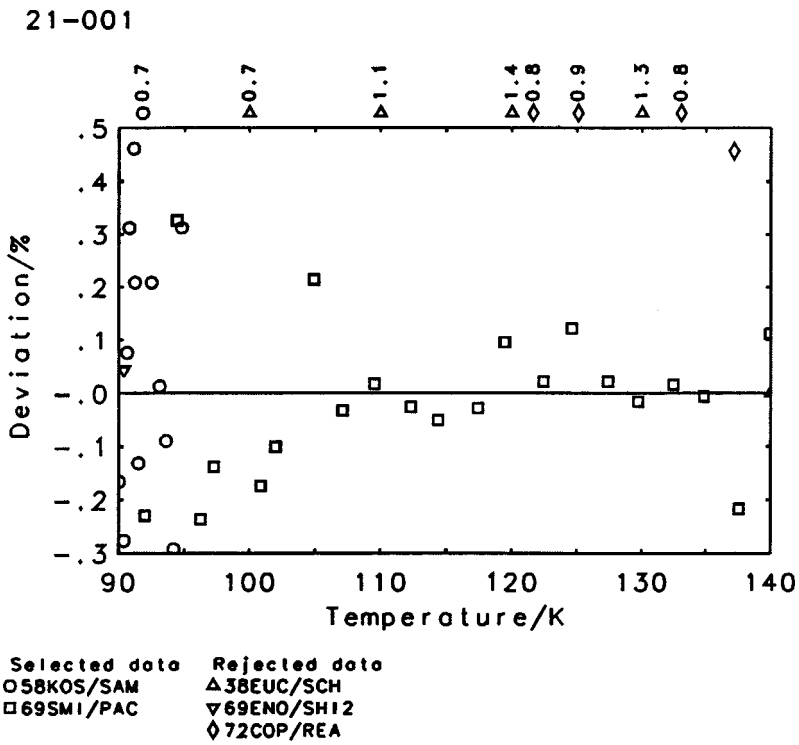
58KOS/SAM data from a graph only

Table 21.1.2. Correlated heat capacities

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R		±
Selected data								
58KOS/SAM	90.0–94.8	14	0.40 #	0.714	2.69–2	0.29	8.58–3	2
69SMI/PAC	92.0–139.9	21	0.20 #	0.700	1.31–2	0.14	−1.37–3	−2
Rejected data								
38EUC/SCH	(1.10–1,1.17,1.07–1,4)		69ENO/SHI2	(4.66–2,0.49,3.49–2,2)				
72COP/REA	(7.41–2,0.79,7.25–2,5)							

Table 21.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	49	35	0.738	2.07−2	0.22	2.61−3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
90.0–139.9		1.30227+1	−6.72786	3.01662			II



Name: 1,1,1-Trifluoroethane
Formula: $C_2H_3F_3$

CAS-RN: 420-46-2
Group No.: 21-005
Molar Mass: 84.04

Table 21.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
44RUS/GOL	165.4–220.7	11	0.10	99.95	melpt	p	BSAO	41YOS/GAR
98MAG	164.8–343.4	80	0.70	99.93	chrom	sat	BSAO	61GOO

Table 21.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
44RUS/GOL	165.4–220.7	11	0.10	0.924	1.18−2	0.09	−1.14−3	−5
98MAG	164.8–343.4	80	0.70	1.062	2.14−1	0.74	1.23−2	18

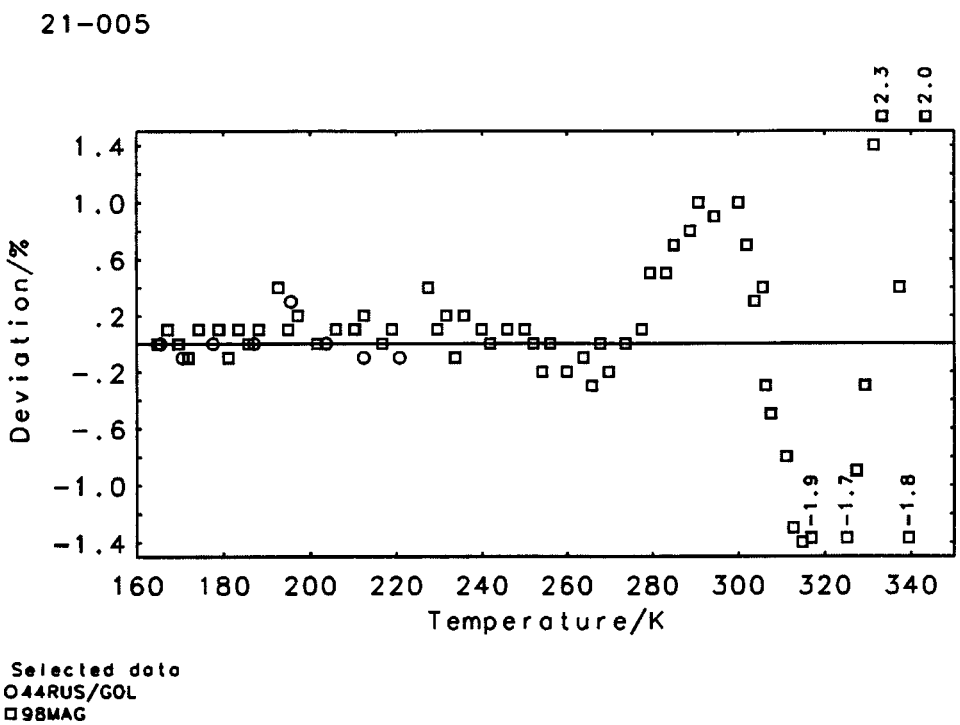
Table 21.5.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	91	91	1.083	2.07–1	0.72	1.07–2	13
sat	91	91	0.737	8.76–2	0.45	8.33–3	23
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
164.8–280.0		9.30610	3.94544	−2.30613	5.99355−1		II
280.0–330.0		−8.43898+2	9.18093+2	−3.28787+2	3.94662+1		IV
330.0–343.4		−3.02931+5	2.75543+5	−8.35485+4	8.44550+3		V
164.8–280.0		1.06075+1	1.76313	−1.08728	3.72614−1		II
280.0–330.0		−5.38048+2	5.89608+2	−2.11032+2	2.53660+1		IV
330.0–343.4		−1.50079+5	1.36536+5	−4.14070+4	4.18657+3		IV

Table 21.5.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	91	91	1.201	3.12–1	0.79	4.76–3	22

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
164.8–343.4	346.30	−2.57393	2.57442−1	1.13207+1	−2.79514	−9.04613−1	2.71412	V



Name: Hexafluorobenzene
Formula: C_6F_6

CAS-RN: 392-56-3
Group No.: 21-010
Molar Mass: 186.06

Table 21.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
65COU/GRE		281.9–305.9	8	0.20	99.97	melpt	*p*	BSAO	63AND/COU1
70MES/FIN		284.8–342.7	8	0.20	99.93	melpt	sat	BSAO	47HUF
82GOR/SIM1	N	284.0–349.7	18	0.50	99.74	melpt	*p*	FSIO	83GOR/SIM
82GOR/SIM2		279.0–353.0	eqn	nosp	99.9	anal	*p*	FSIO	83GOR/SIM
87WIL/LAI		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

82GOR/SIM1 same data in 82GOR/GRI

Name: 1,2-Difluorobenzene
Formula: $C_6H_4F_2$

CAS-RN: 367-11-3
Group No.: 21-016
Molar Mass: 114.09

Table 21.16.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
63SCO/MES	N	229.0–357.2	20	0.20	99.998	melpt	sat	BSAO	47HUF
91LIC		225.3	1	2.00	99.	anal	*p*	BDCT	89BRE/LIC

63SCO/MES smoothed value at 298.15 K in 62GOO/LAC

Name: 1,3-Difluorobenzene
Formula: $C_6H_4F_2$

CAS-RN: 372-18-9
Group No.: 21-017
Molar Mass: 114.09

Table 21.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
70MES/FIN	N	214.3–354.9	15	0.20	99.999	melpt	sat	BSAO	47HUF
91LIC		204.0	1	2.00	99.	anal	*p*	BDCT	89BRE/LIC

70MES/FIN smoothed value at 298.15 K in 62GOO/LAC

Name: 1,4-Difluorobenzene
Formula: $C_6H_4F_2$

CAS-RN: 540-36-3
Group No.: 21-018
Molar Mass: 114.09

Table 21.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
62GOO/LAC	N	298.1	1	nosp	not specified		*p*	not specified	
91LIC	N	238.0–324.0	eqn	2.00	99.	anal	*p*	BDCT	89BRE/LIC

62GOO/LAC origin of data is not clear
91LIC low temperature limit is below n.m.t.; undercooled liquid

Table 21.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
62GOO/LAC	298.1	1	0.50 #	0.622	5.89–2	0.31	−5.89–2	−1
91LIC	238.0–324.4	10	2.00	0.297	1.15–1	0.59	9.63–2	9

Table 21.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	11	11	0.376	1.23−1	0.64	8.22−2	8

Temp. range K	A_1	A_2	Level of uncertainty
238.0–324.4	1.40138+1	1.67429	V

Name: Hexadecafluoroheptane
Formula: C_7F_{16}

CAS-RN: 335-57-9
Group No.: 21-022
Molar Mass: 388.05

Table 21.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
51OLI/GRI1	221.9–310.0	10 S	0.20	99.94	melpt	sat	BSAO	43RUE/HUF
57YAR/KAY	295.0–345.0	eqn	1.10	not specified		p	BSIO	75PED/KAY
97STE/CHI2	300.0–470.0	10	1.00	99.97	chrom	sat	BDHT	89KNI/ARC

Table 21.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
51OLI/GRI1	221.9–310.0	10	0.20	0.228	2.18–2	0.05	−1.71–3	−1
97STE/CHI2	300.0–470.0	10	1.00	2.095	1.62	2.10	1.31–1	2
Rejected data								
57YAR/KAY	(7.18−1,1.42,−7.05−1,−9)							

Table 21.22.3. Parameters of cubic spline polynomials

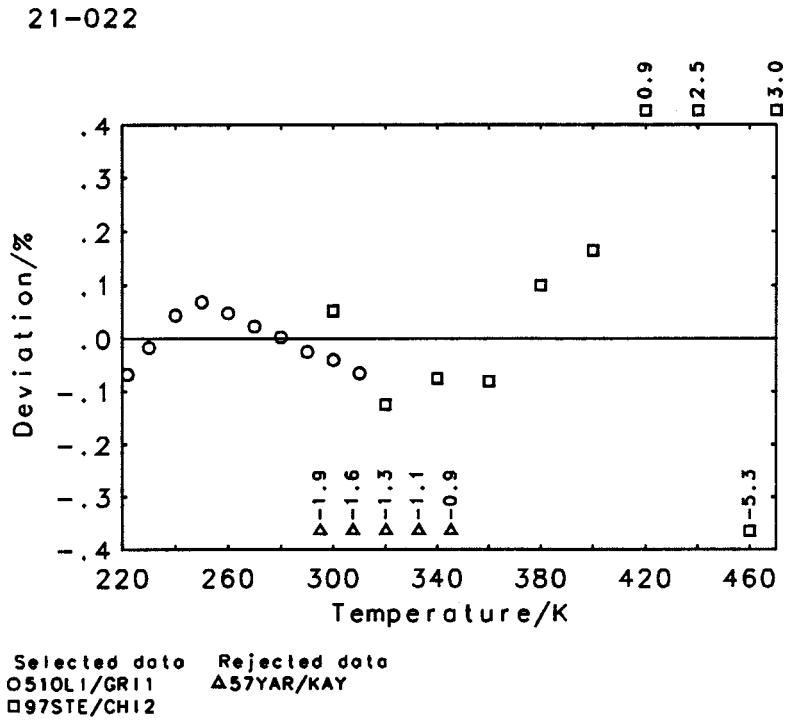
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	29	20	1.720	1.33	1.71	6.48–2	1
sat	29	20	1.049	7.22–1	1.04	3.25–2	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
221.9–430.0	2.87965+1	8.66306	−8.49044−1	1.23279−1	III
430.0–470.0	−4.10255+4	2.86512+4	−6.66190+3	5.16484+2	V
221.9–430.0	3.02751+1	6.80646	−8.15833−2	1.88636−2	III
430.0–470.0	−2.44345+4	1.70753+4	−3.96949+3	3.07725+2	V

Table 21.22.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	29	20	0.288	1.46–1	0.25	1.84–2	5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
221.9–470.0	474.80	−2.70258	3.50776−1	2.43069+1	5.27572+1	−3.16186+1	7.04356	IV



Name: Difluoromethane
Formula: CH_2F_2

CAS-RN: 75-10-5
Group No.: 21-034
Molar Mass: 52.02

Table 21.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96LUD/MAG	141.2–342.2	101	0.70	99.94	anal	sat	BSAO	61GOO

Table 21.34.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	101	101	0.486	5.46−2	0.34	4.47−4	−3
sat	101	101	0.373	3.61−2	0.26	2.07−4	5

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
141.2–260.0	1.07387+1	2.47424−1	−1.13523	3.87077−1	IV
260.0–320.0	−1.40100+2	1.74292+2	−6.80755+1	8.96917	IV
320.0–342.2	−1.83313+4	1.72286+4	−5.39754+3	5.64122+2	IV
141.2–260.0	1.10069+1	−3.08467−1	−7.62033−1	3.05663−1	IV
260.0–320.0	−8.36697+1	1.08934+2	−4.27783+1	5.69236	IV
320.0–342.2	−1.08289+4	1.01825+4	−3.19078+3	3.33609+2	IV

Table 21.34.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	101	92	0.438	3.31−2	0.31	2.86−4	−4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
150.0–342.2	351.35	−2.54682	2.68218−1	8.09230	6.53929	−2.15841+1	1.21412+1	IV

Name: Pentafluoroethane
Formula: C_2HF_5

CAS-RN: 354-33-6
Group No.: 21-035
Molar Mass: 120.02

Table 21.35.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93DU/SUV3	N	187.1–225.0	11 S	nosp	not specified		p	not specified	
96LUD/MAG		175.9–278.0	93	0.70	99.736	anal	sat	BSAO	61GOO

93DU/SUV3 table is based on experimental data from the database at the National Institute of Standards and Technology (NIST)

Table 21.35.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93DU/SUV3	187.1–225.0	11	1.00 #	0.629	9.98−2	0.63	4.03−2	5
96LUD/MAG	175.9–278.0	93	0.70	0.356	3.95−2	0.25	−2.06−3	−14

Table 21.35.3. Parameters of regression polynomial

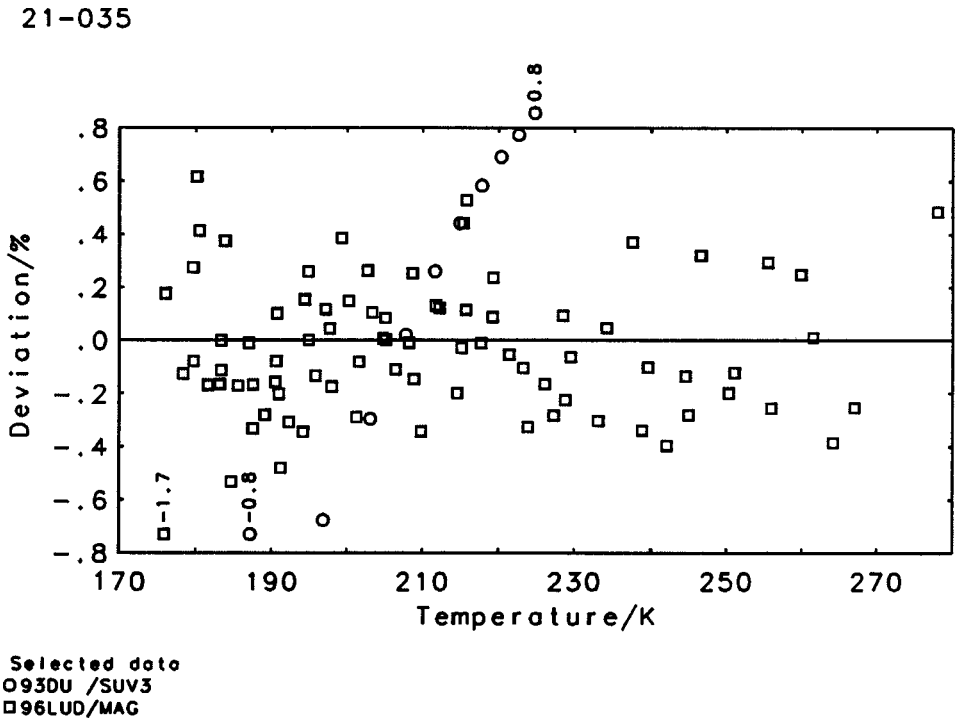
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	104	104	0.402	5.05−2	0.32	2.42−3	−9
sat	104	104	0.395	4.95−2	0.31	2.33−3	−8

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
175.9–278.0	3.93992	1.42448+1	−6.75695	1.25822	III
175.9–278.0	6.84907	9.78813	−4.46906	8.64196−1	III

Table 21.35.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	104	104	0.393	4.84−2	0.31	1.96−3	−7

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
175.9–278.0	339.40	−1.67282	3.51224−1	1.19475+1	1.99185	III



Name: 1,1,1,2-Tetrafluoroethane
Formula: $C_2H_2F_4$

CAS-RN: 811-97-2
Group No.: 21-036
Molar Mass: 102.03

Table 21.36.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92DU/SUV	N	174.1–247.1	26 S	nosp	not specified		*p*	not specified	
92DU/SUV	in original paper all data in the step 1 K								

Table 21.36.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	26	26	0.031	4.44–3	0.03	2.20–6	4
sat	26	26	0.032	4.65–3	0.03	2.27–6	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
174.2–200.0	1.27436+2	−1.72216+2	8.63585+1	−1.42523+1	IV
200.0–247.1	1.57516+1	−4.68922	2.59533	−2.91742−1	IV
174.2–200.0	1.29611+2	−1.75659+2	8.81717+1	−1.45698+1	IV
200.0–247.1	1.54984+1	−4.49011	2.58714	−3.05680−1	IV

Table 21.36.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	26	21	0.159	2.31–2	0.16	6.24–5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
179.1–247.1	374.25	−8.13281−1	1.13697	1.13069+1	1.45435−1	IV

Name: 1,1-Difluoroethane
Formula: $C_2H_4F_2$

CAS-RN: 75-37-6
Group No.: 21-037
Molar Mass: 66.05

Table 21.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98MAG	162.6–314.9	66	0.70	99.962	chrom	sat	BSAO	61GOO

Table 21.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	66	66	0.198	1.85–2	0.14	5.27–5	−4
sat	66	66	0.186	1.73–2	0.13	4.31–5	−2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
162.6–314.9	9.75145	3.41476	−2.03230	4.72437−1	IV
162.6–314.9	1.12439+1	1.19775	−9.41433−1	2.94346−1	IV

Table 21.37.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	66	66	0.430	4.00–2	0.30	2.04–4	5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
162.6–314.9	386.40	−4.45041−1	7.59697−1	1.03207+1	6.51777−2	IV

Name: 1,1,1,2,2,3,3-Heptafluoropropane
Formula: C_3HF_7

CAS-RN: 2252-84-8
Group No.: 21-038
Molar Mass: 170.03

Table 21.38.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.254	3.00	not specified		p	BDHT	92HWA/DES

Name: 1,1,1,2,3,3,3-Heptafluoropropane
Formula: C_3HF_7

CAS-RN: 431-89-0
Group No.: 21-039
Molar Mass: 170.03

Table 21.39.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.258	3.00	not specified		p	BDHT	92HWA/DES

Name: 1,1,1,2,2,3-Hexafluoropropane
Formula: $C_3H_2F_6$

CAS-RN: 677-56-5
Group No.: 21-040
Molar Mass: 152.04

Table 21.40.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.426	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,1,2,3,3-Hexafluoropropane
Formula: $C_3H_2F_6$

CAS-RN: 431-63-0
Group No.: 21-041
Molar Mass: 152.04

Table 21.41.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.304	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,1,3,3,3-Hexafluoropropane
Formula: $C_3H_2F_6$

CAS-RN: 690-39-1
Group No.: 21-042
Molar Mass: 152.04

Table 21.42.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.371	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,1,2,2-Pentafluoropropane
Formula: $C_3H_3F_5$

CAS-RN: 1814-88-6
Group No.: 21-043
Molar Mass: 134.05

Table 21.43.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.457	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,1,3,3-Pentafluoropropane
Formula: $C_3H_3F_5$

CAS-RN: 460-73-1
Group No.: 21-044
Molar Mass: 134.05

Table 21.44.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.422	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,2,2,3-Pentafluoropropane
Formula: $C_3H_3F_5$

CAS-RN: 679-86-7
Group No.: 21-045
Molar Mass: 134.05

Table 21.45.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.454	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,2,2-Tetrafluoropropane
Formula: $C_3H_4F_4$

CAS-RN: 40723-63-5
Group No.: 21-046
Molar Mass: 116.06

Table 21.46.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.590	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,1,2,2,3,3,4,4-Nonafluorobutane
Formula: C_4HF_9

CAS-RN: 375-17-7
Group No.: 21-047
Molar Mass: 220.04

Table 21.47.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.223	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,1,2,2,3,4,4-Octafluorobutane
Formula: $C_4H_2F_8$

CAS-RN: 662-35-1
Group No.: 21-048
Molar Mass: 202.05

Table 21.48.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.342	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,2,2,3,3,4,4-Octafluorobutane
Formula: $C_4H_2F_8$

CAS-RN: 377-36-6
Group No.: 21-049
Molar Mass: 202.05

Table 21.49.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.333	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,1,2,2,3,3-Heptafluorobutane
Formula: $C_4H_3F_7$

CAS-RN: 662-00-0
Group No.: 21-050
Molar Mass: 184.06

Table 21.50.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.383	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1,1,1,2,3,4,5,5,5-Nonafluoro-4-(trifluoromethyl)-2-pentene
Formula: C_6F_{12}

CAS-RN: 2070-70-4
Group No.: 21-051
Molar Mass: 300.05

Table 21.51.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98MUS/NAZ	293.1–313.1	2	1.50	99.	anal	*p*	BDIO	96MUS

Table 21.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
293.1–313.1	1.87886+1	6.13480	V

Name: Hexacosafluorododecane
Formula: $C_{12}F_{26}$

CAS-RN: 307-59-5
Group No.: 21-052
Molar Mass: 638.09

Table 21.52.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94JIN/BOL	370.0–380.0	2	5.00	98.0	anal	*p*	BDHT	90JIN/WUN

Table 21.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
370.0–380.0	7.06954+1	6.49476	VI

Name: Triacontafluorotetradecane
Formula: $C_{14}F_{30}$

CAS-RN: 307-62-0
Group No.: 21-053
Molar Mass: 738.11

Table 21.53.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94JIN/BOL	400.0–410.0	2	5.00	98.0	anal	*p*	BDHT	90JIN/WUN

Table 21.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
400.0–410.0	9.78289+1	3.36762	VI

Name: Tetratriacontafluorohexadecane
Formula: $C_{16}F_{34}$

CAS-RN: 355-49-7
Group No.: 21-054
Molar Mass: 838.12

Table 21.54.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94JIN/BOL	420.0–440.0	3	5.00	98.0	anal	*p*	BDHT	90JIN/WUN

Table 21.54.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	3	0.051	3.24–1	0.25	5.44–4	1

Temp. range K	A_1	A_2	Level of uncertainty
420.0–440.0	1.06617+2	4.92081	VI

Name: Dotetracontafluoroeicosane
Formula: $C_{20}F_{42}$

CAS-RN: 37589-57-4
Group No.: 21-055
Molar Mass: 1038.15

Table 21.55.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94JIN/BOL	460.0–470.0	2	5.00	98.0	anal	*p*	BDHT	90JIN/WUN

Table 21.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
460.0–470.0	1.11431+2	1.16664+1	VI

Name: Pentacontafluorotetracosane
Formula: $C_{24}F_{50}$

CAS-RN: 1766-41-2
Group No.: 21-056
Molar Mass: 1238.18

Table 21.56.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94JIN/BOL	480.0–500.0	3	5.00	98.0	anal	*p*	BDHT	90JIN/WUN

Table 21.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	3	0.026	2.55–1	0.13	2.24–4	−1

Temp. range K	A_1	A_2	Level of uncertainty
480.0–500.0	1.38198+2	1.19195+1	VI

Name: Tetrachloromethane
Formula: CCl_4

CAS-RN: 56-23-5
Group No.: 22-001
Molar Mass: 153.82

Table 22.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
12SCH2		293.1–323.1	3	nosp	not specified		*p*	BSIO	12SCH1
22LAT		253.8–290.0	3	2.00	not specified		*p*	BSIO	20GIB/LAT
24WIL/DAN		303.0–331.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
25WIL/DAN		293.1–333.1	5 S	nosp	not specified		*p*	BSAO	24WIL/DAN
33KOL/UDO	N	288.3	1	nosp	not specified		*p*	BSIT	34KOL/UDO
36LOR/BLA		260.0–330.0	8 S	1.50	not specified		*p*	DSIO	26AND/LYN
37STU		260.0–320.0	7 S	nosp	not specified		*p*	BDHO	37STU
37VOL		298.1	1	nosp	not specified		*p*	BSIO	37VOL
39PHI		301.1	1	nosp	not specified		*p*	BSIO	49WEI
41ZHD		278.6–319.2	3	nosp	not specified		*p*	BSIT	34KOL/UDO
44HIC/HOO		253.8–298.5	13	nosp	99.98	melpt	*p*	BSIO	38HIC
48KUR		299.1	1	nosp	not specified		avg	DSIO	47KUR
49TSC/RIC3		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
55STA/TUP		295.9–338.8	7	1.00	not specified		*p*	BSAO	55STA/TUP
57HAR/MOE		254.4–303.3	6	0.50	not specified		*p*	BSIO	57HAR/MOE
67GRA		308.1–338.1	7	1.00	not specified		*p*	BSIO	67GRA
67RAS/GAN		293.1–333.1	3 S	0.50	not specified		*p*	BSAO	67RAS/GAN
71DES/BHA		298.1–318.1	3 S	nosp	not specified		*p*	BSIO	58MUR/VAN
71VAN		255.0–300.0	10 S	nosp	99.97	chrom	sat	BSAO	72VAN
72ARE/VAN		252.6–256.1	3	nosp	99.97	melpt	*p*	BSAO	72VAN
72REC/SAD		298.1–298.1	2	0.30	not specified		*p*	BSIO	70REC
73SUB/RAJ		298.1–323.1	3	0.30	not specified		*p*	BSIO	64MOE/THO
74WIL/ZET		273.1–323.1	6	nosp	not specified		*p*	BSAO	64ARN1
75GRO/BEN		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED

Table 22.1.1. Experimental heat capacities—Continued

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
76FOR/BEN1		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
76FOR/BEN2		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
78GRO/WIL		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
79GRO/HAM		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
79WIL/FAR		298.1	1	0.30	99.5	chrom	*p*	FSIT	71PIC/LED
81ATA/ELS		293.1	1	2.50	not specified		*p*	BDHO	81ATA/ELS
82TAN		293.1–303.1	3	nosp	99.99	chrom	*p*	FSIT	71PIC/LED
85NKI/CHA		298.0	1	0.30	not specified		*p*	FSIT	71PIC/LED
89LAI/ROD		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
89PET/PES1		258.1–318.1	4	nosp	not specified		*p*	BSAO	83KUK/KOR
93PES/PET	N	298.1	1	0.10	not specified		*p*	BSAO	83KUK/KOR
93SHE		298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

33KOL/UDO same datum in 34KOL/UDO
93PES/PET water content below 0.01%

Name: Trichloromethane
Formula: $CHCl_3$

CAS-RN: 67-66-3
Group No.: 22-002
Molar Mass: 119.38

Table 22.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
12SCH1		223.1–328.1	9	nosp	not specified		*p*	BSIO	12SCH1
21TRE		295.5–321.8	7	nosp	not specified		*p*	BSIO	49WEI
24WIL/DAN		295.0–318.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
25WIL/DAN		293.1–323.1	4 S	nosp	not specified		*p*	BSAO	24WIL/DAN
39PHI		303.5	1	nosp	not specified		*p*	BSIO	49WEI
47SKU		293.1	1	0.30	not specified		*p*	BSAO	47SKU
48KUR		252.9–305.8	4	nosp	not specified		avg	DSIO	47KUR
49TSC/RIC3		293.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
55STA/TUP		284.0–329.0	11	1.00	not specified		*p*	BSAO	55STA/TUP
57HAR/MOE		245.9–303.2	8	0.50	not specified		*p*	BSIO	57HAR/MOE
67RAS/GAN		293.1–333.1	3 S	0.50	not specified		*p*	BSAO	67RAS/GAN
85HEP/KOO		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
86ALP/PES	N	258.1–318.1	4	0.20	not specified		*p*	BSAO	83KUK/KOR
87GRO/ROU		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
89BAR/KOO1		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
89BAR/KOO2		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
89ING		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
90YAM/OGA		298.1	1	nosp	99.97	chrom	*p*	FSIO	85OGA/MUR
91GRO/ROU		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
93GRO/ROU		298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED
93SHE		298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU
94GRO/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
95FEN/DOH		298.1	1	nosp	99.99	anal	*p*	FSIT	71PIC/LED
97CON/GIA		298.1	1	nosp	not specified		*p*	FSIT	88CON/GIA

86ALP/PES same data in 89PET/PES and 90ALP/PES

Name: 1,2-Dichloroethane
Formula: $C_2H_4Cl_2$

CAS-RN: 107-06-2
Group No.: 22-018
Molar Mass: 98.96

Table 22.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
12SCH1		293.1–323.1	3	nosp	not specified		*p*	BSIO	12SCH1
39RAI	N	240.0–322.0	15	2.00	99.96	melpt	*p*	BDHO	37STU
40PIT1		238.7–307.5	6	0.20	99.942	melpt	*p*	BSIO	28LAT/GRE
48KUR		270.5–322.1	4	nosp	not specified		avg	DSIO	47KUR
48TSC5		294.1	1	nosp	not specified		*p*	BSIO	48TSC1
48TSC6		294.1	1	nosp	not specified		*p*	BSIO	48TSC1
49TSC/RIC3		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
51SIE/CRU	N	293.1	1	nosp	not specified		*p*	not specified	
55RUI2		280.8–323.7	4	nosp	not specified		*p*	BSIO	55RUI1
55STA/TUP		284.1–348.0	14	1.00	not specified		*p*	BSAO	55STA/TUP
67RAS/GAN		293.1–353.1	4 S	0.50	not specified		*p*	BSAO	67RAS/GAN
69WIL/SCH		293.1–313.1	3	0.40	not specified		*p*	BDAO	65FIN/GRU
77WIL/GRO		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
79WIL/FAR		298.1	1	0.30	99.5	melpt	*p*	FSIT	71PIC/LED
79WIL/GRO		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
85LAI/ROU		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
89PRA/RAJ		318.1–333.1	4	3.00	not specified		*p*	BDHT	89PRA/RAJ
93HAL		298.1	1	0.15	99.9	chrom	*p*	DDCT	74SUU/WAD
93SHE		308.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

39RAI data from a graph only
51SIE/CRU heat of mixing calorimeter used

Name: 1,2-Dichloropropane
Formula: $C_3H_6Cl_2$

CAS-RN: 78-87-5
Group No.: 22-023
Molar Mass: 112.99

Table 22.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
48KUR	305.9–359.3	3	nosp	not specified		avg	DSIO	47KUR
97STE/CHI2	300.0–570.0	15	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 22.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
97STE/CHI2	300.0–570.0	15	1.00	1.358	4.86–1	1.36	1.94–2	−1
Rejected data								
48KUR	(5.36–1,2.62,2.62–1,1)							

Table 22.23.3. Parameters of cubic spline polynomials

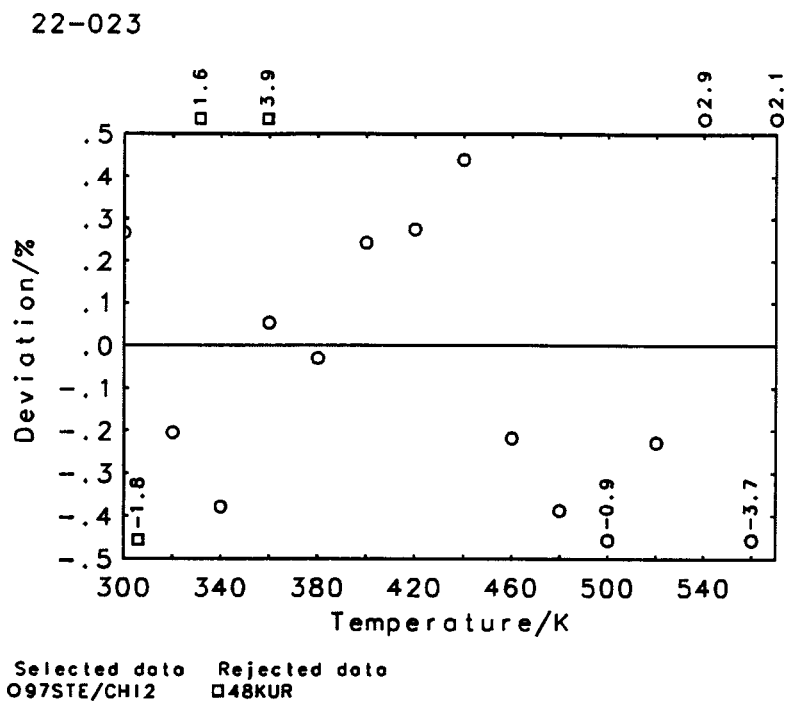
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	18	15	1.664	5.95−1	1.66	1.94−2	−1
sat	18	15	1.055	3.22−1	1.05	6.14−3	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–530.0	−1.26141+1	2.33608+1	−5.98958	5.62495−1	IV
530.0–570.0	−4.35981+4	2.46944+4	−4.66090+3	2.93324+2	V
300.0–530.0	−5.21531−1	1.33025+1	−3.21591	3.08406−1	IV
530.0–570.0	−2.60666+4	1.47677+4	−2.78707+3	1.75393+2	V

Table 22.23.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	18	15	0.636	1.54−1	0.64	3.36−3	3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–570.0	578.00	−2.15476	3.04201−1	1.47650+1	3.81573	IV



Name: 1,3-Dichloropropane
Formula: $C_3H_6Cl_2$

CAS-RN: 142-28-9
Group No.: 22-024
Molar Mass: 112.99

Table 22.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93HAL	298.1	1	0.15	99.9	chrom	*p*	DDCT	74SUU/WAD
93SHE	308.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 22.24.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93HAL	298.1	1	0.15	0.000	0.00	0.00	0.00	0
93SHE	308.1	1	0.50 #	0.000	0.00	0.00	0.00	0

Table 22.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
298.1–308.1		1.24281+1	2.16488				IV

Name: 1,4-Dichlorobutane
Formula: $C_4H_8Cl_2$

CAS-RN: 110-56-5
Group No.: 22-028
Molar Mass: 127.01

Table 22.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
85LAI/WIL	298.1	1	0.30	99.5	estim	p	FSIT	71PIC/LED
93HAL	298.1	1	0.15	99.9	chrom	p	DDCT	74SUU/WAD
93SHE	308.1	1	nosp	99.9	chrom	p	DDCT	71KON/SUU

Table 22.28.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
85LAI/WIL	298.1	1	0.30	0.595	3.94–2	0.18	−3.94–2	−1
93HAL	298.1	1	0.15	0.298	9.90–3	0.04	9.90–3	1
93SHE	308.1	1	0.50 #	0.000	0.00	0.00	0.00	0

Table 22.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	3	0.665	4.06–2	0.18	−9.84–3	0
Temp. range K		A_1	A_2				Level of uncertainty
298.1–308.1		9.27439	4.30847				IV

Name: 1-Chlorobutane
Formula: C_4H_9Cl

CAS-RN: 109-69-3
Group No.: 22-029
Molar Mass: 92.57

Table 22.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
61ROU	300.9–309.0	12	nosp	not specified		*p*	BSAO	61ROU
85LAI/WIL	298.1	1	0.30	99.5	estim	*p*	FSIT	71PIC/LED
93GRO/ROU	298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Name: 2-Chloro-2-methylpropane
Formula: C_4H_9Cl

CAS-RN: 507-20-0
Group No.: 22-031
Molar Mass: 92.57

Table 22.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
50KUS/CRO	251.6–259.6	4	2.00	not specified		*p*	BDHO	50KUS/CRO
66DWO/GUI	252.4–272.7	8	2.00	99.75	melpt	*p*	BSAO	66DWO/GUI
92KAL/KOH	293.1–313.1	2	1.00	98.8	chrom	*p*	FSIT	71PIC/LED
93SHE	298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

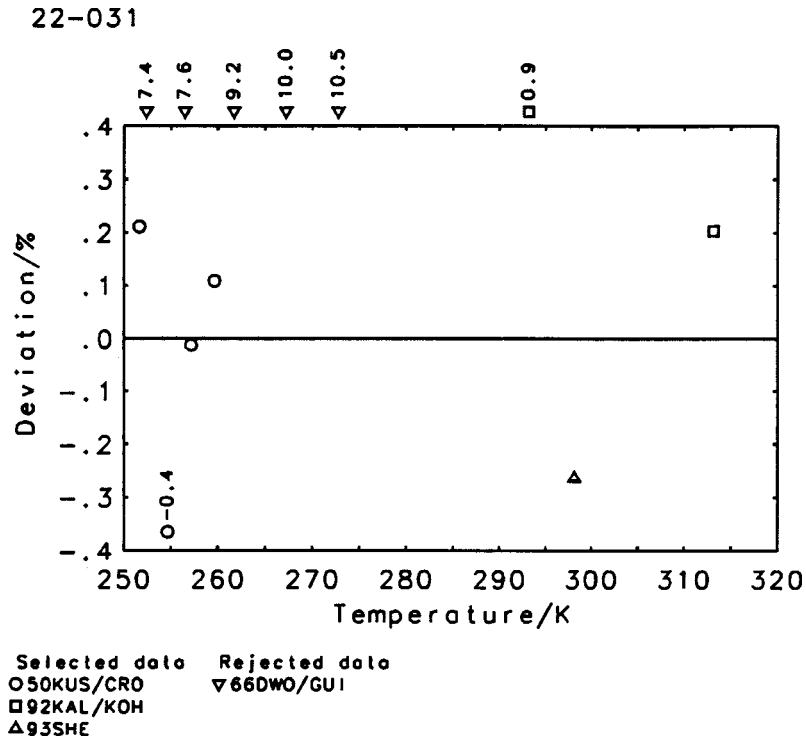
Table 22.31.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
50KUS/CRO	251.6–259.6	4	2.00	0.126	4.59–2	0.25	−6.12–3	0
92KAL/KOH	293.1–313.1	2	1.00	0.650	1.27–1	0.65	1.08–1	2
93SHE	298.1	1	0.50 #	0.527	5.13–2	0.26	−5.13–2	−1
Rejected data								
66DWO/GUI	(1.95,9.54,1.93,8)							

Table 22.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	15	7	0.544	1.04–1	0.54	2.00–2	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
251.6–313.1	4.73508+1	−2.35849+1	4.78133	V



Name: 1,5-Dichloropentane
Formula: $C_5H_{10}Cl_2$

CAS-RN: 628-76-2
Group No.: 22-033
Molar Mass: 141.04

Table 22.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93HAL	298.1	1	0.15	99.9	chrom	*p*	DDCT	74SUU/WAD
93SHE	308.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 22.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93HAL	298.1	1	0.15	0.000	0.00	0.00	0.00	0
93SHE	308.1	1	0.50 #	0.000	0.00	0.00	0.00	0

Table 22.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.56254+1	3.36761	IV

Name: 1,2,4-Trichlorobenzene
Formula: $C_6H_3Cl_3$

CAS-RN: 120-82-1
Group No.: 22-035
Molar Mass: 181.45

Table 22.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
69WIL/ROT	293.1–303.1	2	0.40	not specified		*p*	BDAO	65FIN/GRU
74PET/TER	298.0–469.2	15	nosp	98.	melpt	*p*	BDCT	74PET/TER
82WIL/ING	298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
86WIL/LAI	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
98ROH/SCH	303.1–323.1	2	0.50	99.87	chrom	*p*	BDCT	83ROU/ROU
99ROH/RUZ	304.4–407.1	33	1.00	99.87	chrom	sat	BDCT	91BAN/GAR

Table 22.35.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
74PET/TER	328.1–469.2	12	5.00 #	0.524	6.77–1	2.62	−3.25–2	0
82WIL/ING	298.1	1	0.30	0.162	1.14–2	0.05	1.14–2	1
86WIL/LAI	298.1	1	0.50 #	0.456	5.35–2	0.23	5.35–2	1
98ROH/SCH	303.1–323.1	2	0.50	0.790	9.39–2	0.40	9.26–2	2
99ROH/RUZ	304.4–407.1	33	1.00	0.284	6.78–2	0.28	−3.12–2	−10
Rejected data								
69WIL/ROT	(4.98–1,2.16,−4.98–1,−1)							

Table 22.35.3. Parameters of regression polynomial

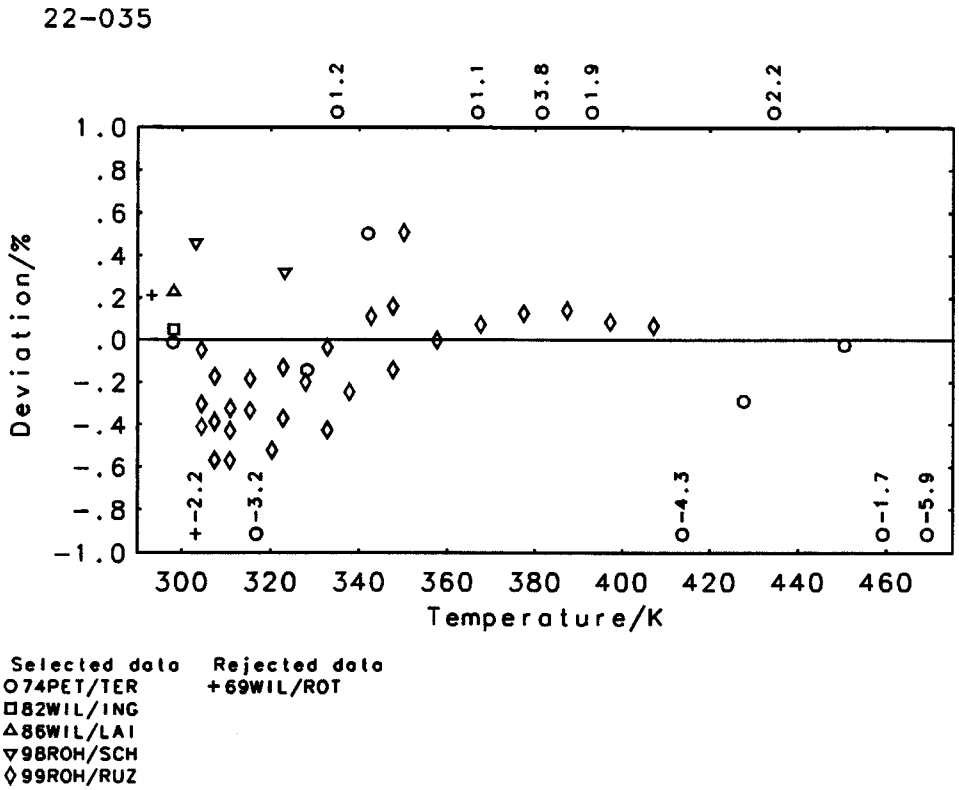
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	54	49	0.398	3.47–1	1.35	−2.38–2	−6

Temp. range K	A_1	A_2	Level of uncertainty
298.1–469.2	1.64160+1	2.33826	V

Table 22.35.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	54	49	1.067	3.13–1	1.22	4.62–2	3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
298.1–469.2	734.90	8.63520+1	1.39289+1	−9.73378	1.33835+2	V



Name: 1,2-Dichlorobenzene
Formula: $C_6H_4Cl_2$

CAS-RN: 95-50-1
Group No.: 22-036
Molar Mass: 147.00

Table 22.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
18NAR	291.1–326.1	4 S	nosp	not specified		avg	DSIO	18NAR
98ROH/SCH	263.1–323.1	4	0.50	99.98	chrom	*p*	BDCT	83ROU/ROU
99ROH/RUZ	307.7–377.2	16	1.00	99.98	chrom	sat	BDCT	91BAN/GAR

Table 22.36.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
98ROH/SCH	263.1–323.1	4	0.50	0.426	4.40–2	0.21	1.52–2	2
99ROH/RUZ	307.7–377.2	16	1.00	0.116	2.45–2	0.12	−1.50–2	−11
			Rejected data					
18NAR	(1.22–1,0.59,−1.07–1,−4)							

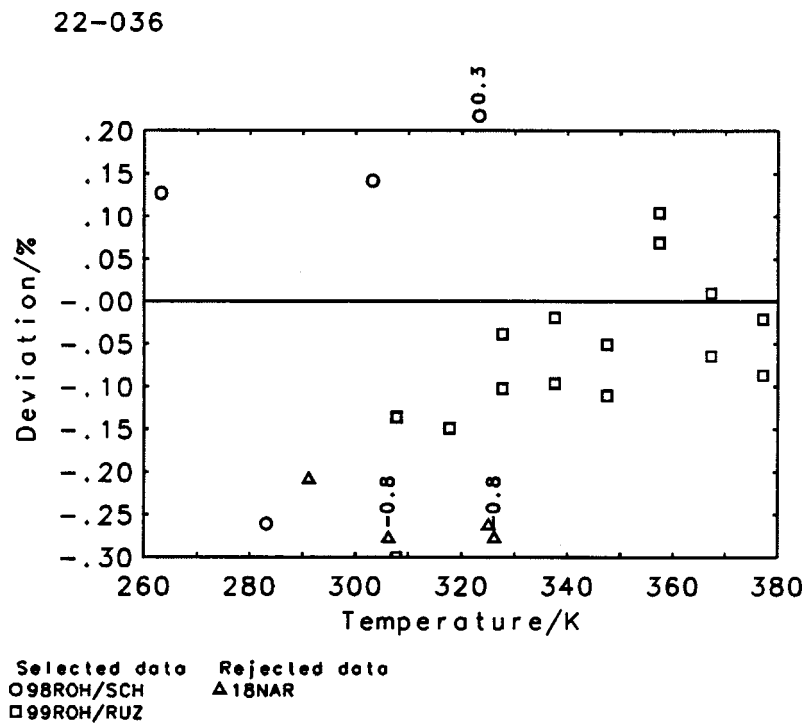
Table 22.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	24	20	0.235	3.20–2	0.15	−8.94–3	−9
Temp. range K		A_1	A_2	A_3			Level of uncertainty
263.1–377.2		1.71023+1	−1.25686−1	4.33991−1			IV

Table 22.36.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	24	20	0.252	3.18−2	0.15	1.29−3	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
263.1–377.2	698.80	−4.75784	1.98491	1.32541+1	2.85114	IV



Name: 1,3-Dichlorobenzene
Formula: $C_6H_4Cl_2$

CAS-RN: 541-73-1
Group No.: 22-037
Molar Mass: 147.00

Table 22.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
18NAR	253.9–327.5	6 S	nosp	not specified		avg	DSIO	18NAR
98ROH/SCH	263.1–323.1	4	0.50	99.55	chrom	*p*	BDCT	83ROU/ROU
99ROH/RUZ	308.0–377.6	24	1.00	99.55	chrom	sat	BDCT	91BAN/GAR

Table 22.37.2. Correlated heat capacities

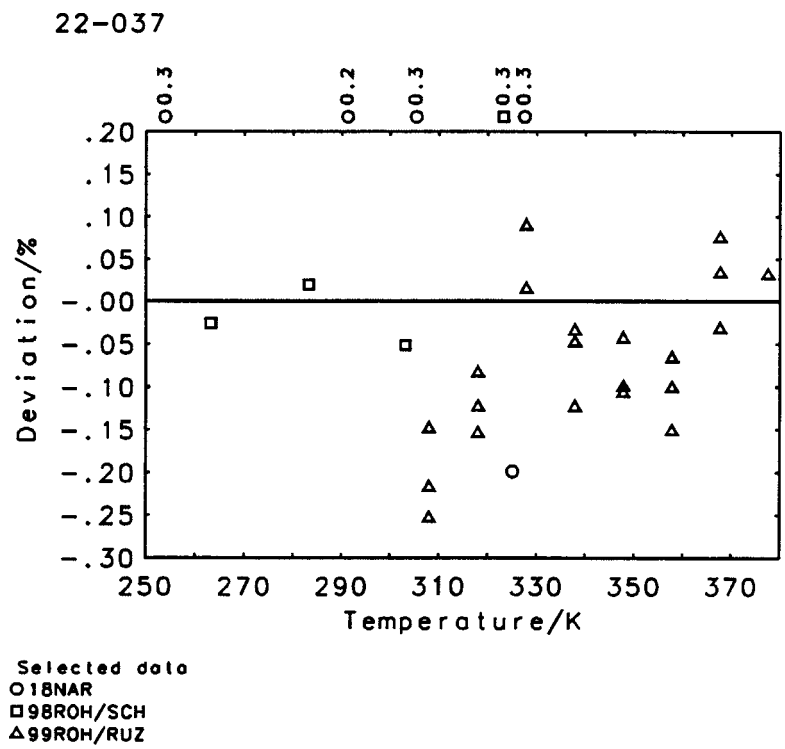
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
18NAR	253.9–327.5	6	2.00 #	0.144	5.93−2	0.29	4.44−2	4
98ROH/SCH	263.1–323.1	4	0.50	0.323	3.42−2	0.16	1.39−2	0
99ROH/RUZ	308.0–377.6	24	1.00	0.110	2.33−2	0.11	−1.19−2	−8

Table 22.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	34	34	0.167	3.60–2	0.17	1.09–3	−4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
253.9–377.6		3.62553+1	−1.81015+1	5.97816	−5.65233−1		IV

Table 22.37.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	34	34	0.217	4.63–2	0.23	5.30–3	6
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
253.9–377.6	682.20	−4.07122	2.38356	1.31488+1	1.73845		IV



Name: 1,4-Dichlorobenzene
Formula: $C_6H_4Cl_2$

CAS-RN: 106-46-7
Group No.: 22-038
Molar Mass: 147.00

Table 22.38.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	334.1	1	nosp	not specified		avg	DSIO	*94BRU
18NAR	N	349.1	1	nosp	not specified		avg	DSIO	18NAR
76DWO/FIG		328.2–329.3	2	nosp	99.93	melpt	sat	BSAO	76DWO/FIG
99ROH/RUZ		332.8–397.3	24	1.00	100.0	chrom	sat	BDCT	91BAN/GAR

*94BRU average value in temperature range 332–346 K
18NAR average value in temperature range 326–372 K

Table 22.38.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
18NAR	349.1	1	2.00 #	0.189	8.34–2	0.38	8.34–2	1
99ROH/RUZ	332.8–397.3	24	1.00	0.211	4.66–2	0.21	−6.71–4	4
Rejected data								
*94BRU	(1.55–1,0.72,−1.55–1,−1)							

Table 22.38.3. Parameters of regression polynomial

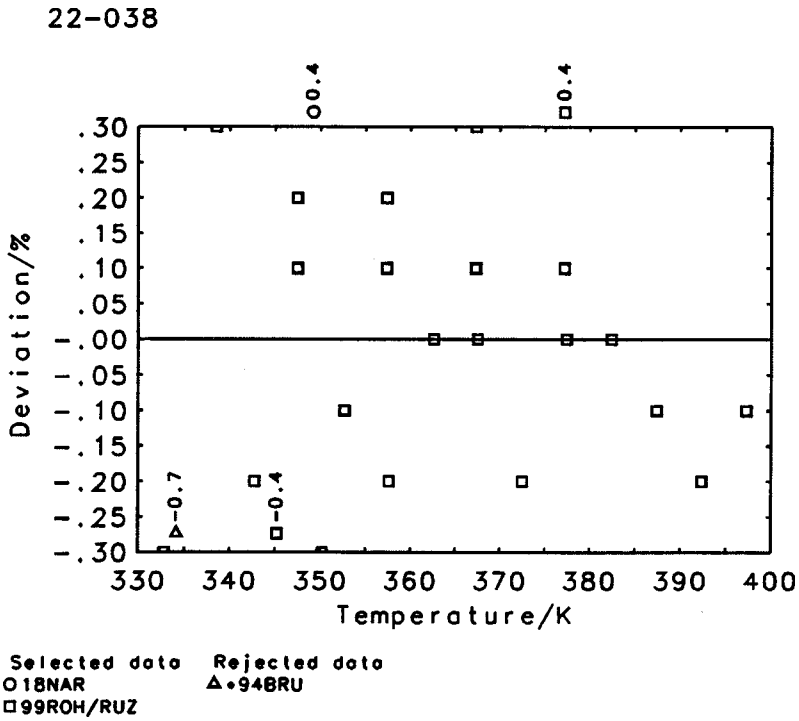
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
sat	28	25	0.219	5.07–2	0.23	2.69–3	5

Temp. range K	A_1	A_2	Level of uncertainty
332.8–397.3	1.20058+1	2.85125	IV

Table 22.38.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
sat	28	25	0.223	5.10–2	0.23	−1.77–3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
332.8–397.3	683.90	3.88216	1.39698–1	1.06891+1	2.69710+1	IV



Name: Chlorobenzene
Formula: C_6H_5Cl

CAS-RN: 108-90-7
Group No.: 22-039
Molar Mass: 112.56

Table 22.39.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		343.8–355.3	3 S	nosp	not specified		avg	DSIO	*81VON
*87SCH		308.6–332.9	6 S	nosp	not specified		avg	DSIO	*86SCH
25WIL/DAN	N	293.1–353.1	4 S	nosp	not specified		*p*	BSAO	24WIL/DAN
37STU		230.0–320.0	10 S	nosp	not specified		*p*	BDHO	37STU
39PHI		305.5	1	nosp	not specified		*p*	BSIO	49WEI
49TSC/RIC3		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
61ROU	N	296.1–318.1	2	nosp	not specified		*p*	BSAO	61ROU
71DES/BHA		298.1–318.1	3 S	nosp	not specified		*p*	BSIO	58MUR/VAN
77FOR/BEN		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
88PER/AIC		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
90RAO/RAJ		318.1–333.1	4	4.00	not specified		*p*	BDHT	89PRA/RAJ
91TAN/ADA		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
92KAL/KOH		293.1–313.1	2	1.00	99.98	chrom	*p*	FSIT	71PIC/LED
93SHE		298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU
94BEN/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
94GRO/ROU		298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED
97TAN/NAK		298.1–303.1	2	nosp	100.0	chrom	*p*	FSIT	71PIC/LED
97TAN/TOY		298.1	1	0.01	99.95	chrom	*p*	FSIT	71PIC/LED

25WIL/DAN origin of data unclear
61ROU constant value in temperature range 296–318 K obtained by the author

Table 22.39.2. Correlated heat capacities

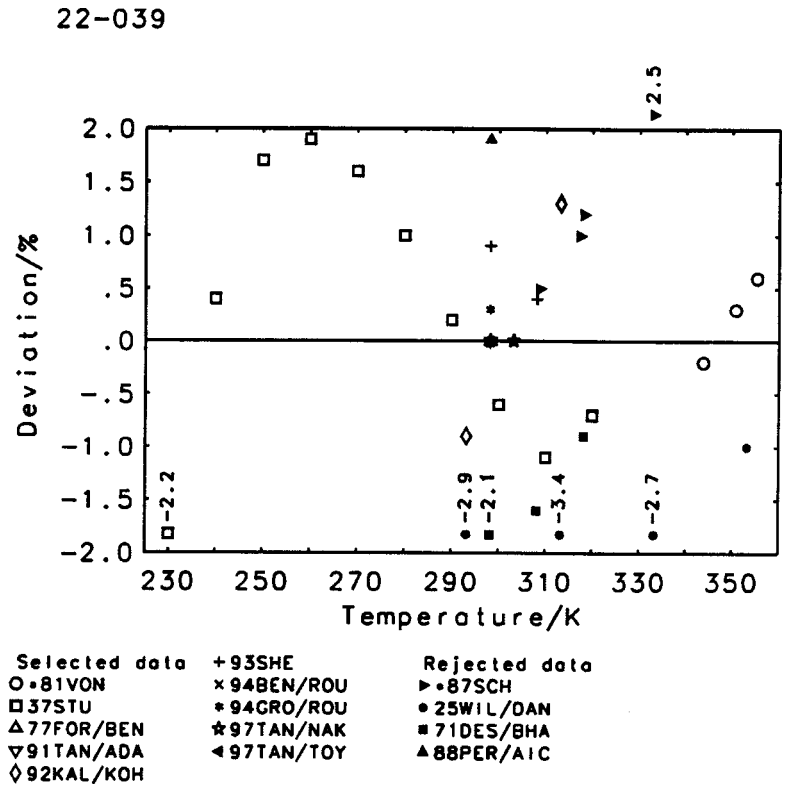
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*81VON	343.8–355.3	3	2.00 #	0.192	7.50–2	0.38	4.63–2	1
37STU	230.0–320.0	10	1.50 #	0.868	2.27–1	1.30	3.78–2	2
77FOR/BEN	298.1	1	0.50 #	0.000	9.54–6	0.00	−9.54–6	0
91TAN/ADA	298.1	1	0.50 #	0.049	4.46–3	0.02	−4.46–3	−1
92KAL/KOH	293.1–313.1	2	1.00	1.100	2.03–1	1.10	3.44–2	0
93SHE	298.1–308.1	2	0.50 #	1.327	1.22–1	0.66	1.13–1	2
94BEN/ROU	298.1	1	0.50 #	0.009	8.53–4	0.00	−8.53–4	0
94GRO/ROU	298.1	1	0.50 #	0.638	5.81–2	0.32	5.81–2	1
97TAN/NAK	298.1–303.1	2	0.50 #	0.045	4.07–3	0.02	−2.32–3	−1
97TAN/TOY	298.1	1	0.01	0.073	1.32–4	0.00	−1.32–4	0
Rejected data								
*87SCH	(3.05–1,1.58,2.60–1,6)		25WIL/DAN	(4.82–1,2.68,−4.57–1,−4)				
39PHI	(6.19–1,3.27,6.19–1,1)		49TSC/RIC3	(6.13–1,3.27,6.13–1,1)				
61ROU	(3.01–1,1.63,1.68–1,0)		71DES/BHA	(2.91–1,1.62,−2.79–1,−3)				
88PER/AIC	(3.60–1,1.95,3.60–1,1)		90RAO/RAJ	(9.19–1,4.64,8.94–1,4)				

Table 22.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	46	24	0.817	1.76–1	01.00	3.58–2	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
230.0–355.3		1.61929+1	−8.71082−1	5.10687−1			V

Table 22.39.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	46	24	1.104	1.81–1	1.05	−9.67–3	−3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
230.0–355.3	632.40	1.06698+1	8.19799	7.79719	3.47173		V



Name: 1-Chloronaphthalene
Formula: $C_{10}H_7Cl$

CAS-RN: 90-13-1
Group No.: 22-044
Molar Mass: 162.62

Table 22.44.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
81GRO/ING	298.1	1	nosp	99.0	chrom	*p*	FSIT	71PIC/LED
86WIL/LAI	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
88COS/VAN	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
94BEN/ROU	298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED

Table 22.44.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
			Selected data					
81GRO/ING	298.1	1	0.50 #	0.114	1.44−2	0.06	1.44−2	1
86WIL/LAI	298.1	1	0.50 #	0.029	3.62−3	0.01	3.62−3	1
94BEN/ROU	298.1	1	0.50 #	0.142	1.80−2	0.07	−1.80−2	−1
			Rejected data					
88COS/VAN	(1.62−1,0.64,1.62−1,1)							

Table 22.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	4	3	0.130	1.65−2	0.07	1.40−5	1
Temp. range K		A_1					Level of uncertainty
298.1−298.1		2.54074+1					III

Name: 1,1,2,3,3,3-Hexachloro-1-propene
Formula: C_3Cl_6

CAS-RN: 1888-71-7
Group No.: 22-050
Molar Mass: 248.75

Table 22.50.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI4	290.0–500.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 22.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	22	22	0.014	3.97–3	0.01	1.13–6	2
sat	22	22	0.000	6.19–7	0.00	−1.73–7	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
290.0–500.0	2.69878+1	−1.21854	3.44287−1	IV
290.0–500.0	2.67100+1	−1.06000	3.22000−1	IV

Table 22.50.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	22	22	0.072	1.99–2	0.07	2.30–5	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
290.0–500.0	680.00	−1.94837	6.20432−1	2.34905+1	1.52963	IV

Name: 1,2-Dichlorobutane
Formula: $C_4H_8Cl_2$

CAS-RN: 616-21-7
Group No.: 22-051
Molar Mass: 127.01

Table 22.51.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HE/AN	298.15	1.540	nosp	99.77	chrom	*p*	not specified	

Name: 2-Chlorobutane
Formula: C_4H_9Cl

CAS-RN: 78-86-4
Group No.: 22-052
Molar Mass: 92.57

Table 22.52.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HE/AN	298.1	1	nosp	99.87	chrom	*p*	not specified	
93SHE	298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 22.52.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93SHE	298.1	1	0.50 #	0.000	0.00	0.00	0.00	0
Rejected data								
92HE/AN	(1.58,7.54,1.58,1)							

Table 22.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	2	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		1.93517+1					V

Name: Chlorocyclopentane
Formula: C_5H_9Cl

CAS-RN: 930-28-9
Group No.: 22-053
Molar Mass: 104.58

Table 22.53.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93DIK/KAB	181.8–300.8	36	0.40	99.92	melpt	p	BSAO	93DIK/KAB

Table 22.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	36	35	0.733	4.95–2	0.29	2.59–4	−2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
181.8–300.8		1.77891+1	−2.84843	1.01953			IV

Table 22.53.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	36	35	0.799	5.41–2	0.32	3.10–4	−2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
181.8–300.8	603.00	2.01154+1	1.37113+1	1.32642	7.37763		IV

Name: 1-Chloropentane
Formula: $C_5H_{11}Cl$

CAS-RN: 543-59-9
Group No.: 22-054
Molar Mass: 106.60

Table 22.54.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 22.54.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.14587+1	3.72842	IV

Name: Pentachlorobenzene
Formula: C_6HCl_5

CAS-RN: 608-93-5
Group No.: 22-055
Molar Mass: 250.34

Table 22.55.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99ROH/RUZ	367.5–436.9	16	1.00	99.92	chrom	sat	BDCT	91BAN/GAR

Table 22.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	16	16	0.063	1.98–2	0.06	2.05–5	−1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
367.5–436.9	2.88437+1	−6.41595−1	3.00225−1	IV

Table 22.55.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	16	16	0.064	2.00–2	0.06	2.10–5	−2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
367.5–436.9	790.00	−3.15305	1.38377	2.51433+1	1.79613	IV

Name: 1,2,3-Trichlorobenzene
Formula: $C_6H_3Cl_3$

CAS-RN: 87-61-6
Group No.: 22-056
Molar Mass: 181.45

Table 22.56.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99ROH/RUZ	332.5–402.4	21	1.00	100.0	chrom	sat	BDCT	91BAN/GAR

Table 22.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	21	21	0.188	4.72–2	0.19	1.58–4	−5

Temp. range K	A_1	A_2	Level of uncertainty
332.5–402.4	1.69821+1	2.21416	IV

Table 22.56.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	21	21	0.192	4.82–2	0.19	1.58–4	−4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
332.5–402.4	733.00	3.27073	1.19887−1	1.59746+1	2.23079+1	V

Name: 1,3,5-Trichlorobenzene
Formula: $C_6H_3Cl_3$

CAS-RN: 108-70-3
Group No.: 22-057
Molar Mass: 181.45

Table 22.57.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99ROH/RUZ	343.1–402.1	20	1.00	100.0	chrom	sat	BDCT	91BAN/GAR

Table 22.57.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	20	20	0.128	3.15–2	0.13	7.35–5	−3

Temp. range K	A_1	A_2	Level of uncertainty
343.1–402.1	1.49911+1	2.69010	IV

Name: Chlorocyclohexane
Formula: $C_6H_{11}Cl$

CAS-RN: 542-18-7
Group No.: 22-058
Molar Mass: 118.61

Table 22.58.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94DIK/KAB	235.0–304.3	13	0.40	99.92	chrom	*p*	BSAO	93DIK/KAB
95KOB/OGU	228.9–300.9	28	0.30	99.98	chrom	sat	BSAO	93FUJ/OGU1
96TAN/TOY1	298.1	1	nosp	99.1	chrom	*p*	FSIT	71PIC/LED

Table 22.58.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94DIK/KAB	235.0–304.3	13	0.40	0.641	5.38–2	0.26	−2.67–2	−2
95KOB/OGU	228.9–300.9	28	0.30	0.236	1.50–2	0.07	6.61–3	8
96TAN/TOY1	298.1	1	0.50 #	0.332	3.59–2	0.17	3.59–2	1

Table 22.58.3. Parameters of regression polynomial

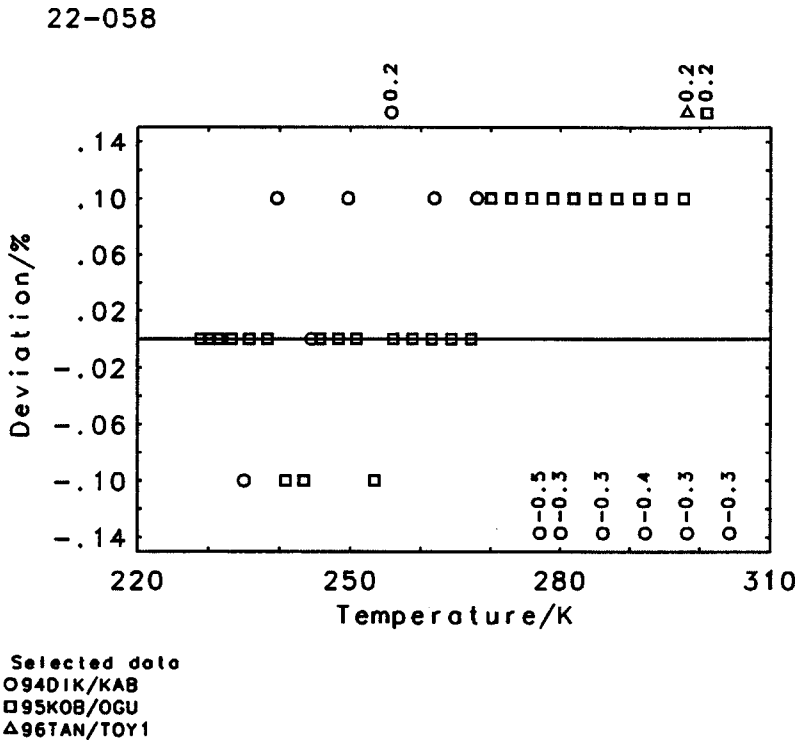
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	42	42	0.424	3.40–2	0.16	−3.01–3	7

Temp. range K	A_1	A_2	A_3	Level of uncertainty
228.9–304.3	1.68933+1	−6.35818−1	7.38105−1	II

Table 22.58.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	42	42	0.430	3.37–2	0.16	−1.78–3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
228.9–304.3	636.00	−3.07827	5.06749	9.84876	4.67478−1	III



Name: 1-Chloro-1-methylcyclopentane
Formula: $C_6H_{11}Cl$

CAS-RN: 6196-85-6
Group No.: 22-059
Molar Mass: 118.61

Table 22.59.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96KAB/BLO	189.2–306.4	34	0.40	99.94	chrom	sat	BDHT	92KAB/KOZ

Table 22.59.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	34	34	0.618	4.99–2	0.25	2.19–4	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
189.2–306.4		9.39957	1.05675+1	−4.10569	6.49380−1		III

Table 22.59.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	34	34	0.629	5.12–2	0.25	2.36–4	9
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
189.2–306.4	560.00	−8.73258–1	3.46361	1.35147+1	5.50422–2		IV

Name: 1-Chlorohexane
Formula: $C_6H_{13}Cl$

CAS-RN: 544-10-5
Group No.: 22-060
Molar Mass: 120.62

Table 22.60.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 22.60.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.13006+1	4.93114	IV

Name: 1-Chloro-1-methylcyclohexane
Formula: $C_7H_{13}Cl$

CAS-RN: 931-78-2
Group No.: 22-061
Molar Mass: 132.63

Table 22.61.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98KAB/BLO	234.5–300.0	9 S	0.40	99.93	chrom	*p*	BSAO	93DIK/KAB

Table 22.61.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	9	9	0.035	3.22–3	0.01	4.24–7	0

Temp. range K	A_1	A_2	Level of uncertainty
234.5–300.0	1.40076+1	3.44276	III

Name: 1-Chloroheptane
Formula: $C_7H_{15}Cl$

CAS-RN: 629-06-1
Group No.: 22-062
Molar Mass: 134.65

Table 22.62.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 22.62.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.33782+1	5.41221	IV

Name: 1-Chlorooctane
Formula: $C_8H_{17}Cl$

CAS-RN: 111-85-3
Group No.: 22-063
Molar Mass: 148.68

Table 22.63.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1–308.1	2	nosp	99.9	chrom	p	DDCT	71KON/SUU

Table 22.63.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.61850+1	5.65273	IV

Name: 1,1′,1″-(Chloromethylidene)trisbenzene
Formula: $C_{19}H_{15}Cl$

CAS-RN: 76-83-5
Group No.: 22-064
Molar Mass: 278.78

Table 22.64.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91NAO/SEK	276.0–412.0	eqn	nosp	not specified		p	BDHT	69PER/COM

Table 22.64.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	36	36	0.001	2.85–2	0.00	4.75–5	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
276.0–412.5	3.39595+3	1.71517+2	−5.67650+1	7.58072	IV

Name: Dibromomethane
Formula: CH_2Br_2

CAS-RN: 74-95-3
Group No.: 23-003
Molar Mass: 173.83

Table 23.3.1. Experimental heat capacities

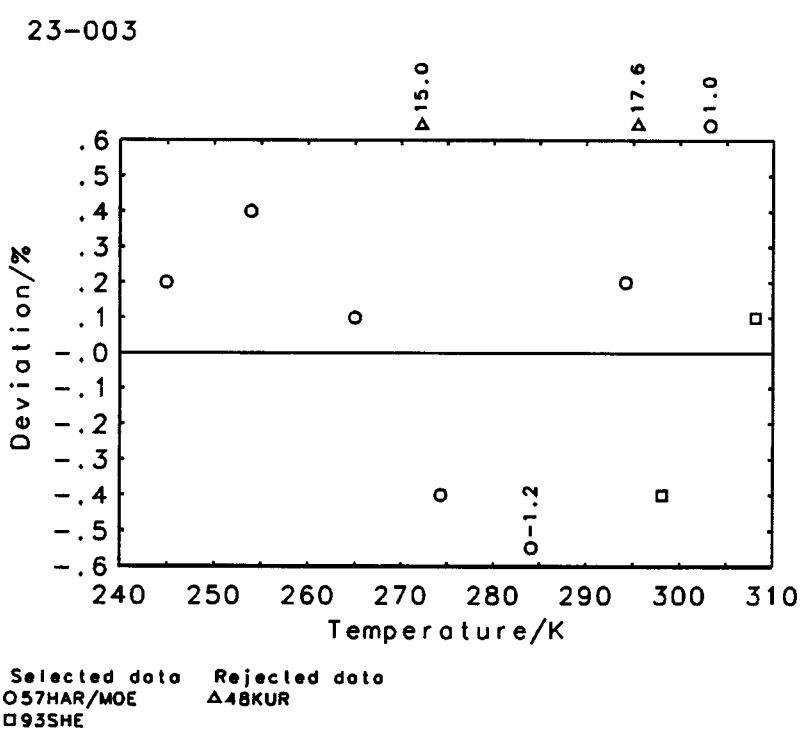
Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
48KUR	272.1–329.9	4	nosp	not specified		avg	DSIO	47KUR
57HAR/MOE	244.9–303.2	7	0.50	not specified		*p*	BSIO	57HAR/MOE
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 23.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
57HAR/MOE	244.9–303.2	7	0.50	1.243	7.80–2	0.62	4.80–3	3
93SHE	298.1–308.1	2	0.50 #	0.540	3.38–2	0.27	−1.32–2	0
Rejected data								
48KUR	(2.60,17.08,2.58,3)							

Table 23.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	13	9	1.276	8.00–2	0.64	7.95–4	3
Temp. range K		A_1	A_2				Level of uncertainty
244.9–308.1		1.26297+1	−2.18224-2				IV



Name: 1,2-Dibromoethane
Formula: $C_2H_4Br_2$

CAS-RN: 106-93-4
Group No.: 23-017
Molar Mass: 187.86

Table 23.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
33LEB/MOE		283.3–298.5	5	nosp	not specified		*p*	BSIO	33LEB/MOE
39RAI	N	283.3–321.7	9	2.00	99.92	melpt	*p*	BDHO	37STU
40PIT1		286.5–318.0	4	0.20	99.74	melpt	*p*	BSIO	28LAT/GRE
48KUR		309.1–345.7	3	nosp	not specified		avg	DSIO	47KUR
49DHO/JUN		293.1	1	nosp	not specified		*p*	BDHO	49WUY/JUN
49TSC/RIC3		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
49WUY/JUN		310.1	1	nosp	not specified		*p*	BDHO	49WUY/JUN
65FIN/GRU		300.0	1	0.40	not specified		*p*	BDAO	65FIN/GRU
69WIL/SCH		293.1–313.1	3	0.40	not specified		*p*	BDAO	65FIN/GRU
93SHE		298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

39RAI data from a graph only

Name: Bromoethane
Formula: C_2H_5Br

CAS-RN: 74-96-4
Group No.: 23-018
Molar Mass: 108.97

Table 23.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
07BAT	N	167.7–244.3	5	nosp	not specified		*p*	BSIO	07BAT
12SCH2		280.6–290.6	3	nosp	not specified		*p*	BSIO	12SCH1
48KUR		256.5–300.0	5	nosp	not specified		avg	DSIO	47KUR
49TSC/RIC3		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
93SHE		298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

07BAT same data in 08BAT

Name: 1,3-Dibromopropane
Formula: $C_3H_6Br_2$

CAS-RN: 109-64-8
Group No.: 23-022
Molar Mass: 201.89

Table 23.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
48KUR	332.3–358.3	3	nosp	not specified		avg	DSIO	47KUR
50CRO/SMY2	243.1–245.6	2	1.40	not specified		*p*	BDHO	50KUS/CRO
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 23.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
48KUR	332.3–358.4	3	5.00 #	0.226	2.34–1	1.13	−4.98–2	−1
50CRO/SMY2	243.1–245.6	2	1.40	0.201	5.26–2	0.28	8.70–3	0
93SHE	298.1–308.1	2	0.50 #	0.138	1.37–2	0.07	−2.24–4	0

Table 23.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	7	7	0.234	1.84−1	0.90	−1.89−2	−1

Temp. range K	A_1	A_2	Level of uncertainty
243.1–358.4	1.40635+1	1.89130	VI

Name: 1-Bromopropane
Formula: C_3H_7Br

CAS-RN: 106-94-5
Group No.: 23-023
Molar Mass: 122.99

Table 23.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON	305.1–323.3	3 S	nosp	not specified		avg	DSIO	*81VON
48KUR	268.1–312.9	3	nosp	not specified		avg	DSIO	47KUR
49TSC/RIC3	298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 23.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*81VON	305.1–323.3	3	3.00 #	0.494	2.36−1	1.48	−1.95−1	−3
93SHE	298.1–308.1	2	0.50 #	0.178	1.46−2	0.09	8.43−3	0
Rejected data								
48KUR	(8.69−1,5.05,8.60−1,2)		49TSC/RIC3	(3.95−1,2.38,3.95−1,1)				

Table 23.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	9	5	0.515	2.36−1	1.48	−1.13−1	−3

Temp. range K	A_1	A_2	Level of uncertainty
298.1–323.3	1.33129+1	9.65645−1	V

Name: 2-Bromopropane
Formula: C_3H_7Br

CAS-RN: 75-26-3
Group No.: 23-024
Molar Mass: 122.99

Table 23.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON	298.0–317.7	4 S	nosp	not specified		avg	DSIO	*81VON
50KUS/CRO	190.1–209.6	7	1.70	not specified		*p*	BDHO	50KUS/CRO
93SHE	298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Name: 1-Bromobutane
Formula: C_4H_9Br

CAS-RN: 109-65-9
Group No.: 23-025
Molar Mass: 137.02

Table 23.25.1. Experimental heat capacities

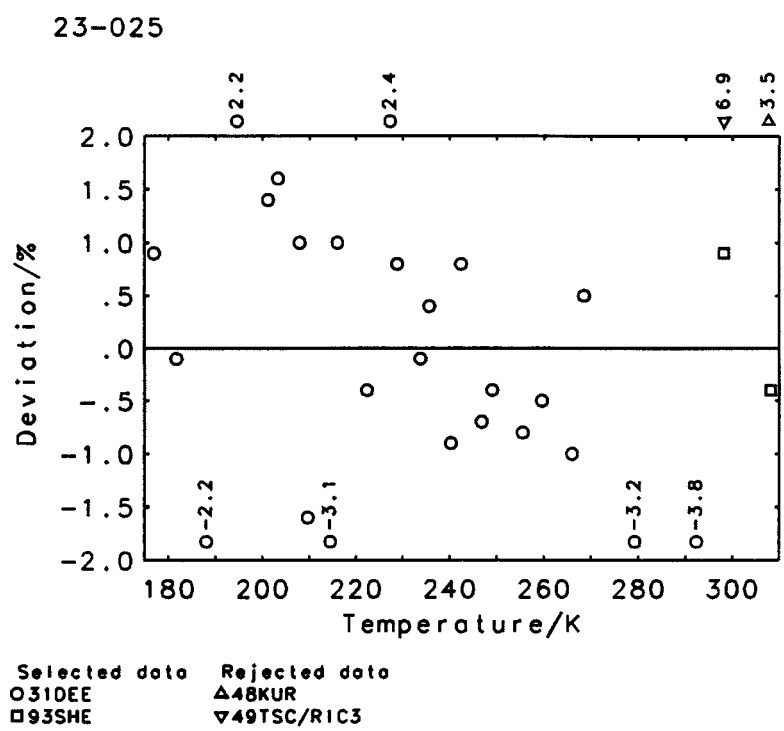
Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
31DEE	176.9–292.3	27	nosp	not specified		*p*	BDAO	31DEE
48KUR	307.6–331.1	2	nosp	not specified		avg	DSIO	47KUR
49TSC/RIC3	298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 23.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
31DEE	176.9–292.3	27	2.00 #	0.929	3.18–1	1.86	−4.22–2	−3
93SHE	298.1–308.1	2	0.50 #	1.437	1.41–1	0.72	4.77–2	0
Rejected data								
48KUR	(7.14–1,3.47,7.14–1,1)		49TSC/RIC3	(1.43,6.87,1.43,1)				

Table 23.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	32	29	1.027	3.26–1	1.90	−3.60–2	−3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
176.9–308.1		2.93689+1	−1.22106+1	2.96593			V



Name: 1-Bromo-2-methylpropane
Formula: C_4H_9Br

CAS-RN: 78-77-3
Group No.: 23-026
Molar Mass: 137.02

Table 23.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
48KUR	306.1–319.1	2	nosp	not specified		avg	DSIO	47KUR
93SHE	298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 23.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93SHE	298.1	1	0.50 #	0.000	0.00	0.00	0.00	0

Table 23.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	3	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		1.96885+1					V

Name: 2-Bromo-2-methylpropane
Formula: C_4H_9Br

CAS-RN: 507-19-7
Group No.: 23-027
Molar Mass: 137.02

Table 23.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
50KUS/CRO	259.6–265.1	3	2.00	not specified		*p*	BDHO	50KUS/CRO
93SHE	298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 23.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
50KUS/CRO	259.6–265.1	3	2.00	0.259	9.40–2	0.52	−6.04–3	−1
93SHE	298.1	1	0.50 #	0.013	1.33–3	0.01	1.33–3	0

Table 23.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	4	4	0.317	1.15–1	0.63	−4.20–3	−1
Temp. range K		A_1	A_2				Level of uncertainty
259.6–298.1		4.97215	5.01611				V

Name: 1-Bromopentane
Formula: $C_5H_{11}Br$

CAS-RN: 110-53-2
Group No.: 23-030
Molar Mass: 151.05

Table 23.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
31DEE	195.8–290.7	10	nosp	not specified		*p*	BDAO	31DEE
50KUS/CRO	190.1–206.6	6	1.50	not specified		*p*	BDHO	50KUS/CRO
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 23.30.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
31DEE	195.8–290.7	10	2.00 #	1.530	6.20–1	3.06	−4.26–1	−8
50KUS/CRO	190.1–206.6	6	1.50	1.301	4.09–1	1.95	2.45–1	0
93SHE	298.1–308.1	2	0.50 #	2.110	2.43–1	1.05	7.36–2	0

Table 23.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	18	18	1.683	5.75–1	2.81	−1.47–1	−8

Temp. range K	A_1	A_2	A_3	Level of uncertainty
190.1–308.1	4.74797+1	−2.41167+1	5.29745	V

Name: Bromobenzene
Formula: C_6H_5Br

CAS-RN: 108-86-1
Group No.: 23-033
Molar Mass: 157.01

Table 23.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		323.0–369.1	5 S	nosp	not specified		avg	DSIO	*81VON
25WIL/DAN		293.1–353.1	4 S	nosp	not specified		*p*	BSAO	24WIL/DAN
34KOL/UDO	N	302.6	1	nosp	not specified		*p*	BSIT	34KOL/UDO
37STU		250.0–320.0	8 S	nosp	not specified		*p*	BDHO	37STU
49TSC/RIC3		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
75MAS/SCO		243.3–296.4	17	nosp	99.998	melpt	sat	BSAO	45SCO/MEY
93SHE		308.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

34KOL/UDO same datum in 34KOL/UDO1

Name: 1-Bromohexane
Formula: $C_6H_{13}Br$

CAS-RN: 111-25-1
Group No.: 23-034
Molar Mass: 165.07

Table 23.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
31DEE	214.0–289.8	12	nosp	not specified		*p*	BDAO	31DEE
49TSC/RIC3	298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

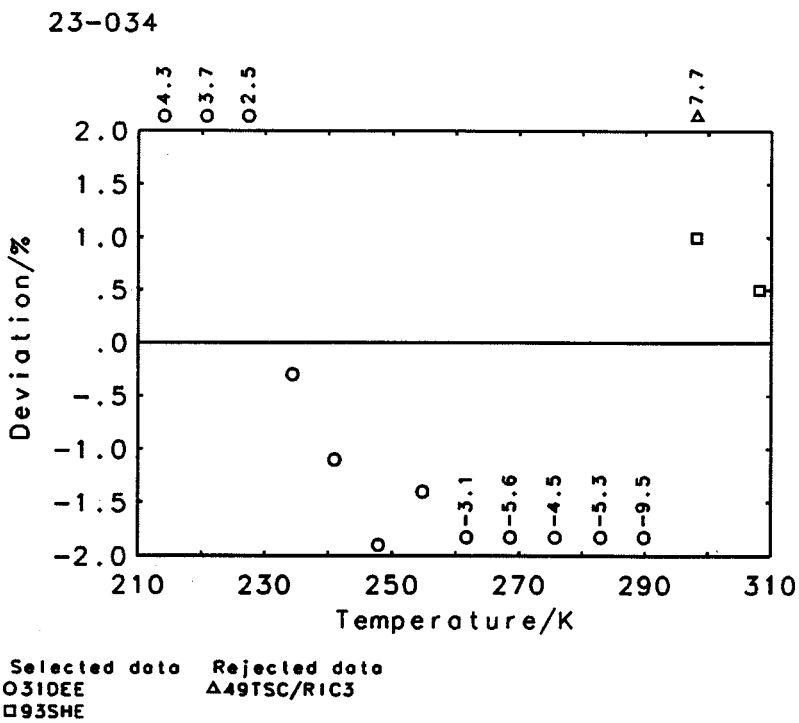
Table 23.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
31DEE	214.0–289.8	12	0.20 #	6.365	2.98–1	1.27	−2.20–2	2
93SHE	298.1–308.1	2	0.50 #	9.569	1.27	4.78	1.23	2
Rejected data								
49TSC/RIC3	(3.44,12.13,3.44,1)							

Table 23.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	15	14	2.261	1.02	4.34	−3.49–1	−4

Temp. range K	A_1	A_2	Level of uncertainty
214.0–308.1	1.06451+1	5.20103	V



Name: 1-Bromoheptane
Formula: $C_7H_{15}Br$

CAS-RN: 629-04-9
Group No.: 23-036
Molar Mass: 179.10

Table 23.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
50CRO/SMY1	222.1–231.1	4	1.00	not specified		p	BDHO	50KUS/CRO
93SHE	298.1–308.1	2	nosp	99.9	chrom	p	DDCT	71KON/SUU

Table 23.36.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
50CRO/SMY1	222.1–231.1	4	1.00	0.895	2.12–1	0.89	−2.40–2	0
93SHE	298.1–308.1	2	0.50 #	1.142	1.71–1	0.57	1.57–2	0

Table 23.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	6	6	1.205	2.44–1	0.98	−1.08–2	0

Temp. range K	A_1	A_2	Level of uncertainty
222.1–308.1	4.74984	8.34450	V

Name: 1-Bromooctane
Formula: $C_8H_{17}Br$

CAS-RN: 111-83-1
Group No.: 23-037
Molar Mass: 193.13

Table 23.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
50CRO/SMY1	222.1–234.1	3	1.00	not specified		p	BDHO	50KUS/CRO
#00BEC/AUF	295.4–360.0	14	0.20	99.95	chrom	sat	BDCT	#00BEC/AUF

Table 23.37.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
50CRO/SMY1	222.1–234.1	3	1.00	0.569	1.78–1	0.57	−6.81–2	−1
#00BEC/AUF	295.4–360.0	14	0.20	0.360	2.55–2	0.07	6.40–4	−2

Table 23.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	17	17	0.446	8.64–2	0.27	−1.15–2	−3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
222.1–360.0	3.01948+1	−1.72650	9.89185–1	III

Name: 1,4-Dibromobutane
Formula: $C_4H_8Br_2$

CAS-RN: 110-52-1
Group No.: 23-041
Molar Mass: 215.92

Table 23.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1–308.1	2	nosp	99.9	chrom	p	DDCT	71KON/SUU

Table 23.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.36726+1	3.12707	IV

Name: 1,4-Dibromobenzene
Formula: $C_6H_4Br_2$

CAS-RN: 106-37-6
Group No.: 23-042
Molar Mass: 235.91

Table 23.42.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	367.15	0.6569	nosp	not specified	avg		DSIO	*94BRU

*94BRU average value in temperature range 363–371 K

Name: Bromocyclohexane
Formula: $C_6H_{11}Br$

CAS-RN: 108-85-0
Group No.: 23-043
Molar Mass: 163.06

Table 23.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU
95KOB/OGU	218.9–303.2	43	0.30	99.91	melpt	sat	BSAO	93FUJ/OGU1

Table 23.43.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93SHE	298.1	1	0.50 #	0.686	7.51–2	0.34	−7.51–2	−1
95KOB/OGU	218.9–303.2	43	0.30	0.091	5.63–3	0.03	6.35–4	3

Table 23.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	44	44	0.144	1.32–2	0.06	−1.09–3	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
218.9–303.2	2.31423+1	−6.54621	2.74642	−2.28725–1	III

Name: Diiodomethane
Formula: CH_2I_2

CAS-RN: 75-11-6
Group No.: 24-001
Molar Mass: 267.84

Table 24.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
48KUR		307.1–363.0	3	nosp	not specified		avg	DSIO	47KUR
93CAR/LAY	N	298.1	1	nosp	not specified		*p*	not specified	
93SHE		298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

93CAR/LAY origin of data is not clear

Table 24.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93SHE	298.1–308.1	2	0.50 #	0.000	0.00	0.00	0.00	0
Rejected data								
48KUR	(2.55,15.72,2.55,1)		93CAR/LAY	(2.53,15.70,2.53,1)				

Table 24.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	6	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.06979+1	9.62170−1	IV

Name: Iodomethane
Formula: CH_3I

CAS-RN: 74-88-4
Group No.: 24-002
Molar Mass: 141.94

Table 24.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
48KUR		254.9–299.6	5	nosp	not specified		avg	DSIO	47KUR
57HAR/MOE		243.4–303.2	8	0.50	not specified		*p*	BSIO	57HAR/MOE
62LOW/MOE		253.2–308.2	7 S	0.50	not specified		*p*	BSIO	57HAR/MOE
84GAI/GRA		213.1–262.6	8	nosp	not specified		*p*	not specified	
93CAR/LAY	N	298.1	1	nosp	not specified		*p*	not specified	
93SHE		298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

93CAR/LAY origin of data is not clear

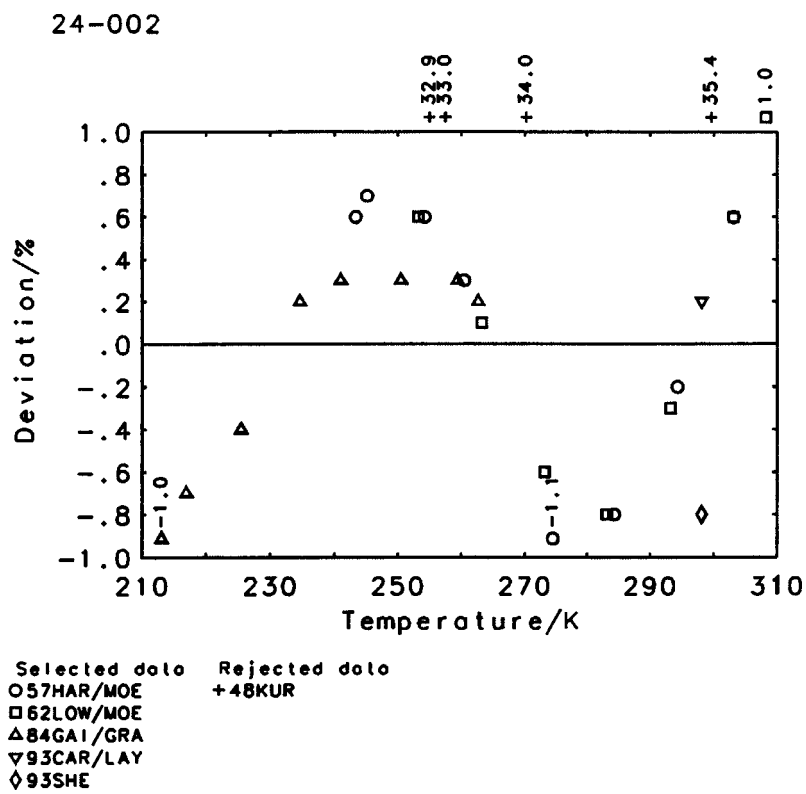
Table 24.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
			Selected data					
57HAR/MOE	243.4–303.2	8	0.50	1.338	6.55–2	0.67	7.13–3	2
62LOW/MOE	253.2–308.2	7	0.50	1.224	6.09–2	0.61	9.25–3	1
84GAI/GRA	213.1–262.6	8	0.70 #	0.697	4.79–2	0.49	−8.68–3	2
93CAR/LAY	298.1	1	1.00 #	0.155	1.54–2	0.15	1.54–2	1
93SHE	298.1	1	0.50 #	1.519	7.49–2	0.76	−7.49–2	−1
			Rejected data					
48KUR	(4.98,33.64,4.97,5)							

Table 24.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	30	25	1.188	6.19–2	0.63	−2.84–4	5

Temp. range K	A_1	A_2	A_3	Level of uncertainty
213.1–308.2	1.57584+1	−4.72289	9.29212−1	IV



Name: Iodoethane
Formula: C_2H_5I

CAS-RN: 75-03-6
Group No.: 24-003
Molar Mass: 155.97

Table 24.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81BER/OGI	243.1–333.1	4 S	nosp	not specified		avg	DSIO	*79BER
48KUR	263.4–316.6	3	nosp	not specified		avg	DSIO	47KUR
93SHE	298.1	1	nosp	99.9	chrom	p	DDCT	71KON/SUU

Table 24.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*81BER/OGI	243.1–333.1	4	3.00 #	0.409	1.61–1	1.23	−1.52–1	−4
93SHE	298.1	1	0.50 #	0.263	1.73–2	0.13	1.73–2	1
Rejected data								
48KUR	(6.27–1,4.46,5.71–1,3)							

Table 24.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	8	5	0.496	1.86–1	1.42	−1.18–1	−3
Temp. range K		A_1	A_2				Level of uncertainty
243.1–333.1		8.84109	1.45410				V

Name: 1-Iodopropane
Formula: C_3H_7I

CAS-RN: 107-08-4
Group No.: 24-004
Molar Mass: 169.99

Table 24.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON	317.3–339.1	4 S	nosp	not specified		avg	DSIO	*81VON
93SHE	298.1–308.1	2	nosp	99.9	chrom	p	DDCT	71KON/SUU

Table 24.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*81VON	317.3–339.1	4	3.00 #	0.119	5.98–2	0.36	−1.32–2	1
93SHE	298.1–308.1	2	0.50 #	0.009	7.79–4	0.00	7.59–4	0

Table 24.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	6	6	0.120	5.98–2	0.36	−8.55–3	1
Temp. range K		A_1	A_2				Level of uncertainty
298.1–339.1		1.06533+1	1.92089				V

Name: 1-Iodo-2-methylpropane
Formula: C_4H_9I

CAS-RN: 513-38-2
Group No.: 24-005
Molar Mass: 184.02

Table 24.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON	315.0–344.5	3 S	nosp	not specified		avg	DSIO	*81VON
93SHE	298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 24.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*81VON	315.0–344.5	3	3.00 #	0.332	2.04–1	01.00	7.05–2	1
93SHE	298.1	1	0.50 #	0.056	5.54–3	0.03	−5.54–3	−1

Table 24.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	4	4	0.408	2.50–1	1.22	5.15–2	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–344.5	1.52809+1	1.55277	V

Name: Iodobenzene
Formula: C_6H_5I

CAS-RN: 591-50-4
Group No.: 24-009
Molar Mass: 204.01

Table 24.9.1. Experimental heat capacities

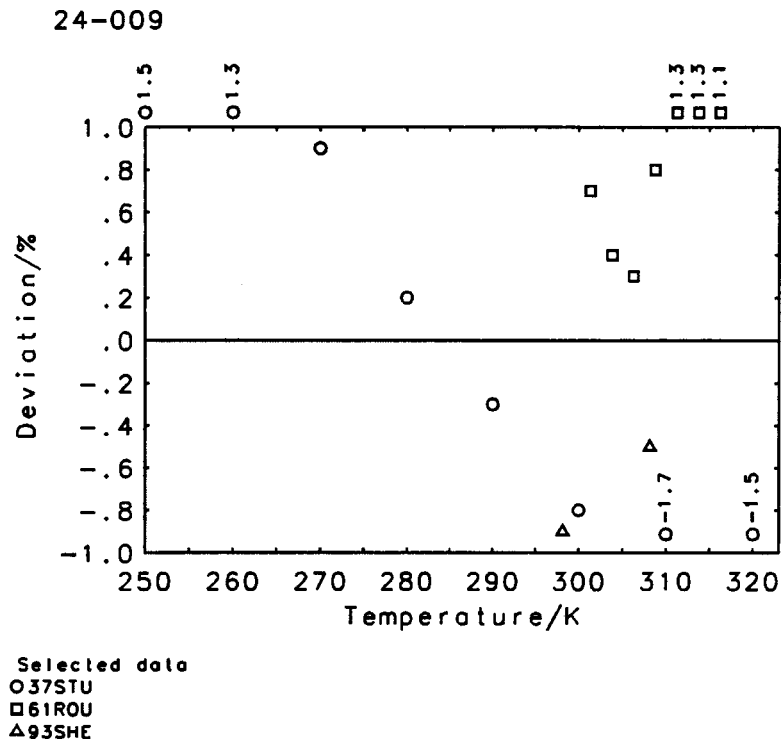
Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
37STU	250.0–320.0	8 S	nosp	not specified		*p*	BDHO	37STU
61ROU	301.3–316.2	7	nosp	not specified		*p*	BSAO	61ROU
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 24.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
37STU	250.0–320.0	8	2.00 #	0.568	2.16–1	1.14	−1.13–2	0
61ROU	301.3–316.2	7	1.00 #	0.910	1.79–1	0.91	1.64–1	7
93SHE	298.1–308.1	2	0.50 #	1.472	1.41–1	0.74	−1.34–1	−2

Table 24.9.3 Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	17	17	0.921	2.06−1	1.07	4.63−2	5
Temp. range K		A_1	A_2				Level of uncertainty
250.0–320.0		1.38502+1	1.80350				V



Name: 1,3-Diiodopropane
Formula: $C_3H_6I_2$

CAS-RN: 627-31-6
Group No.: 24-010
Molar Mass: 295.89

Table 24.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1–308.1	2	nosp	99.9	chrom	p	DDCT	71KON/SUU

Table 24.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
298.1–308.1		1.28196+1	2.52569				IV

Name: 2-Iodopropane
Formula: C_3H_7I

CAS-RN: 75-30-9
Group No.: 24-011
Molar Mass: 169.99

Table 24.11.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.15	0.8077	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Name: 1-Iodobutane
Formula: C_4H_9I

CAS-RN: 542-69-8
Group No.: 24-012
Molar Mass: 184.02

Table 24.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 24.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.04613+1	3.12707	IV

Name: 2-Iodobutane
Formula: C_4H_9I

CAS-RN: 513-48-4
Group No.: 24-013
Molar Mass: 184.02

Table 24.13.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.15	0.8983	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Name: 1-Iodopentane
Formula: $C_5H_{11}I$

CAS-RN: 628-17-1
Group No.: 24-014
Molar Mass: 198.05

Table 24.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 24.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.28855+1	3.48787	IV

Name: 1-Iodohexane
Formula: $C_6H_{13}I$

CAS-RN: 638-45-9
Group No.: 24-015
Molar Mass: 212.07

Table 24.15.1. Experimental heat capacities

Reference	Temp. rang K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 24.15.3 Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.38513+1	4.32975	IV

Name: 1-Iodoheptane
Formula: $C_7H_{15}I$

CAS-RN: 4282-40-0
Group No.: 24-016
Molar Mass: 226.10

Table 24.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93SHE	298.1–308.1	2	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

Table 24.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	1.52237+1	5.05140	IV

Name: Dichlorodifluoromethane
Formula: CCl_2F_2

CAS-RN: 75-71-8
Group No.: 25-004
Molar Mass: 120.91

Table 25.4.1 Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
31BUF/FLE	N	230.1–290.1	2	4.00	not specified		avg	not specified	
39RIE3		194.4–293.5	12	1.00	not specified		sat	BSIO	39RIE3
55MCH/EIS	N	169.0–253.4	17	nosp	not specified		sat	BSIO	36AST/MES

31BUF/FLE the first datum from drop calorimetry; the second datum from isoperibol calorimetry
55MCH/EIS source of data was Cryogenic Laboratory, The Pennsylvania State University

Table 25.4.2 Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
39RIE3	194.4–293.5	12	1.00	0.855	1.10–1	0.85	−7.84–3	0
55MCH/EIS	169.0–253.4	17	0.40 #	0.773	4.01–2	0.31	1.34–3	0
Rejected data								
31BUF/FLE	(9.04–1,5.87,6.12–1,0)							

Table 25.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	31	29	0.853	8.15–2	0.63	−2.46–3	0
sat	31	29	0.867	8.11–2	0.63	−3.32–3	−1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
169.0–293.5	1.09253+1	−1.95506−1	4.46794−1	IV
169.0–293.5	1.04247+1	3.16041−1	3.17051−1	IV

Table 25.4.4 Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	31	29	1.022	7.45–2	0.58	1.22–3	−5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
169.0–293.5	384.95	1.77817	7.11773−1	7.27819	1.33063+1	−9.84623	4.58487	IV

Name: 1,2-Dichloro-1,1,2,2-tetrafluoroethane
Formula: $C_2Cl_2F_4$

CAS-RN: 76-14-2
Group No.: 25-012
Molar Mass: 170.92

Table 25.12.1 Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
60MAR	N	237.1–275.9	2	nosp	not specified		sat	not specified	
66VAS2		224.5–315.2	23	0.70	not specified		sat	BDAO	64VAS2
81KOL/KOS		182.0–295.9	21	0.10	99.79	melpt	sat	BSAO	62KOL/SER

60MAR unpublished data: J. G. Aston, private communication (1955) and R. C. McHarness, private communication (1951)

Name: 1,1,2-Trichloro-1,2,2-trifluoroethane
Formula: $C_2Cl_3F_3$

CAS-RN: 76-13-1
Group No.: 25-014
Molar Mass: 187.38

Table 25.14.1 Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
38RIE	N	242.9–333.9	19	0.50	not specified		sat	BSIO	39RIE3
40BEN/MCH		261.6–336.4	6	nosp	not specified		sat	BSIO	40BEN/MCH
54BUB	N	253.1–458.1	22 S	3.30	not specified		*p*	BDAO	75RAS/GRI
81KOL/KOS		240.5–298.9	10	0.10	99.81	melpt	sat	BSAO	62KOL/SER
88VES/ZAB		298.1–318.1	5	0.30	100.0	chrom	*p*	BSAO	79VES/ZAB
92FEN/COS		298.1	1	nosp	99.99	chrom	*p*	FSIT	71PIC/LED

38RIE same data in 39RIE1
54BUB C_p at saturation line extrapolated from high pressure measurements

Name: 2-Bromo-2-chloro-1,1,1-trifluoroethane
Formula: $C_2HBrClF_3$

CAS-RN: 151-67-7
Group No.: 25-017
Molar Mass: 197.38

Table 25.17.1 Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
88VES/ZAB	298.1–318.1	5	0.30	99.0	chrom	*p*	BSAO	79VES/ZAB
93DOH/COS	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED

Name: 1,1,2-Trichloro-1,2-difluoroethane
Formula: $C_2HCl_3F_2$

CAS-RN: 354-15-4
Group No.: 25-018
Molar Mass: 169.38

Table 25.18.1 Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92LEB/KUL1	104.8–328.1	82	0.20	98.9	chrom	*p*	BSAO	76LEB/LIT
97VAR/DRU2	126.6–326.8	99	0.20	99.39	chrom	*p*	BSAO	97VAR/DRU1

Table 25.18.2 Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
92LEB/KUL1	104.8–328.1	82	0.20	2.565	9.85–2	0.51	1.01–3	4
Rejected data								
97VAR/DRU2	(4.29–1,2.18,−3.29–1,−99)							

Table 25.18.3 Parameters of regression polynomial

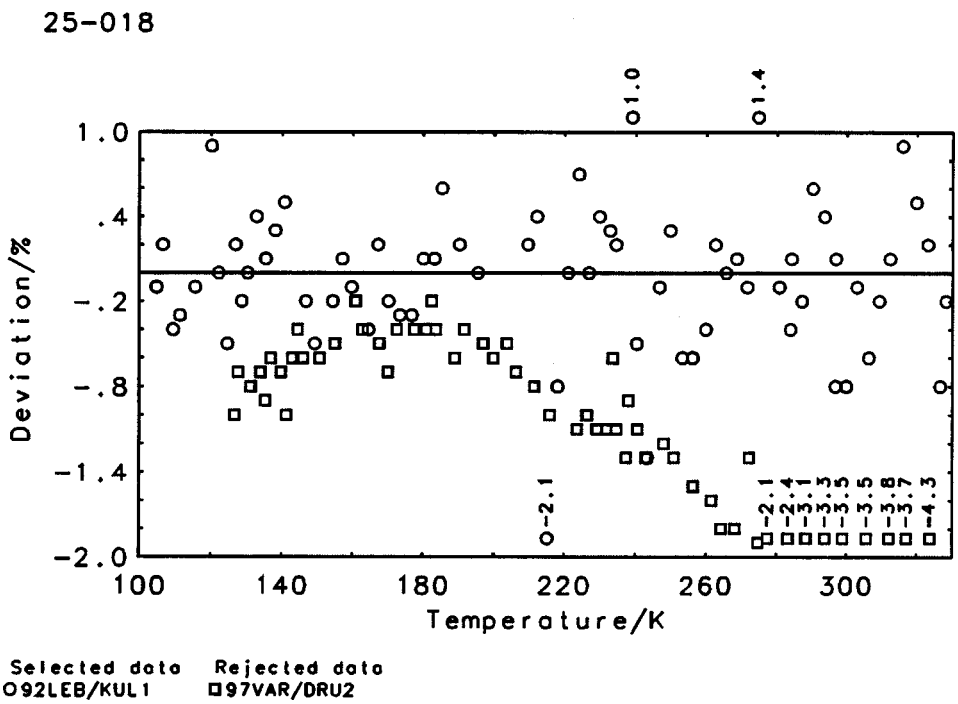
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	181	82	2.630	1.01–1	0.53	1.01–3	4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
104.8–328.1	2.23408+1	−5.98599	2.58632	−2.71272−1	III

Table 25.18.4 Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	181	82	4.535	1.73−1	0.91	2.96−3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
104.8–328.1	525.10	1.10306+1	6.65475	1.14720+1	4.57094	IV



Name: 1,1-Dichloro-1,2-difluoroethane
Formula: $C_2H_2Cl_2F_2$

CAS-RN: 1842-05-3
Group No.: 25-019
Molar Mass: 134.94

Table 25.19.1 Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92LEB/KUL1	173.5–313.4	27	0.20	99.6	melpt	*p*	BSAO	76LEB/LIT

Table 25.19.3 Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	27	26	1.453	5.11−2	0.29	2.62−4	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
173.5–307.6	1.74233	−1.09581	4.64319−1	III

Name: 1-Bromo-4-chlorobenzene
Formula: C_6H_4BrCl

CAS-RN: 106-39-8
Group No.: 25-033
Molar Mass: 191.45

Table 25.33.1 Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
18NAR	355.3	1	nosp	not specified		avg	DSIO	18NAR
#00VAN/OON1	339.6–369.0	19	0.20	99.97	melpt	p	BSAO	98VAN/VAN

Table 25.33.2 Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
#00VAN/OON1	339.6–369.0	19	0.20	0.356	1.59–2	0.07	2.26–5	1
Rejected data								
18NAR	(5.61–1,2.44,5.61–1,1)							

Table 25.33.3 Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	19	0.377	1.68–2	0.08	2.26–5	1

Temp. range K	A_1	A_2	Level of uncertainty
339.6–369.0	1.28277+1	2.71204	III

Name: 2-Chloro-1,1,1,2-tetrafluoroethane
Formula: C_2HClF_4

CAS-RN: 2837-89-0
Group No.: 25-036
Molar Mass: 136.48

Table 25.36.1 Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93DU/SUV2	N	216.6–261.1	11 S	nosp	not specified		p	not specified	

93DU/SUV2 table is based on experimental data from the database at the National Institute of Standards and Technology (NIST)

Table 25.36.3 Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	11	11	0.005	9.04–4	0.01	−9.71–6	0
sat	11	11	0.005	9.13–4	0.01	3.99–6	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
216.6–261.1	1.96171+2	−1.95628+2	7.02572+1	−8.29074	IV
216.6–261.1	1.94133+2	−1.93172+2	6.92941+1	−8.16920	IV

Name: 1,2-Dichloro-1,1,2-trifluoroethane
Formula: $C_2HCl_2F_3$

CAS-RN: 354-23-4
Group No.: 25-037
Molar Mass: 152.93

Table 25.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99DRU/VAR	138.8–296.3	75	0.30	99.51	melpt	*p*	BSAO	97VAR/DRU1

Table 25.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	75	75	0.365	1.94–2	0.11	3.92–5	−4
sat	75	75	0.372	1.98–2	0.11	4.16–5	−5

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
138.8–296.3	2.21496+1	−7.72151	3.57936	−4.44704−1	III
138.8–296.3	2.23041+1	−7.95675	3.69472	−4.62900−1	III

Table 25.37.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	75	75	0.452	2.43–2	0.14	6.31–5	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
138.8–296.3	461.40	2.46869+2	2.41427+1	−8.84074	2.44834+2	5.27103	2.06832+2	III

Name: 2,2-Dichloro-1,1,1-trifluoroethane
Formula: $C_2HCl_2F_3$

CAS-RN: 306-83-2
Group No.: 25-038
Molar Mass: 152.93

Table 25.38.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91DU/SUV		298.1	1	nosp	not specified		*p*	not specified	
91NAK		275.6–300.0	4	0.40	99.82	anal	*p*	FSAO	89SAI/SAT
93DU/SUV1	N	249.5–301.0	11 S	nosp	not specified		*p*	not specified	

93DU/SUV1 table is based on experimental data from the database at the National Institute of Standards and Technology (NIST)

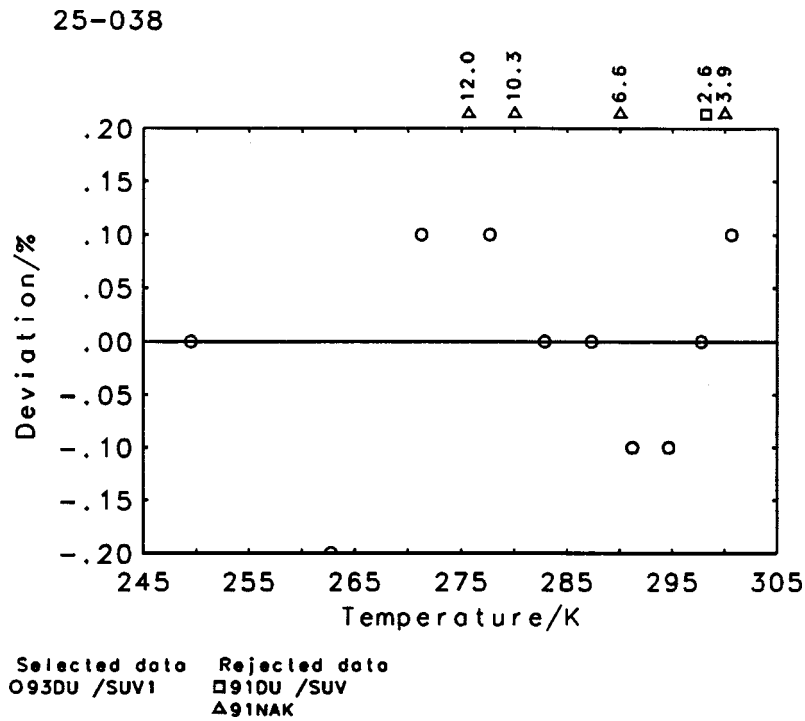
Table 25.38.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93DU/SUV1	249.5–301.0	11	1.00 #	0.080	1.33–2	0.08	1.27–4	1
Rejected data								
91DU/SUV	(4.85–1,2.59,4.85–1,1)		91NAK	(1.63,8.77,1.53,4)				

Table 25.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	16	11	0.101	1.67−2	0.10	1.27−4	1
sat	16	11	0.094	1.57−2	0.09	−1.39−4	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
249.5–301.0	4.92962+2	−5.29861+2	1.92952+2	−2.30228+1	IV
249.5–301.0	4.90061+2	−5.26789+2	1.91887+2	−2.29024+1	IV



Name: 1,2,2-Trichloro-1,1-difluoroethane
Formula: $C_2HCl_3F_2$

CAS-RN: 354-21-2
Group No.: 25-039
Molar Mass: 169.38

Table 25.39.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97DRU/VAR	N	123.2–325.6	104	0.20	99.87	chrom	p	BSAO	97VAR/DRU1
97DRU/VAR	same data in 97VAR/DRU2								

Table 25.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	104	104	0.995	3.62−2	0.20	1.37−4	6

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
123.2–325.6	2.13398+1	−5.51787	2.58118	−3.13662−1	III

Table 25.39.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	104	73	1.164	4.30−2	0.23	1.90−4	−7

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
144.0–325.6	524.00	−1.39090	1.03144	1.56551+1	4.68907−1	V

Name: 1,1-Dichloro-1-fluoroethane
Formula: $C_2H_3Cl_2F$

CAS-RN: 1717-00-6
Group No.: 25-040
Molar Mass: 116.95

Table 25.40.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91DU/SUV	298.15	1.155	nosp	not specified		p	not specified	

Name: 1-Chloro-1,1,2,3,3,3-hexafluoropropane
Formula: C_3HClF_6

CAS-RN: 359-58-0
Group No.: 25-041
Molar Mass: 186.48

Table 25.41.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.205	3.00	not specified		p	BDHT	92HWA/DES

Name: 2-Chloro-1,1,1,3,3,3-hexafluoropropane
Formula: C_3HClF_6

CAS-RN: 431-87-8
Group No.: 25-042
Molar Mass: 186.48

Table 25.42.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.207	3.00	not specified		p	BDHT	92HWA/DES

Name: 1,2-Dichloro-1,1,3,3,3-pentafluoropropane
Formula: $C_3HCl_2F_5$

CAS-RN: 431-86-7
Group No.: 25-043
Molar Mass: 202.94

Table 25.43.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.087	3.00	not specified		p	BDHT	92HWA/DES

Name: 2,3-Dichloro-1,1,1,2,3-pentafluoropropane
Formula: $C_3HCl_2F_5$

CAS-RN: 422-48-0
Group No.: 25-044
Molar Mass: 202.94

Table 25.44.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.087	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 3-Chloro-1,1,1,2,2-pentafluoropropane
Formula: $C_3H_2ClF_5$

CAS-RN: 422-02-6
Group No.: 25-045
Molar Mass: 168.49

Table 25.45.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.275	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 2,3-Dichloro-1,1,1,3-tetrafluoropropane
Formula: $C_3H_2Cl_2F_4$

CAS-RN: 146916-90-7
Group No.: 25-046
Molar Mass: 184.95

Table 25.46.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.176	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 2,3-Dichloro-1,1,1-trifluoropropane
Formula: $C_3H_3Cl_2F_3$

CAS-RN: 338-75-0
Group No.: 25-047
Molar Mass: 166.96

Table 25.47.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.234	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 4-Chloro-1,1,2,2,3,3-hexafluorocyclobutane
Formula: C_4HClF_6

CAS-RN: 132186-30-2
Group No.: 25-048
Molar Mass: 198.50

Table 25.48.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.158	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 1-Chloro-4-iodobenzene
Formula: C_6H_4ClI

CAS-RN: 637-87-6
Group No.: 25-049
Molar Mass: 238.45

Table 25.49.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00VAN/OON1	329.8–368.6	25	0.20	99.83	melpt	*p*	BSAO	98VAN/VAN

Table 25.49.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	25	25	0.332	1.51−2	0.07	1.88−5	−1

Temp. range K	A_1	A_2	Level of uncertainty
329.8–368.6	1.40694+1	2.49758	III

Name: 1-Bromo-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluorooctane
Formula: C_8BrF_{17}

CAS-RN: 423-55-2
Group No.: 25-050
Molar Mass: 498.96

Table 25.50.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97VAR/DRU1	280.0–346.4	34	0.20	99.92	melpt	p	BSAO	97VAR/DRU1

Table 25.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	34	34	0.261	3.06−2	0.05	2.83−5	−2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
280.0–346.4	1.76997+1	4.11604+1	−1.58012+1	2.19704	IV

Name: Ethanamine
Formula: C_2H_7N

CAS-RN: 75-04-7
Group No.: 31-002
Molar Mass: 45.08

Table 31.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
33POH/MEH	N	273.1	1	3.00	not specified		p	BSIO	33POH/MEH
58JAF		298.1	1	nosp	not specified		p	not specified	

33POH/MEH temperature not specified; estimated by the compilers

Table 31.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
58JAF	298.1	1	0.50 #	0.000	0.00	0.00	0.00	0

Table 31.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	1.56353+1	IV

Name: *N*-Ethylethanamine
Formula: $C_4H_{11}N$

CAS-RN: 109-89-7
Group No.: 31-011
Molar Mass: 73.14

Table 31.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
36KUR/VOS	N	311.6	1	nosp	not specified		avg	DSIO	36KUR/VOS
65KAU/BIT		293.1–323.1	4 S	1.00	not specified		p	FSIO	65KAU/BIT
85COS/PAT9		283.1–313.1	3 S	nosp	99.5	chrom	p	FSIT	71PIC/LED
91PES/NIK	N	298.1	1	nosp	not specified		p	BSAO	83KUK/KOR

36KUR/VOS average value in temperature range 290–333 K
91PES/NIK water content below 0.05%

Name: *N*-(2-Aminoethyl)-1,2-ethanediamine
Formula: $C_4H_{13}N_3$

CAS-RN: 111-40-0
Group No.: 31-015
Molar Mass: 103.17

Table 31.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
88BOB/KAM	313.1–493.1	10	6.00	97.	chrom	sat	BDCT	86MER/BEN
97STE/CHI4	290.0–550.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 31.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
97STE/CHI4	290.0–550.0	27	1.00	0.029	1.11–2	0.03	2.40–5	−2
Rejected data								
88BOB/KAM	(2.14,6.75,−1.90,−10)							

Table 31.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	37	27	0.031	1.17–2	0.03	2.40–5	−2
sat	37	27	0.000	1.56–6	0.00	5.65–7	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
290.0–550.0	3.92690+1	−4.84339	9.67736−1	IV
290.0–550.0	3.87200+1	−4.54000	9.26600−1	IV

Table 31.15.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	37	27	0.356	1.31−1	0.36	7.86−4	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
290.0–550.0	678.00	−3.45766	1.22513	2.79866+1	2.43963	IV

Name: *N*,*N*-Diethylethanamine
Formula: $C_6H_{15}N$

CAS-RN: 121-44-8
Group No.: 31-023
Molar Mass: 101.19

Table 31.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON	319.7–330.0	3 S	nosp	not specified		avg	DSIO	*81VON
65KAU/BIT	293.1–343.1	6	1.00	not specified		*p*	FSIO	65KAU/BIT
80ROU/ROB	278.1–288.1	2	0.30	not specified		*p*	FSIT	71PIC/LED
85HEP/KOO	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91GRO/ROU	298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
93GRO/ROU	298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
94GRO/ROU	298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED

Name: 1-Hexanamine
Formula: $C_6H_{15}N$

CAS-RN: 111-26-2
Group No.: 31-024
Molar Mass: 101.19

Table 31.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
71KON/WAD	298.1	1	nosp	99.8	chrom	*p*	BSIO	70LKB/COM
77BEL/BUB	298.1	1	nosp	not specified		*p*	BDCT	68WAD

Name: *N*-Propyl-1-propanamine
Formula: $C_6H_{15}N$

CAS-RN: 142-84-7
Group No.: 31-025
Molar Mass: 101.19

Table 31.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
01KAH	N	334.1	1	nosp	not specified		avg	DSIO	01KAH
91PES/NIK	N	298.1	1	nosp	not specified		*p*	BSAO	83KUK/KOR

01KAH average value in temperture range 294–374 K
91PES/NIK water content below 0.05%

Table 31.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
91PES/NIK	298.1	1	0.50 #	0.000	0.00	0.00	0.00	0

Table 31.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	3.04047+1	IV

Name: 2-Methylbenzenamine
Formula: C_7H_9N

CAS-RN: 95-53-4
Group No.: 31-029
Molar Mass: 107.16

Table 31.29.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		330.8–392.2	4 S	nosp	not specified		avg	DSIO	*81VON
*87SCH	N	320.3–348.5	6 S	nosp	not specified		p	DSIO	*86SCH
02LOU2	N	381.0–382.0	2	nosp	not specified		avg	DSIO	*98LOU
34KOL/UDO	N	302.5	1	nosp	not specified		p	BSIT	34KOL/UDO
34RAD/JUL		288.1	1	nosp	not specified		p	BSIO	49WEI
88GUS/MIR2		303.1–463.1	9	1.90	not specified		p	BDHT	84GUS/MIR
90MEV/LIC		249.5	1	3.00	99.	anal	p	BDCT	89BRE/LIC
94STE/CHI	N	235.2–441.1	26	0.10	99.925	melpt	sat	BSAO	88STE/ARC
94STE/CHI		460.0–700.0	13 S	1.00	99.925	melpt	sat	BDHT	89KNI/ARC
#00CEN/LIP		313.1–371.1	26	2.00	99.97	chrom	p	BDCT	91BAN/GAR

*87SCH two data points near the upper temperature limit are misprinted; corrected to comply with equation presented by the author
02LOU2 average value in temperature range 295–468 K
34KOL/UDO same datum in 34KOL/UDO1
94STE/CHI low temperature limit is below n.m.t.(258.7 K); undercooled liquid

Table 31.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
94STE/CHI	235.2–441.1	26	0.10	0.289	7.92–3	0.03	6.87–4	0
94STE/CHI	460.0–700.0	13	1.00	0.754	3.06–1	0.75	−6.36–2	−7
#00CEN/LIP	313.1–371.1	26	1.00 #	0.268	7.48–2	0.27	−3.32–2	−4
			Rejected data					
*81VON	(5.76–1,2.06,−5.72–1,−4)		*87SCH	(5.31–1,1.90,5.16–1,6)				
02LOU2	(4.32–1,1.54,−4.17–1,−2)		34KOL/UDO	(1.17,4.63,−1.17,−1)				
34RAD/JUL	(1.79,7.37,−1.79,−1)		88GUS/MIR2	(6.70,30.58,−6.70,−9)				
90MEV/LIC	(3.09–1,1.23,−3.09–1,−1)							

Table 31.29.3. Parameters of cubic spline polynomials

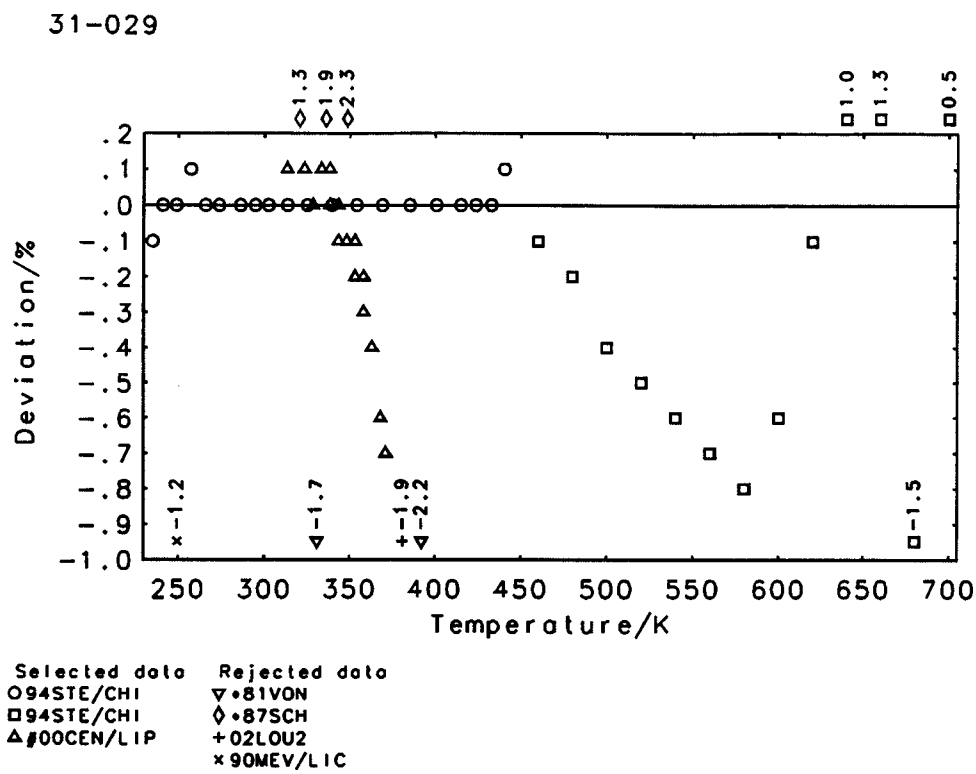
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	89	65	0.440	1.52−1	0.40	−2.57−2	−11
sat	89	65	0.354	1.06−1	0.30	−2.46−2	−10

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
235.2–400.0	3.45268+1	−1.00217+1	3.19712	−2.56233−1	II
400.0–630.0	1.47972+1	4.77551	−5.02192−1	5.20433−2	IV
630.0–700.0	−9.76675+3	4.66265+3	−7.39848+2	3.91709+1	IV
235.2–400.0	3.45599+1	−1.00564+1	3.20908	−2.57588−1	II
400.0–630.0	1.76567+1	2.62095	3.97415−2	6.52410−3	IV
630.0–700.0	−6.10308+3	2.91726+3	−4.62601+2	2.44849+1	IV

Table 31.29.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	89	65	6.890	3.67−1	1.07	1.14−1	30

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
235.2–700.0	716.50	−3.90240	2.22143−1	2.16886+1	3.24879	4.25429	1.19801	V



Name: 3-Methylbenzenamine
Formula: C_7H_9N

CAS-RN: 108-44-1
Group No.: 31-030
Molar Mass: 107.16

Table 31.30.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
34KOL/UDO	N	302.7	1	nosp	not specified		*p*	BSIT	34KOL/UDO
88GUS/MIR2		303.1–463.1	9	1.90	not specified		*p*	BDHT	84GUS/MIR
90MEV/LIC		241.6	1	3.00	99.	anal	*p*	BDCT	89BRE/LIC
#00CEN/LIP		313.2–371.2	26	2.00	99.7	chrom	*p*	BDCT	91BAN/GAR
#00CEN/LIP		263.1–353.1	10	0.50	99.7	chrom	*p*	BDCT	83ROU/ROU

34KOL/UDO2 same datum in 34KOL/UDO1

Table 31.30.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
90MEV/LIC	241.6	1	3.00	0.030	2.23–2	0.09	2.23–2	1
#00CEN/LIP	313.2–371.1	26	2.00	0.322	1.73–1	0.64	−1.52–1	−26
#00CEN/LIP	263.1–353.1	10	0.50	0.257	3.51–2	0.13	2.50–2	6
Rejected data								
34KOL/UDO	(3.50–1,1.34,−3.50–1,−1)		88GUS/MIR2	(6.34,30.41,−6.34,−4)				

Table 31.30.3. Parameters of regression polynomial

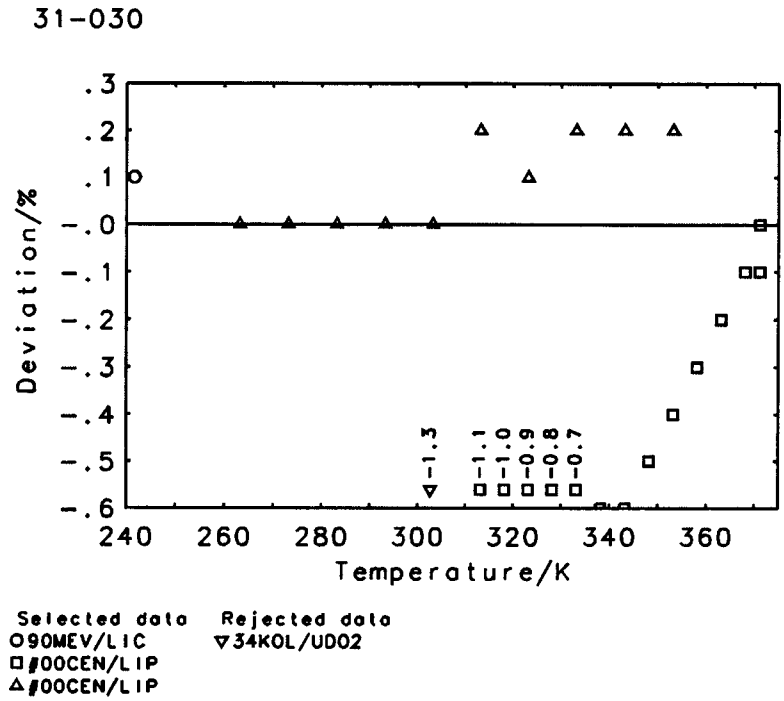
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	47	37	0.310	1.50–1	0.56	−9.91–2	−19

Temp. range K	A_1	A_2	Level of uncertainty
241.6–371.1	1.86869+1	2.56034	IV

Table 31.30.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	47	37	0.581	9.67–2	0.36	9.95–4	−10

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
241.6–371.1	709.00	−3.38737	3.25642	1.83645+1	8.80895−1	IV



Name: 4-Methylbenzenamine
Formula: C_7H_9N

CAS-RN: 106-49-0
Group No.: 31-031
Molar Mass: 107.16

Table 31.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
90MEV/LIC	323.0–368.0	eqn	3.00	99.	anal	*p*	BDCT	89BRE/LIC
#00CEN/LIP	328.3–353.1	12	2.00	99.7	chrom	*p*	BDCT	91BAN/GAR
#00CEN/LIP	323.1–353.1	4	0.50	99.7	chrom	*p*	BDCT	83ROU/ROU

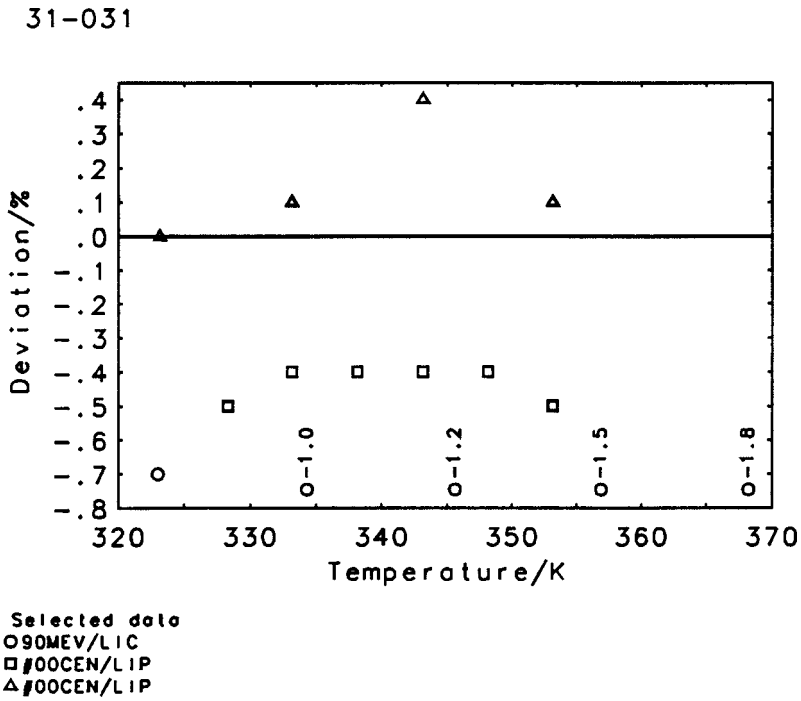
Table 31.31.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
90MEV/LIC	323.0–368.2	5	3.00	0.428	3.52–1	1.28	−3.35–1	−5
#00CEN/LIP	328.3–353.1	12	2.00	0.220	1.20–1	0.44	−1.19–1	−12
#00CEN/LIP	323.1–353.1	4	0.50	0.387	5.33–2	0.19	3.47–2	2

Table 31.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	21	21	0.332	2.06–1	0.75	−1.41–1	−15

Temp. range K	A_1	A_2	Level of uncertainty
323.0–368.2	1.76283+1	2.86690	IV



Name: *N*,*N*-Dimethylbenzenamine
Formula: $C_8H_{11}N$

CAS-RN: 121-69-7
Group No.: 31-033
Molar Mass: 121.18

Table 31.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		329.5–388.1	4 S	nosp	not specified		avg	DSIO	*81VON
*87SCH		318.0–348.3	6 S	nosp	not specified		*p*	DSIO	*86SCH
02LOU2	N	376.8–378.0	2	nosp	not specified		avg	DSIO	*98LOU
16BRA		283.1	1	nosp	not specified		avg	DSTO	16BRA
34KOL/UDO	N	302.3	1	nosp	not specified		*p*	BSIT	34KOL/UDO
34RAD/JUL		289.1	1	nosp	not specified		*p*	BSIO	49WEI
57CRU/JOS		293.1	1	2.00	not specified		*p*	BSIO	57CRU/JOS
97VER		298.1	1	nosp	100.00	chrom	*p*	BDHT	69PER/COM

02LOU2 average value in temperature range 294–459 K
34KOL/UDO same datum in 34KOL/UDO1

Name: 2,6-Dimethylbenzenamine
Formula: $C_8H_{11}N$

CAS-RN: 87-62-7
Group No.: 31-034
Molar Mass: 121.18

Table 31.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86STE/CHI	284.6–450.0	19 S	nosp	99.99	melpt	sat	BSAO	47HUF
#00VER2	298.1	1	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: *N*-Phenylbenzenamine
Formula: $C_{12}H_{11}N$

CAS-RN: 122-39-4
Group No.: 31-042
Molar Mass: 169.23

Table 31.42.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*84BAT	N	326.1–339.1	2	nosp	not specified		*p*	not specified	
*99STI/SWA	N	340.5	1	nosp	not specified		avg	DSIO	*81VON
13CAM	N	327.1–329.1	2	nosp	not specified		*p*	BSIO	13CAM

*84BAT error 0.5% (information in 29WAS)
*99STI/SWA average value in temperature range 330–352 K
13CAM error 0.5% (information in 29WAS)

Table 31.42.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*84BAT	326.1–339.1	2	5.00 #	0.609	1.21	3.04	1.15	2
*99STI/SWA	340.5	1	5.00 #	0.199	4.00–1	01.00	−4.00–1	−1
13CAM	327.1–329.1	2	5.00 #	0.446	8.37–1	2.23	−8.37–1	−2

Table 31.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	5	5	0.627	1.22	3.13	4.58–2	−1

Temp. range K	A_1	A_2	Level of uncertainty
326.1–340.5	−1.92922+1	1.75651+1	V

Name: *N*,*N*-Dimethyl-2-propanamine
Formula: $C_5H_{13}N$

CAS-RN: 996-35-0
Group No.: 31-046
Molar Mass: 87.16

Table 31.46.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99ZIJ/WIT	278.00	2.320	nosp	not specified		*p*	BSIO	99ZIJ/WIT

Name: *N*-(1-Methylethyl)-2-propanamine
Formula: $C_6H_{15}N$

CAS-RN: 108-18-9
Group No.: 31-047
Molar Mass: 101.19

Table 31.47.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99ZIJ/WIT	278.00	2.630	nosp	not specified		*p*	BSIO	99ZIJ/WIT

Name: 2,4-Dimethylbenzenamine
Formula: $C_8H_{11}N$

CAS-RN: 95-68-1
Group No.: 31-048
Molar Mass: 121.18

Table 31.48.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97VER	298.15	1.970	nosp	99.95	chrom	*p*	BDHT	69PER/COM

Name: 2,5-Dimethylbenzenamine
Formula: $C_8H_{11}N$

CAS-RN: 95-78-3
Group No.: 31-049
Molar Mass: 121.18

Table 31.49.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97VER	298.15	1.890	nosp	100.00	chrom	*p*	BDHT	69PER/COM

Name: *N*-Ethylbenzenamine
Formula: $C_8H_{11}N$

CAS-RN: 103-69-5
Group No.: 31-050
Molar Mass: 121.18

Table 31.50.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97VER	298.15	1.840	nosp	100.00	chrom	*p*	BDHT	69PER/COM

Name: 2-Ethylbenzenamine
Formula: $C_8H_{11}N$

CAS-RN: 578-54-1
Group No.: 31-051
Molar Mass: 121.18

Table 31.51.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00VER2	298.15	1.630	nosp	99.99	chrom	*p*	BDHT	69PER/COM

?
Name: α-Methylbenzenemethanamine
Formula: $C_8H_{11}N$

CAS-RN: 618-36-0
Group No.: 31-052
Molar Mass: 121.18

Table 31.52.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER2	298.15	1.460	nosp	99.96	chrom	*p*	BDHT	69PER/COM

Name: 1-Octanamine
Formula: $C_8H_{19}N$

CAS-RN: 111-86-4
Group No.: 31-053
Molar Mass: 129.25

Table 31.53.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
82PFE/KUC		298.1	1	nosp	not specified		*p*	BDCT	68WAD
93STE/CHI2	N	300.0–620.0	17	1.00	99.95	chrom	sat	BDHT	89KNI/ARC
93STE/CHI2	same data in 96STE/CHI2								

Table 31.53.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
93STE/CHI2	300.0–620.0	17	1.00	0.314	1.77–1	0.31	1.31–3	2

Table 31.53.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	18	17	0.373	2.10–1	0.37	1.31–3	2
sat	18	17	0.240	1.29–1	0.24	4.82–4	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–540.0	1.40353+1	1.27940+1	−2.34770	2.24142−1	IV
540.0–620.0	−2.29218+3	1.29402+3	−2.39612+2	1.48701+1	IV
300.0–540.0	1.46798+1	1.20662+1	−2.09238	1.95755−1	IV
540.0–620.0	−1.31515+3	7.50862+2	−1.38906+2	8.64106	IV

Table 31.53.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	18	17	0.295	1.40–1	0.29	4.60–4	3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–620.0	641.00	−4.00830	2.24105−1	2.61924+1	1.79229+1	IV

Name: α,α-Dimethylbenzenemethanamine
Formula: $C_9H_{13}N$

CAS-RN: 585-32-0
Group No.: 31-054
Molar Mass: 135.21

Table 31.54.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER2	298.15	1.630	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: *N*,*N*-Dimethylbenzenemethanamine
Formula: $C_9H_{13}N$

CAS-RN: 103-83-3
Group No.: 31-055
Molar Mass: 135.21

Table 31.55.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER2	298.15	2.000	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 2-(1-Methylethyl)benzenamine
Formula: $C_9H_{13}N$

CAS-RN: 643-28-7
Group No.: 31-056
Molar Mass: 135.21

Table 31.56.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00VER2	298.15	2.010	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 1-Naphthalenamine
Formula: $C_{10}H_9N$

CAS-RN: 134-32-7
Group No.: 31-057
Molar Mass: 143.19

Table 31.57.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	344.6	1	nosp	not specified		avg	DSIO	*94BRU
*99STI/SWA	N	339.0	1	nosp	not specified		avg	DSIO	*81VON
*13CAM	N	324.9–327.9	2	nosp	not specified		*p*	BSIO	13CAM

*94BRU average value in temperature range 333–356 K
*99STI/SWA average value in temperature range 326–352 K
13CAM error 0.5% (information in 29WAS)

Table 31.57.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*94BRU	344.6	1	3.00 #	0.048	4.59–2	0.14	−4.59–2	−1
13CAM	324.9–327.9	2	3.00 #	0.315	3.24–1	0.94	2.90–2	0
Rejected data								
*99STI/SWA	(3.09,10.44,−3.09,−1)							

Table 31.57.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	4	3	0.448	4.61–1	1.34	4.04–3	−1

Temp. range K	A_1	A_2	Level of uncertainty
324.9–344.6	7.46590+1	−1.23873+1	VI

Name: 2,6-Diethylbenzenamine
Formula: $C_{10}H_{15}N$

CAS-RN: 579-66-8
Group No.: 31-058
Molar Mass: 149.24

Table 31.58.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00VER2	298.15	2.050	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 2-(1,1-Dimethylethyl)benzenamine
Formula: $C_{10}H_{15}N$

CAS-RN: 6310-21-0
Group No.: 31-059
Molar Mass: 149.24

Table 31.59.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00VER2	298.15	1.840	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: *N*,*N*-Dimethyloctanamine
Formula: $C_{10}H_{23}N$

CAS-RN: 7378-99-6
Group No.: 31-060
Molar Mass: 157.30

Table 31.60.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97VER	298.15	1.760	nosp	99.95	chrom	*p*	BDHT	69PER/COM

Name: 1-Decanamine
Formula: $C_{10}H_{23}N$

CAS-RN: 2016-57-1
Group No.: 31-061
Molar Mass: 157.30

Table 31.61.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
77BEL/BUB	298.15	2.429	nosp	not specified		*p*	BDCT	68WAD

Name: Octamethylethenetetramine
Formula: $C_{10}H_{24}N_4$

CAS-RN: 996-70-3
Group No.: 31-062
Molar Mass: 200.33

Table 31.62.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI4	N	290.0–480.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

97STE/CHI4 the original equation gives negative heat capacities; the sign of the 2nd parameter was changed to positive

Table 31.62.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	20	0.008	4.01−3	0.01	1.33−6	−2
sat	20	20	0.000	3.34−6	0.00	9.54−7	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
290.0–480.0	2.71350+1	4.89309	3.31419−1	IV
290.0–480.0	2.68310+1	5.07000	3.06000−1	IV

Table 31.62.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	20	0.020	1.02−2	0.02	5.72−6	−3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
290.0–480.0	680.00	−4.79173	1.49242−1	2.47650+1	3.84622+1	IV

Name: 2,6-Bis(1-methylethyl)benzenamine
Formula: $C_{12}H_{19}N$

CAS-RN: 24544-04-5
Group No.: 31-063
Molar Mass: 177.29

Table 31.63.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00VER2	298.15	1.630	nosp	99.99	chrom	p	BDHT	69PER/COM

Name: *N*-Octyl-1-octanamine
Formula: $C_{16}H_{35}N$

CAS-RN: 1120-48-5
Group No.: 31-064
Molar Mass: 241.46

Table 31.64.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86DJO/LAU		315.0	1	nosp	not specified		p	BDHT	69PER/COM
93STE/CHI2	N	300.0–600.0	16	1.00	99.95	chrom	sat	BDHT	89KNI/ARC
93STE/CHI2	same data in 96STE/CHI2								

Table 31.64.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93STE/CHI2	300.0–600.0	16	1.00	0.044	3.40−2	0.04	3.79−5	−2
Rejected data								
86DJO/LAU	(1.66+1,20.85,1.66+1,1)							

Table 31.64.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	17	16	0.051	3.93−2	0.05	3.79−5	−2
sat	17	16	0.045	3.45−2	0.04	3.65−5	−2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–600.0	−9.56055	3.69008+1	−5.57010	3.76343−1	IV
300.0–600.0	−8.01969	3.57090+1	−5.26824	3.51300−1	IV

Table 31.64.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	17	16	0.051	4.07−2	0.05	2.46−5	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
300.0–600.0	734.00	−1.70062	1.36895	1.94358	1.92288+2	−1.54712+2	4.86443+1	IV

Name: *N*,*N*-Dioctyl-1-octanamine
Formula: $C_{24}H_{51}N$

CAS-RN: 1116-76-3
Group No.: 31-065
Molar Mass: 353.68

Table 31.65.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93STE/CHI2	N	298.1–635.0	18	1.00	99.95	chrom	sat	BDHT	89KNI/ARC
93STE/CHI2	same data in 96STE/CHI2								

Table 31.65.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	18	18	0.414	4.86−1	0.41	3.62−3	4

Temp. range K	A_1	A_2	Level of uncertainty
298.1–635.0	4.40178+1	1.54669+1	IV

Name: Acetonitrile
Formula: C_2H_3N

CAS-RN: 75-05-8
Group No.: 32-002
Molar Mass: 41.05

Table 32.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
00LOU	N	321.7	1	nosp	not specified		avg	DSIO	*98LOU
07WAL		291.1	1	nosp	not specified		avg	DSIO	07WAL
65PUT/MCE		234.2–300.6	9	0.30	99.72	melpt	*p*	BSIO	55TAY/JOH
71GOP/GAM		318.0–333.0	eqn	1.00	not specified		*p*	BSAO	71GOP/GAM
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	*p*	BDHT	71DU/COM
78DEV/HEU		298.1	1	1.00	99.8	chrom	*p*	BSIO	70LKB/COM
79DEV/SOM		298.1	1	1.00	99.8	chrom	*p*	BSIO	70LKB/COM
84GUS/MIR		303.1–343.1	3 S	1.60	not specified		*p*	BDHT	84GUS/MIR
87MIR/SHA		253.0–353.0	6	1.90	not specified		*p*	BDHT	84GUS/MIR
90ALP/PES	N	258.1–318.1	4	0.10	not specified		*p*	BSAO	83KUK/KOR
91GRO/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
91KAL/KOH		293.1–313.1	2	1.00	99.95	anal	*p*	FSIT	71PIC/LED
92KOL/KUL1	N	283.1–328.1	2	0.05	not specified		*p*	BSAO	75VYU/ZVE
92KOL/KUL2	N	283.1–323.1	6	0.05	not specified		*p*	BSAO	75VYU/ZVE
92MIY/TAM2		298.1	1	nosp	99.9	chrom	*p*	FSIO	85OGA/MUR
92PIE/SOM		278.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
93NAK/CHU		298.1	1	0.50	99.94	chrom	*p*	FSIO	85OGA/MUR
97HOV/ROU		298.1–298.1	2	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
97NIS/TAM		308.1	1	nosp	99.99	chrom	*p*	FSIO	85OGA/MUR

00LOU average value in temperature range 294–350 K
71HAL/BAL suspect value
90ALP/PES content of water 0.03%
92KOL/KUL1 content of water 0.01% by Karl Fischer method; remaining two data points identical with those in 92KOL/KUL2
92KOL/KUL2 content of water 0.01% by Karl Fischer method; misprint in C_p value 2.2259 corrected to 2.2559

Table 32.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
65PUT/MCE	234.2–300.6	9	0.30 #	0.691	2.25–2	0.21	−1.67–2	−5
71GOP/GAM	318.0–333.0	6	1.00	0.854	9.65–2	0.85	9.01–2	6
78DEV/HEU	298.1	1	1.00	0.076	8.33–3	0.08	8.33–3	1
92KOL/KUL1	283.1–328.1	2	0.30 #	1.669	5.50–2	0.50	3.21–2	0
92KOL/KUL2	283.1–323.1	6	0.30 #	1.115	3.68–2	0.33	8.33–3	0
92PIE/SOM	278.1	1	0.50 #	0.476	2.58–2	0.24	−2.58–2	−1

Rejected data

00LOU	(1.47–2,0.13,1.47–2,1)	07WAL	(2.64–1,2.47,−2.64–1,−1)
71HAL/BAL	(1.09,10.97,−1.09,−1)	79DEV/SOM	(8.33–3,0.08,8.33–3,1)
84GUS/MIR	(1.53,16.02,−1.52,−2)	87MIR/SHA	(1.70,18.66,−1.68,−5)
90ALP/PES	(2.37–1,2.14,1.76–1,2)	91GRO/ROU	(2.08–1,1.92,−2.08–1,−1)
91KAL/KOH	(6.29–1,6.10,−6.05–1,−2)	92MIY/TAM2	(1.92–1,1.78,−1.92–1,−1)
93NAK/CHU	(1.92–1,1.78,−1.92–1,−1)	97HOV/ROU	(1.02–1,0.93,−9.87–2,−2)
97NIS/TAM	(2.23–1,2.05,−2.23–1,−1)		

Table 32.2.3. Parameters of regression polynomial

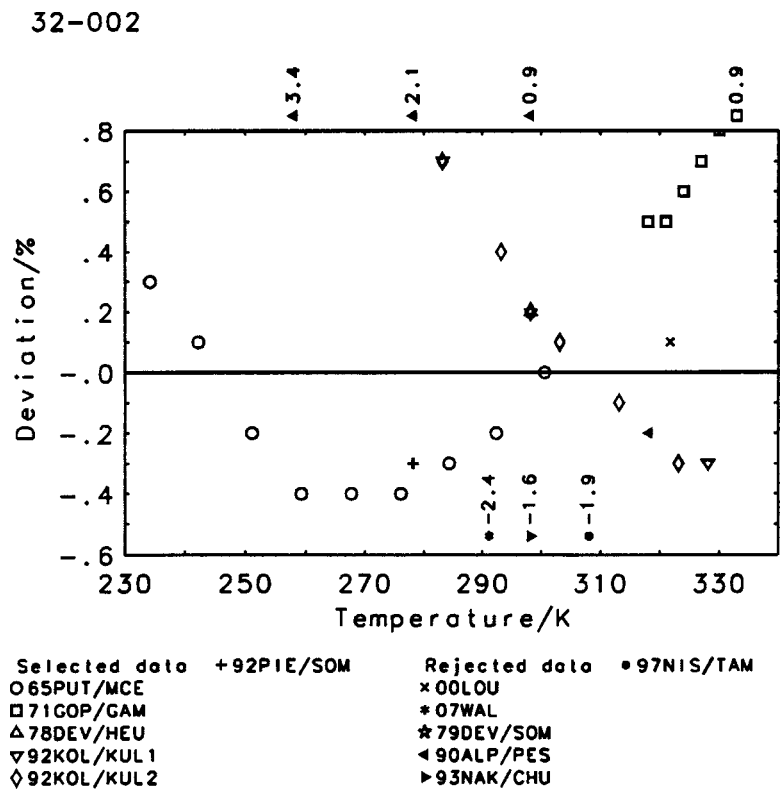
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	50	25	1.084	5.30–2	0.48	1.66–2	3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
234.2–333.0	7.64495	1.57191	−1.49141–1	III

Table 32.2.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	50	25	1.196	4.30−2	0.39	1.31−3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
234.2–333.0	545.50	−5.08391−2	1.56605−4	8.71674	4.12601	III



Name: 2-Propenenitrile
Formula: C_3H_3N

CAS-RN: 107-13-1
Group No.: 32-004
Molar Mass: 53.06

Table 32.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
45DAV/WIE		294.6–312.9	4	nosp	99.	anal	avg	DSIO	45DAV/WIE
67LEB/RAB3		190.1–300.0	13 S	0.50	not specified		p	BSAO	56POP/KOL
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	p	BDHT	71DU/COM
72FIN/MES		196.7–347.1	18	0.20	99.92	melpt	sat	BSAO	47HUF
87MIR/SHA		213.0–333.0	7	1.90	not specified		p	BDHT	84GUS/MIR
97HOV/ROU		298.1	1	nosp	99.	anal	p	FSIT	71PIC/LED

71HAL/BAL suspect value

Name: Propanenitrile
Formula: C_3H_5N

CAS-RN: 107-12-0
Group No.: 32-005
Molar Mass: 55.08

Table 32.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81BER/OGI		243.1–363.1	5 S	nosp	not specified		avg	DSIO	*79BER
00LOU	N	330.3	1	nosp	not specified		avg	DSIO	*98LOU
07WAL		290.1	1	nosp	not specified		*p*	DSIO	07WAL
62WEB/KIL		185.4–297.0	24	0.30	99.958	melpt	*p*	BSIO	55TAY/JOH
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	*p*	BDHT	71DU/COM
85GUS/MIR		303.1–363.1	4	1.70	not specified		*p*	BDHT	84GUS/MIR
87MIR/SHA		193.0–353.0	9	1.90	not specified		*p*	BDHT	84GUS/MIR
97HOV/ROU		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

00LOU average value in temperature range 292–368 K
71HAL/BAL suspect value

Name: Benzonitrile
Formula: C_7H_5N

CAS-RN: 100-47-0
Group No.: 32-021
Molar Mass: 103.12

Table 32.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
00LOU	N	376.6	1	nosp	not specified		avg	DSIO	*98LOU
83BYK/LEB2	N	265.3–328.9	14	0.30	99.88	melpt	*p*	BSAO	76LEB/LIT
85LAI/ROD		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
85TAN/NAK		283.1–318.1	3	0.30	99.9	chrom	*p*	FSIT	71PIC/LED
87MIR/SHA		273.0–453.0	10	1.90	not specified		*p*	BDHT	84GUS/MIR
97TAN/NAK	N	298.1–303.1	2	nosp	not specified		*p*	FSIT	71PIC/LED

00LOU average value in temperature range 294–459 K
83BYK/LEB2 smoothed values in 84LEB/BYK2
97TAN/NAK sample contained a small amount of water <0.1%

Name: *endo*-Bicyclo[2.2.1]heptane-2-carbonitrile
Formula: $C_8H_{11}N$

CAS-RN: 3211-87-8
Group No.: 32-025
Molar Mass: 121.18

Table 32.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
62SER/KOL		340.0–350.0	2 S	nosp	99.88	melpt	*p*	BSAO	62KOL/SER
70KOL/SER	N	332.3–340.2	4	0.15	99.88	melpt	sat	BSAO	62KOL/SER

70KOL/SER smoothed values in 62SER/KOL

Table 32.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
70KOL/SER	332.3–340.2	4	0.15	0.539	2.10–2	0.08	3.39–5	0
Rejected data								
62SER/KOL	(4.01–3,0.02,4.01–3,1)							

Table 32.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	6	6	0.540	2.12−2	0.08	4.80−5	0

Temp. range K	A_1	A_2	Level of uncertainty
332.3–350.0	8.92416	5.06580	III

Name: *exo*-Bicyclo[2.2.1]heptane-2-carbonitrile
Formula: $C_8H_{11}N$

CAS-RN: 3211-90-3
Group No.: 32-026
Molar Mass: 121.18

Table 32.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
62SER/KOL		300.0–310.0	2 S	nosp	99.82	melpt	*p*	BSAO	62KOL/SER
70KOL/SER	N	304.1–311.5	5	0.15	99.82	melpt	sat	BSAO	62KOL/SER

70KOL/SER smoothed values in 62SER/KOL

Table 32.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
62SER/KOL	300.0–310.0	2	0.50 #	0.080	9.62−3	0.04	8.12−3	2
70KOL/SER	304.1–311.5	5	0.15	0.899	3.30−2	0.13	−2.03−4	1

Table 32.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	7	7	0.900	3.35−2	0.14	2.18−3	3

Temp. range K	A_1	A_2	Level of uncertainty
300.0–311.5	7.60384	5.43695	III

Name: Isocyanocyclohexane
Formula: $C_7H_{11}N$

CAS-RN: 931-53-3
Group No.: 32-027
Molar Mass: 109.17

Table 32.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91KIS/PIN	N	281.3–298.1	2	nosp	99.965	melpt	*p*	BSAO	91KIS/PIN

91KIS/PIN data from a graph only

Table 32.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
281.3–298.1	1.26893+1	3.65111	IV

Name: Benzeneacetonitrile
Formula: C_8H_7N

CAS-RN: 140-29-4
Group No.: 32-028
Molar Mass: 117.15

Table 32.28.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00VER1	298.15	1.440	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 4′-Propyl[1,1′-biphenyl]-4-carbonitrile
Formula: $C_{16}H_{15}N$

CAS-RN: 58743-76-3
Group No.: 32-029
Molar Mass: 221.30

Table 32.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91ASA/SOR	340.0–380.0	5 S	nosp	99.89	melpt	*p*	BSAO	83YOS/SOR1

Table 32.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	5	5	0.192	2.88−2	0.06	2.67−5	2

Temp. range K	A_1	A_2	Level of uncertainty
340.0–380.0	2.38269+1	7.27961	III

Name: [*trans(trans)*]-4′-Propyl-[1,1′-bicyclohexyl]-4-carbonitrile
Formula: $C_{16}H_{27}N$

CAS-RN: 65355-35-3
Group No.: 32-030
Molar Mass: 233.40

Table 32.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91ASA/SOR	360.0–380.0	3 S	nosp	99.9	melpt	*p*	BSAO	83YOS/SOR1

Table 32.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	3	0.000	0.00	0.00	−2.42−5	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
360.0–380.0	5.60075+2	−2.72483+2	3.71040+1	III

Name: Piperazine
Formula: $C_4H_{10}N_2$

CAS-RN: 110-85-0
Group No.: 33-007
Molar Mass: 86.14

Table 33.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
88BOB/KAM	413.1–473.1	4	6.00	97.	chrom	sat	BDCT	86MER/BEN
97STE/CHI4	385.0–505.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 33.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
97STE/CHI4	385.0–505.0	25	1.00	0.007	2.23–3	0.01	1.37–6	0
Rejected data								
88BOB/KAM	(1.15,3.84,1.09,4)							

Table 33.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	29	25	0.008	2.38–3	0.01	1.37–6	0
sat	29	25	0.000	2.42–6	0.00	1.14–6	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
385.0–505.0	3.64303	5.32653	9.59349–2	IV
385.0–505.0	2.14000	6.08400	9.59349–2	IV

Table 33.7.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	29	25	0.004	1.08–3	0.00	−2.14–6	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
385.0–505.0	652.80	−7.88230–1	4.11134–3	2.57659	3.77801+1	IV

Name: Pyridine
Formula: C_5H_5N

CAS-RN: 110-86-1
Group No.: 33-008
Molar Mass: 79.10

Table 33.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
00LOU	N	337.7	1	nosp	not specified		avg	DSIO	*98LOU
03CON/WHI		308.6–333.1	6	nosp	not specified		avg	DSIO	03CON/WHI
16BRA		283.1–323.1	2	nosp	not specified		avg	DSTO	16BRA
17MAT/KRA		294.1	1	nosp	not specified		*p*	BSIO	49WEI
31SWI/RYB2	N	290.1	1	nosp	not specified		*p*	BDHT	31SWI/RYB2
34RAD/JUL		289.1	1	nosp	not specified		*p*	BSIO	49WEI
36PAR/TOD1	N	230.0–300.0	8 S	0.70	not specified		*p*	BSIO	25PAR
36PEA/BAK		233.1–298.1	8 S	nosp	not specified		*p*	BSIO	36PEA/BAK
47PUS/FED		284.0–306.9	5	nosp	not specified		*p*	DSIO	47PUS/FED
57MCC/DOU		239.7–346.7	13	0.20	99.92	melpt	sat	BSAO	47HUF
58SWI/ZIE1	N	332.1–348.8	2	nosp	not specified		avg	DSIO	58SWI/ZIE1
67RAS/GAN		293.1–353.1	4 S	0.50	not specified		*p*	BSAO	67RAS/GAN
92LAI/ROD		298.1	1	nosp	99.8	anal	*p*	FSIT	71PIC/LED
93NAN/BHA		303.1	1	nosp	not specified		*p*	BSIO	93NAN/BHA
94GRO/ROU		298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED
94LAI/WIL		298.1	1	nosp	99.8	anal	*p*	FSIT	71PIC/LED
96CHI/STE		360.0–560.0	11 S	1.00	99.9	chrom	sat	BDHT	89KNI/ARC

00LOU average value in temperature range 295–381 K
31SWI/RYB2 same datum in 31SWI/RYB1
36PAR/TOD1 high sample purity
58SWI/ZIE1 average values in temperature ranges 295–369 K and 295–402 K

Table 33.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
57MCC/DOU	239.7–346.7	13	0.20	0.091	2.97–3	0.02	−3.39–4	−2
96CHI/STE	360.0–560.0	11	1.00	0.291	6.92–2	0.29	1.05–2	5
Rejected data								
00LOU	(1.85–1,1.08,1.85–1,1)		03CON/WHI	(8.49–2,0.51,−4.08–2,−2)				
16BRA	(1.89–1,1.16,−5.79–2,0)		17MAT/KRA	(3.10–1,1.99,−3.10–1,−1)				
31SWI/RYB2	(5.15–1,3.16,5.15–1,1)		34RAD/JUL	(1.70–1,1.09,−1.70–1,−1)				
36PAR/TOD1	(1.67–1,1.05,1.49–1,7)		36PEA/BAK	(3.45–1,2.43,−9.62–2,1)				
47PUS/FED	(1.93–1,1.22,−1.18–1,−3)		58SWI/ZIE1	(7.67–1,4.31,7.64–1,2)				
67RAS/GAN	(2.00–1,1.16,1.81–1,4)		92LAI/ROD	(1.47–1,0.93,−1.47–1,−1)				
93NAN/BHA	(1.73,9.71,1.73,1)		94GRO/ROU	(1.37–1,0.87,−1.37–1,−1)				
94LAI/WIL	(1.63–1,1.03,−1.63–1,−1)							

Table 33.8.3. Parameters of cubic spline polynomials

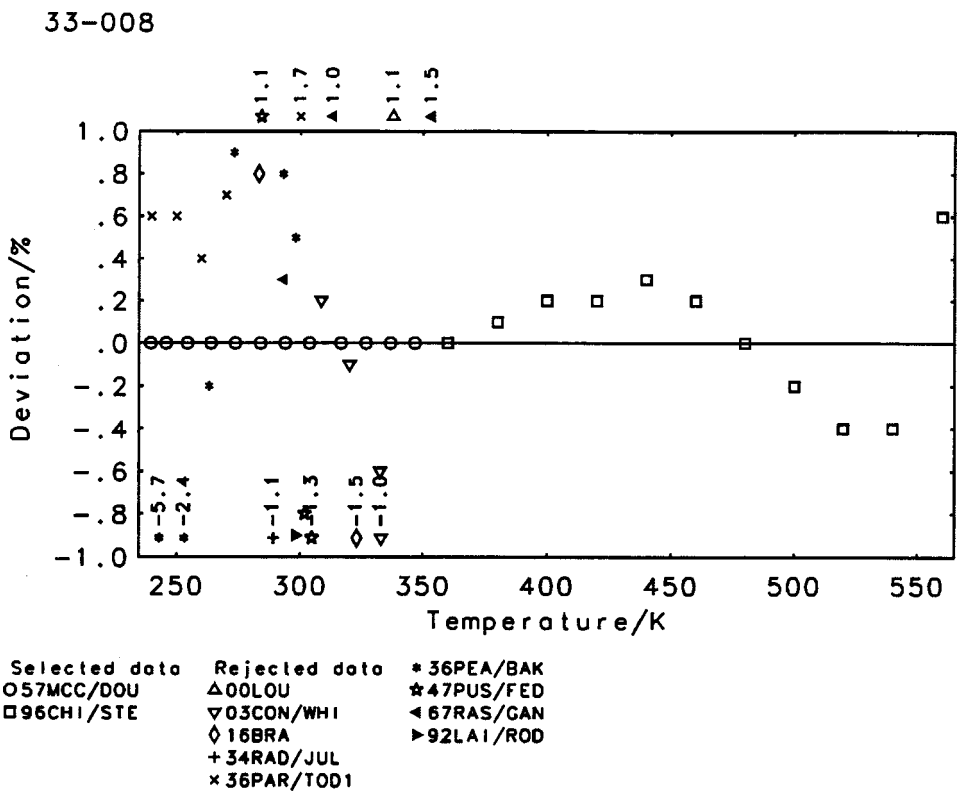
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	67	24	0.234	5.27–2	0.22	4.64–3	3
sat	67	24	0.134	2.43–2	0.10	1.91–3	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
239.7–350.0	1.51863+1	−2.80185	1.31862	−9.79324−2	II
350.0–560.0	4.63252	6.24426	−1.26598	1.48220−1	IV
239.7–350.0	1.44307+1	−2.02288	1.05351	−6.81397−2	II
350.0–560.0	1.03394+1	1.48393	5.15615−2	2.72838−2	IV

Table 33.8.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	67	24	0.286	4.57–2	0.19	−1.09–3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
239.7–560.0	620.00	−1.25405	1.34769−2	1.15487+1	3.25601	6.81733	3.83162	IV



Name: Piperidine
Formula: $C_5H_{11}N$

CAS-RN: 110-89-4
Group No.: 33-012
Molar Mass: 85.15

Table 33.12.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
00LOU	N	331.6	1	nosp	not specified		avg	DSIO	*98LOU
34RAD/JUL		290.1	1	nosp	not specified		*p*	BSIO	49WEI
36KUR/VOS	N	311.1	1	nosp	not specified		avg	DSIO	36KUR/VOS
64MOE/THO		297.4–327.3	4	0.50	not specified		*p*	BSIO	64MOE/THO
76CON/GIA		298.1	1	nosp	not specified		*p*	BDCT	76CON/GIA
88MES/TOD	N	267.3–361.9	12	0.05	99.941	melpt	sat	BSAO	47HUF
92LAI/ROD		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
94LAI/WIL		298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED

00LOU average value in temperature range 293–371 K
36KUR/VOS average value in temperature range 290–333 K
88MES/TOD same data in 87MES/TOD and smoothed data in 86STE/CHI

Name: 2-Methylpyridine
Formula: C_6H_7N

CAS-RN: 109-06-8
Group No.: 33-013
Molar Mass: 93.13

Table 33.13.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
01KAH	N	346.1	1	nosp	not specified		avg	DSIO	01KAH
03CON/WHI		321.1–343.1	8	nosp	not specified		avg	DSIO	03CON/WHI
63SCO/HUB		209.9–369.0	19	0.20	99.9	melpt	sat	BSAO	47HUF
99CHI/KNI		400.0–560.0	9 S	1.00	99.9	melpt	sat	BDHT	89KNI/ARC

01KAH average value in temperature range 295–397 K

Table 33.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
03CON/WHI	321.1–343.1	8	1.00 #	0.298	6.09–2	0.30	3.48–2	4
63SCO/HUB	209.9–369.0	19	0.20	0.238	9.28–3	0.05	−1.18–3	0
99CHI/KNI	400.0–560.0	9	1.00	0.311	8.03–2	0.31	3.23–2	4
Rejected data								
01KAH	(2.57–1,1.26,−2.57–1,−1)							

Table 33.13.3. Parameters of cubic spline polynomials

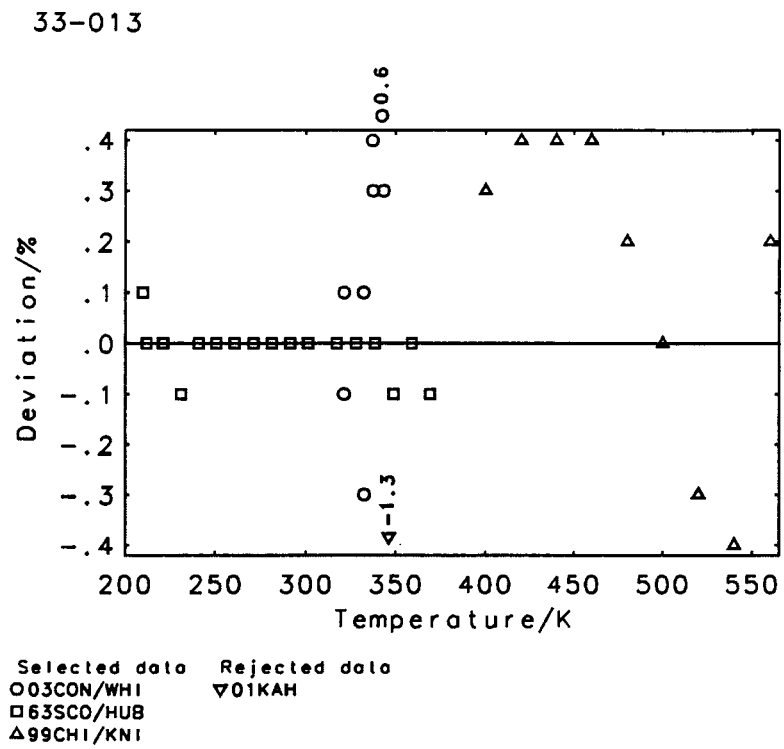
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	37	36	0.293	5.37–2	0.23	1.52–2	8
sat	37	36	0.313	4.99–2	0.22	1.70–2	8

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
209.9–340.0	2.37260+1	−9.06926	3.48555	−3.25295−1	II
340.0–560.0	5.32498	7.16692	−1.28980	1.42877−1	IV
209.9–340.0	2.32013+1	−8.48894	3.27555	−3.00430−1	II
340.0–560.0	9.75883	3.37208	−2.12980−1	4.15828−2	IV

Table 33.13.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	37	36	2.505	1.18−1	0.58	1.60−2	−8

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
209.9–560.0	621.00	8.64910−1	4.31072−3	1.35402+1	6.51225	1.01230+1	5.72341	IV



Name: 3-Methylpyridine
Formula: C_6H_7N

CAS-RN: 108-99-6
Group No.: 33-014
Molar Mass: 93.13

Table 33.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
03CON/WHI	320.5–348.3	8	nosp	not specified		avg	DSIO	03CON/WHI
63SCO/GOO	257.5–387.9	16	0.20	99.88	melpt	sat	BSAO	47HUF
99CHI/KNI	400.0–560.0	9 S	1.00	99.93	melpt	sat	BDHT	89KNI/ARC

Table 33.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
03CON/WHI	320.5–348.3	8	1.00 #	0.490	9.89−2	0.49	5.85−2	4
63SCO/GOO	257.5–387.9	16	0.20	0.181	7.28−3	0.04	−1.63−3	−4
99CHI/KNI	400.0–560.0	9	1.00	0.159	3.96−2	0.16	2.18−2	4

Table 33.14.3. Parameters of cubic spline polynomials

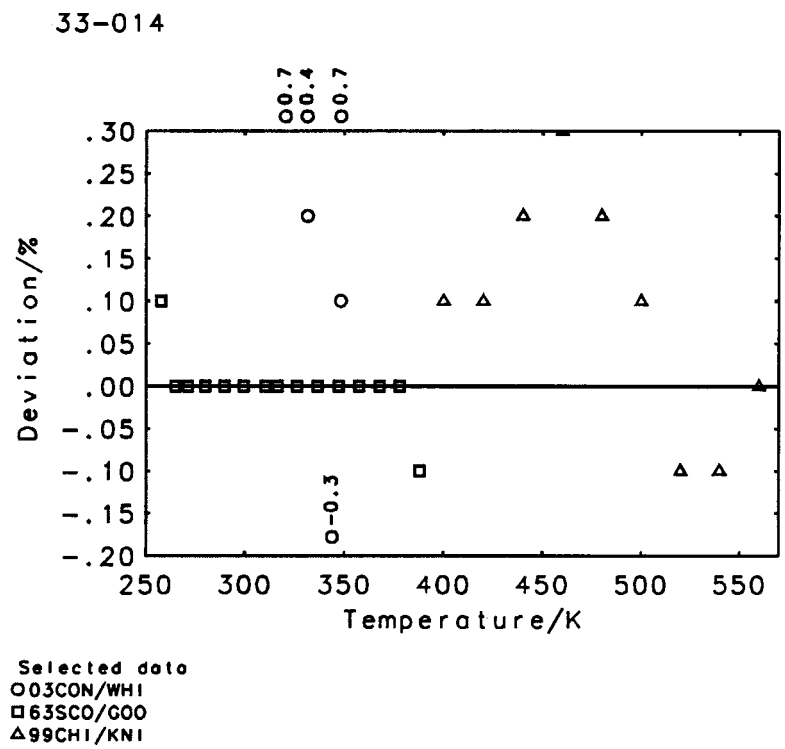
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	33	33	0.309	5.77−2	0.28	1.93−2	4
sat	33	33	0.319	5.80−2	0.28	1.98−2	7

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
257.5–370.0	1.96048+1	−4.56237	1.94680	−1.59016−1	II
370.0–560.0	5.67693	6.73053	−1.10534	1.15951−1	IV
257.5–370.0	1.92557+1	−4.23937	1.84887	−1.49306−1	II
370.0–560.0	9.81193	3.41772	−2.20615−1	3.71340−2	IV

Table 33.14.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	33	33	0.864	9.21−2	0.39	1.26−2	−2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
257.5–560.0	645.00	−2.86767	1.60530−1	1.11484+1	1.28069+1	IV



Name: 4-Methylpyridine
Formula: C_6H_7N

CAS-RN: 108-89-4
Group No.: 33-015
Molar Mass: 93.13

Table 33.15.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
88MES/TOD	N	283.2–394.8	16	0.05	99.967	melpt	sat	BSAO	47HUF
99CHI/KNI		420.0–560.0	8 S	1.00	99.93	melpt	sat	BDHT	89KNI/ARC

88MES/TOD same data in 87MES/TOD and smoothed data in 86STE/CHI

Table 33.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
88MES/TOD	283.1–394.9	16	0.05	0.442	4.62–3	0.02	2.29–5	2
99CHI/KNI	420.0–560.0	8	1.00	0.138	3.78–2	0.14	−1.61–2	−6

Table 33.15.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	24	24	0.416	2.49–2	0.09	−5.36–3	−4
sat	24	24	0.400	1.11–2	0.04	−2.48–3	−4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
283.2–400.0	1.84907+1	−3.45402	1.57883	−1.17233−1	II
400.0–560.0	5.54138	6.25798	−8.49167−1	8.51002−2	IV
283.2–400.0	1.90002+1	−3.94975	1.73904	−1.34425−1	II
400.0–560.0	9.45220	3.21122	−5.12002−2	1.47620−2	IV

Table 33.15.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	24	24	0.553	8.38–2	0.31	−2.02–2	−4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
283.1–560.0	646.00	3.28009	5.21276−2	1.36909+1	8.96082	1.19609+1	6.93308	IV

Name: 2,4-Dimethyl-1*H*-pyrrole
Formula: C_6H_9N

CAS-RN: 625-82-1
Group No.: 33-016
Molar Mass: 95.14

Table 33.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86STE/CHI	268.4–450.0	22 S	nosp	99.979	melpt	sat	BSAO	47HUF
94CHI/HOS2	272.8–441.0	19	0.10	99.98	melpt	sat	BSAO	88STE/ARC

Table 33.16.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
94CHI/HOS2	272.8–441.0	19	0.10	0.175	4.25–3	0.02	2.01–6	−2
			Rejected data					
86STE/CHI	(3.27–2,0.12,−2.11–2,−18)							

Table 33.16.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	41	19	0.204	4.95–3	0.02	2.01–6	−2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
272.8–340.0	2.14764+1	−8.53282	4.63307	−5.31985−1	II
340.0–441.0	−6.57180	1.62156+1	−2.64587	1.81637−1	II

Table 33.16.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	41	19	0.523	1.34–2	0.05	6.63–6	−2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
272.8–441.0	671.00	1.48726+1	9.81701−1	5.07390	5.63294+1	II

Name: 2,3-Dimethylpyridine
Formula: C_7H_9N

CAS-RN: 583-61-9
Group No.: 33-024
Molar Mass: 107.16

Table 33.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86STE/CHI	258.6–450.0	23 S	nosp	99.86	melpt	sat	BSAO	47HUF
94CHI/HOS1	266.7–441.2	20	0.10	99.85	melpt	sat	BSAO	88STE/ARC
95STE/CHI2	460.0–640.0	10 S	1.00	99.85	melpt	sat	BDHT	89KNI/ARC

Table 33.24.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
94CHI/HOS1	266.7–441.3	20	0.10	0.318	8.02–3	0.03	−2.31–4	4
95STE/CHI2	460.0–640.0	10	1.00	0.374	1.42–1	0.37	4.82–2	8
			Rejected data					
86STE/CHI	(1.94–2,0.07,−1.20–2,−17)							

Table 33.24.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	53	30	0.378	9.19−2	0.24	1.59−2	12
sat	53	30	0.343	6.67−2	0.19	1.53−2	13

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
266.7–470.0	2.13071+1	−3.28745	1.61952	−1.16620−1	II
470.0–590.0	−1.05855+2	7.78799+1	−1.56501+1	1.10818	IV
590.0–640.0	−1.64002+4	8.36312+3	−1.41993+3	8.04460+1	IV
266.7–470.0	2.18290+1	−3.78952	1.77943	−1.33479−1	II
470.0–590.0	−7.21004+1	5.61654+1	−1.09769+1	7.71229−1	IV
590.0–640.0	−9.64091+3	4.92166+3	−8.35637+2	4.73622+1	IV

Table 33.24.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	53	30	1.805	4.21−1	1.08	−1.14−1	−6

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
266.7–640.0	655.40	−3.63159	2.17054−1	1.33285+1	1.51903+1	V

Name: 2,4-Dimethylpyridine
Formula: C_7H_9N

CAS-RN: 108-47-4
Group No.: 33-025
Molar Mass: 107.16

Table 33.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86STE/CHI	209.4–450.0	28 S	nosp	99.44	melpt	sat	BSAO	47HUF
94CHI/HOS1	207.4–440.2	29	0.10	99.8	melpt	sat	BSAO	88STE/ARC
95STE/CHI2	460.0–620.0	9 S	1.00	99.8	melpt	sat	BDHT	89KNI/ARC

Table 33.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94CHI/HOS1	207.4–440.2	28	0.10	0.739	1.76−2	0.07	−3.25−5	5
95STE/CHI2	460.0–620.0	9	1.00	0.294	1.11−1	0.29	1.78−2	7
Rejected data								
86STE/CHI	(1.29−2,0.05,−2.55−3,0)							

Table 33.25.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	66	37	0.720	6.19–2	0.17	4.31–3	12
sat	66	37	0.682	4.71–2	0.14	5.19–3	11

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
207.4–400.0	2.45428+1	−7.07613	2.80298	−2.32546−1	II
400.0–550.0	−7.18802	1.67220+1	−3.14655	2.63249−1	IV
550.0–620.0	−2.31155+3	1.27365+3	−2.31679+2	1.41137+1	IV
207.4–400.0	2.47121+1	−7.26207	2.86987	−2.40424−1	II
400.0–550.0	−2.06215	1.28187+1	−2.15032	1.77925−1	IV
550.0–620.0	−1.33825+3	7.41649+2	−1.34665+2	8.20911	IV

Table 33.25.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	66	37	3.087	6.11–1	1.62	−8.69–2	−6

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
207.4–620.0	647.00	−1.01583	5.29410−3	1.65502+1	4.47637	1.06979+1	7.39079	V

Name: 2,5-Dimethylpyridine
Formula: C_7H_9N

CAS-RN: 589-93-5
Group No.: 33-026
Molar Mass: 107.16

Table 33.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86STE/CHI	259.1–450.0	23 S	nosp	99.64	melpt	sat	BSAO	47HUF
94CHI/HOS1	253.9–441.1	22	0.20	99.65	melpt	sat	BSAO	88STE/ARC
95STE/CHI2	460.0–620.0	9 S	1.00	99.65	melpt	sat	BDHT	89KNI/ARC

Table 33.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94CHI/HOS1	253.9–441.1	22	0.20	0.465	2.30–2	0.09	−1.15–4	1
95STE/CHI2	460.0–620.0	9	1.00	0.436	1.50–1	0.44	1.11–2	−3
Rejected data								
86STE/CHI	(7.04–2,0.26,−3.23–2,−8)							

Table 33.26.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	54	31	0.499	9.10−2	0.27	3.13−3	−2
sat	54	31	0.414	6.40−2	0.20	3.66−3	−4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
253.9–550.0	1.56602+1	1.14140	3.24711−1	1.11290−2	II
550.0–620.0	−3.07167+3	1.68514+3	−3.05857+2	1.85676+1	IV
253.9–550.0	1.69939+1	−1.07099−1	7.09780−1	−2.80124−2	II
550.0–620.0	−1.91375+3	1.05303+3	−1.90769+2	1.15768+1	IV

Table 33.26.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	54	31	1.095	1.25−1	0.38	−2.69−2	−2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
253.9–620.0	644.20	−3.48050	1.93587−1	1.25139+1	1.56440+1	IV

Name: 2,6-Dimethylpyridine
Formula: C_7H_9N

CAS-RN: 108-48-5
Group No.: 33-027
Molar Mass: 107.16

Table 33.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86STE/CHI	267.0–440.0	21 S	nosp	99.884	melpt	sat	BSAO	47HUF
93PER/QUI	288.1–318.1	6	nosp	99.9	chrom	*p*	FSIT	71PIC/LED
94CHI/HOS1	272.6–435.3	27	0.10	99.9	melpt	sat	BSAO	88STE/ARC
95STE/CHI2	460.0–600.0	8 S	1.00	99.90	melpt	sat	BDHT	89KNI/ARC

Table 33.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94CHI/HOS1	272.6–435.3	27	0.10	0.351	8.75−3	0.04	−1.77−4	1
95STE/CHI2	460.0–600.0	8	1.00	0.566	2.02−1	0.57	6.43−2	2
Rejected data								
86STE/CHI	(2.65−2,0.10,−1.53−2,−13)		93PER/QUI	(1.49,6.20,1.48,6)				

Table 33.27.3. Parameters of cubic spline polynomials

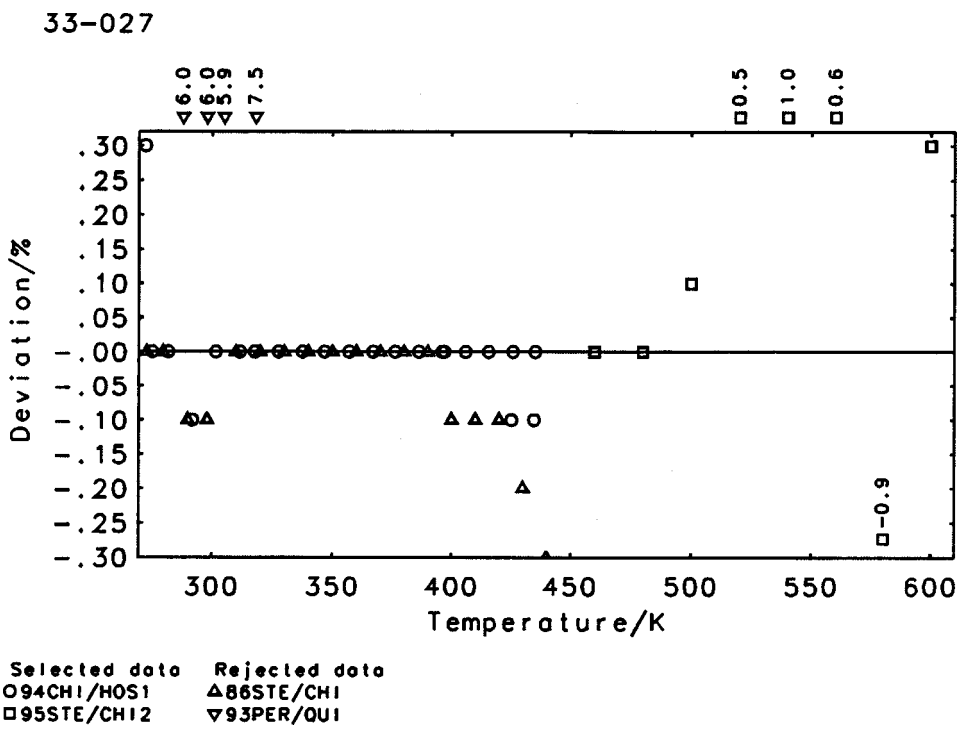
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	62	35	0.443	1.05−1	0.29	1.46−2	3
sat	62	35	0.350	6.40−2	0.19	9.36−3	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
272.6–520.0	1.48696+1	1.14493	4.90649−1	−1.36343−2	II
520.0–600.0	−1.96302+3	1.14223+3	−2.18950+2	1.40531+1	IV
272.6–520.0	1.60980+1	3.20483−4	8.44498−1	−4.99595−2	II
520.0–600.0	−1.22270+3	7.14690+2	−1.36596+2	8.76032	IV

Table 33.27.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	62	35	0.948	2.34−1	0.64	−5.58−2	−5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
272.6–600.0	623.80	−3.33659	1.66524−1	1.18146+1	1.67136+1	V



Name: 3,4-Dimethylpyridine
Formula: C_7H_9N

CAS-RN: 583-58-4
Group No.: 33-028
Molar Mass: 107.16

Table 33.28.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
84POD/RAC	N	264.6–378.0	76	1.00	not specified		sat	BSAO	84POD/RAC
86STE/CHI		262.7–450.0	22 S	nosp	99.71	melpt	sat	BSAO	47HUF
94CHI/HOS1		257.1–440.0	24	0.10	99.71	melpt	sat	BSAO	88STE/ARC
95STE/CHI2		460.0–660.0	11 S	1.00	99.71	melpt	sat	BDHT	89KNI/ARC

84POD/RAC only a graph given in the paper; experimental values provided by the author

Table 33.28.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
94CHI/HOS1	257.1–440.0	24	0.10	0.639	1.58–2	0.06	−8.43–5	2
95STE/CHI2	460.0–660.0	11	1.00	0.575	2.05–1	0.57	2.41–2	−3
Rejected data								
84POD/RAC	(3.94–1,1.62,2.66–1,60)		86STE/CHI	(3.72–2,0.13,−1.77–2,−7)				

Table 33.28.3. Parameters of cubic spline polynomials

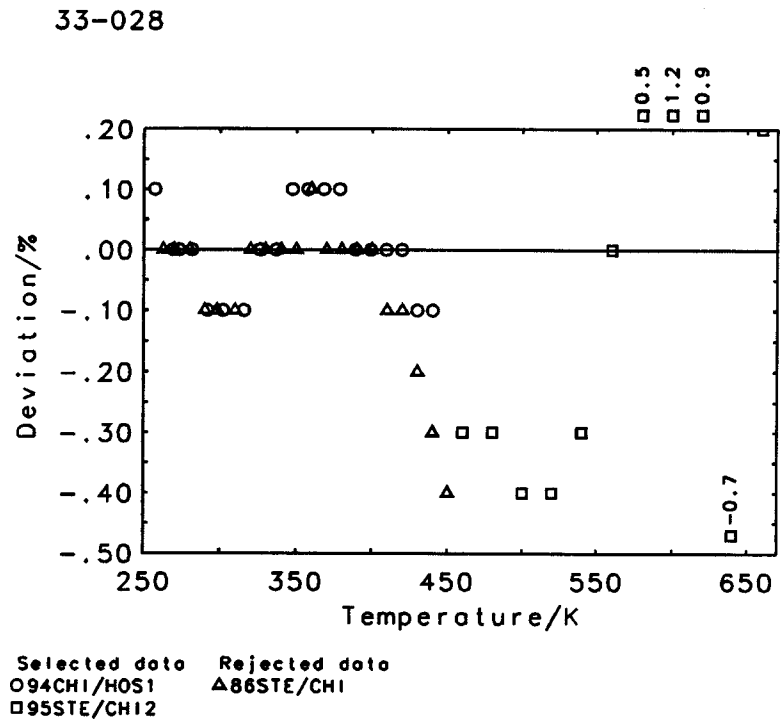
Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	133	35	0.669	1.25–1	0.35	7.52–3	−1
sat	133	35	0.569	8.71–2	0.25	7.10–3	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
257.1–580.0	2.27968+1	−3.59956	1.54519	−1.02281−1	II
580.0–660.0	−3.06368+3	1.59285+3	−2.73705+2	1.57167+1	IV
257.1–580.0	2.36564+1	−4.39421	1.78725	−1.26580−1	II
580.0–660.0	−1.94776+3	1.01530+3	−1.74023+2	9.97744	IV

Table 33.28.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	133	35	2.157	6.23–1	1.63	−1.35–1	−7

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
257.1–660.0	683.80	−2.24155	3.69063–2	1.67356+1	7.28774	8.50874	2.86793	V



Name: 3,5-Dimethylpyridine
Formula: C_7H_9N

CAS-RN: 591-22-0
Group No.: 33-029
Molar Mass: 107.16

Table 33.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86STE/CHI	266.8–450.0	22 S	nosp	99.812	melpt	sat	BSAO	47HUF
94CHI/HOS1	274.0–444.6	19	0.10	99.85	melpt	sat	BSAO	88STE/ARC
95STE/CHI2	460.0–640.0	10 S	1.00	99.85	melpt	sat	BDHT	89KNI/ARC

Table 33.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94CHI/HOS1	274.0–444.6	19	0.10	0.458	1.11–2	0.05	−2.02–4	1
95STE/CHI2	460.0–640.0	10	1.00	0.398	1.43–1	0.40	4.15–2	0
Rejected data								
86STE/CHI	(1.69–2,0.06,−8.51–3,−4)							

Table 33.29.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	51	29	0.481	9.26−2	0.26	1.42−2	1
sat	51	29	0.393	6.22−2	0.18	1.34−2	6

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
274.0–560.0	1.75853+1	−6.87410−1	8.99997−1	−4.99111−2	II
560.0–640.0	−2.06755+3	1.11635+3	−1.98570+2	1.18233+1	IV
274.0–560.0	1.87014+1	−1.69828	1.20242	−7.98039−2	II
560.0–640.0	−1.28091+3	6.94520+2	−1.23122+2	7.32048	IV

Table 33.29.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	51	29	1.362	3.96−1	1.06	−8.39−2	−9

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
274.0–640.0	667.20	−2.73382	7.09301−2	1.37202+1	1.25552+1	5.40477	7.29739−1	V

Name: 1-Methyl-1*H*-imidazole
Formula: $C_4H_6N_2$

CAS-RN: 616-47-7
Group No.: 33-047
Molar Mass: 82.11

Table 33.47.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99MO/YAN	278.1–370.1	20	1.50	99.995	chrom	*p*	BDHT	99MO/YAN

Table 33.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	20	0.187	6.55−2	0.28	3.12−4	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
278.1–370.1	−9.71410+1	9.93687+1	−2.76867+1	2.60835	V

Name: 1-Methyl-1*H*-pyrazole
Formula: $C_4H_6N_2$

CAS-RN: 930-36-9
Group No.: 33-048
Molar Mass: 82.11

Table 33.48.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99MO/YAN	278.1–370.1	20	1.50	99.995	chrom	*p*	BDHT	99MO/YAN

Table 33.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	20	0.304	1.03−1	0.46	7.44−4	−4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
278.1–370.1	−1.76537+2	1.85062+2	−5.86111+1	6.29076	V

Name: 1,4,5,6-Tetrahydropyrimidine
Formula: $C_4H_8N_2$

CAS-RN: 1606-49-1
Group No.: 33-049
Molar Mass: 84.12

Table 33.49.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93STE/CHI2	N	298.15	1.878	1.00	99.95	chrom	p	BDHT	89KNI/ARC
93STE/CHI2	same datum in 96STE/CHI2								

Name: [1,2,4]Triazolo[1,5-*a*]pyrimidine
Formula: $C_5H_4N_4$

CAS-RN: 275-02-5
Group No.: 33-050
Molar Mass: 120.11

Table 33.50.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI4	420.0–525.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 33.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	22	22	0.000	1.04−6	0.00	−5.20−7	0

Temp. range K	A_1	A_2	Level of uncertainty
420.0–525.0	1.41060+1	2.62000	IV

Name: 1-Ethyl-1*H*-imidazole
Formula: $C_5H_8N_2$

CAS-RN: 7098-07-9
Group No.: 33-051
Molar Mass: 96.13

Table 33.51.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99RIB/RIB	280.1–365.2	18	1.50	99.8	anal	p	BDHT	94CHE/FER

Table 33.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	18	18	0.419	1.50−1	0.63	1.56−3	−6

Temp. range K	A_1	A_2	A_3	Level of uncertainty
280.1–365.2	2.44984+1	−4.89346	1.40524	V

Name: 1-Ethyl-1*H*-pyrazole
Formula: $C_5H_8N_2$

CAS-RN: 2817-71-2
Group No.: 33-052
Molar Mass: 96.13

Table 33.52.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99RIB/RIB	280.3–365.4	18	1.50	99.55	anal	*p*	BDHT	94CHE/FER

Table 33.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	18	18	0.766	2.72−1	1.15	4.99−3	−2

Temp. range K	A_1	A_2	Level of uncertainty
280.3–365.4	−2.16103	8.24471	V

Name: 1-Phenyl-1*H*-imidazole
Formula: $C_9H_8N_2$

CAS-RN: 7164-98-9
Group No.: 33-053
Molar Mass: 144.18

Table 33.53.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00RIB/RIB	268.2–381.2	24	1.50	99.87	chrom	*p*	BDHT	99MO/YAN

Table 33.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	24	24	0.206	9.52−2	0.31	5.16−4	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
268.2–381.2	3.20365+1	−5.92266	1.73783	V

Name: 1-Phenyl-1*H*-pyrazole
Formula: $C_9H_8N_2$

CAS-RN: 1126-00-7
Group No.: 33-054
Molar Mass: 144.18

Table 33.54.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00RIB/RIB	268.2–381.2	24	1.50	99.99	chrom	*p*	BDHT	99MO/YAN

Table 33.54.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	24	24	0.166	7.41–2	0.25	3.25–4	−6

Temp. range K	A_1	A_2	A_3	Level of uncertainty
268.2–381.2	9.54797	7.10078	−3.16458–1	V

Name: *trans*-(±)-Decahydroquinoline
Formula: $C_9H_{17}N$

CAS-RN: 105728-23-2
Group No.: 33-055
Molar Mass: 139.24

Table 33.55.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94STE/CHI	328.9–440.3	13	0.10	99.984	melpt	sat	BSAO	88STE/ARC

Table 33.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	13	13	0.133	4.53–3	0.01	6.46–6	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
328.9–440.3	5.88105+1	−2.71574+1	7.66551	−5.75137−1	II

Table 33.55.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	13	13	0.870	3.03–2	0.09	3.86–5	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
328.9–440.3	705.00	−9.62303	2.71438	1.68127+1	8.52889	III

Name: 1-(Phenylmethyl)-1*H*-pyrazole
Formula: $C_{10}H_{10}N_2$

CAS-RN: 10199-67-4
Group No.: 33-056
Molar Mass: 158.20

Table 33.56.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99MO/YAN	280.0–392.0	25	1.50	99.995	chrom	*p*	BDHT	99MO/YAN

Table 33.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	25	25	0.001	3.31–4	0.00	−3.20–6	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
280.0–392.0	1.73706+2	−1.38524+2	4.34371+1	−4.36168	V

Name: Diphenyldiazene
Formula: $C_{12}H_{10}N_2$

CAS-RN: 103-33-3
Group No.: 34-011
Molar Mass: 182.22

Table 34.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	350.6	1	nosp	not specified		avg	DSIO	*94BRU
08BOG/WIN	N	356.6	1	nosp	not specified		avg	DSIO	08BOG/WIN

*94BRU average value in temperature range 343–358 K
08BOG/WIN average value in temperature range 341–372 K

Table 34.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
Selected data								
*94BRU	350.6	1	5.00 #	0.437	8.61–1	2.18	8.61–1	1
08BOG/WIN	356.6	1	5.00 #	0.418	7.90–1	2.09	−7.90–1	−1

Table 34.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
C	2	2	0.604	1.17	3.02	3.53–2	0

Temp. range K	A_1	Level of uncertainty
350.6–356.6	3.85698+1	VI

Name: (*E*)-Diphenyldiazene
Formula: $C_{12}H_{10}N_2$

CAS-RN: 17082-12-1
Group No.: 34-012
Molar Mass: 182.22

Table 34.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
84VAN/BOU	344.6–356.2	4	nosp	99.87	melpt	*p*	BSAO	79SCH/OFF
85BOU/DEL	343.6–408.4	27	nosp	99.84	melpt	*p*	BSAO	85BOU/DEL
96STE/CHI3	355.0–635.0	14	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 34.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
85BOU/DEL	343.6–408.4	27	0.50 #	0.260	5.08–2	0.13	−9.02–3	−1
96STE/CHI2	355.0–635.0	14	1.00	0.396	1.68–1	0.40	7.20–2	4
Rejected data								
84VAN/BOU	(1.91–1,0.52,−1.89–1,−4)							

Table 34.12.3. Parameters of cubic spline polynomials

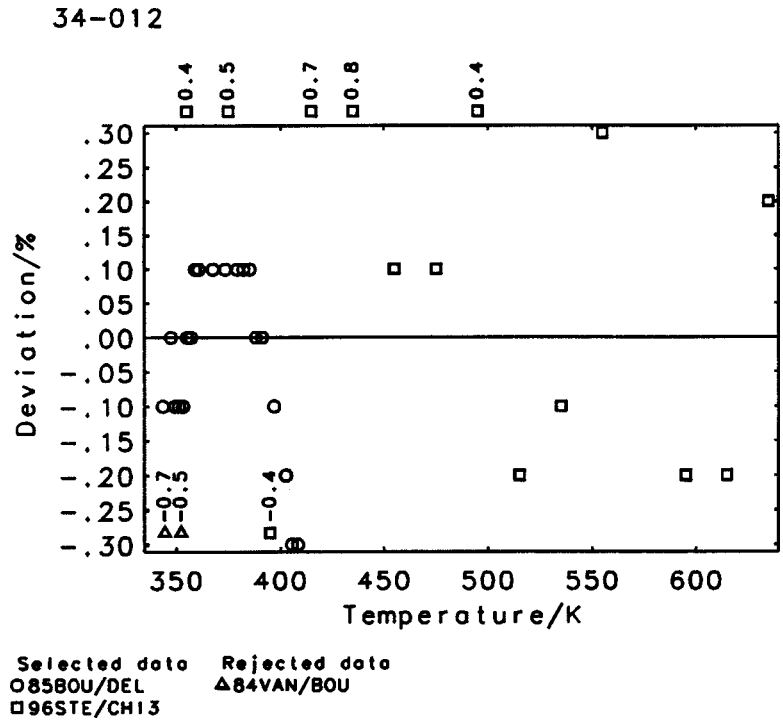
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	45	41	0.334	1.14–1	0.27	1.87–2	3
sat	45	41	0.335	1.13–1	0.27	1.87–2	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
343.6–500.0	7.28195+1	−3.49979+1	9.65244	−7.41769−1	IV
500.0–635.0	−1.47656+2	9.72873+1	−1.68046+1	1.02203	IV
343.6–500.0	7.32400+1	−3.53131+1	9.73063	−7.48185−1	IV
500.0–635.0	−1.44816+2	9.55207+1	−1.64361+1	9.96266−1	IV

Table 34.12.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	45	41	0.448	1.94–1	0.42	1.89–2	−11

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
343.6–635.0	830.00	5.35612+1	3.03579	1.92402+1	6.96822+1	5.66097+1	2.85280+1	IV



Name: Cyanoguanidine
Formula: $C_2H_4N_4$

CAS-RN: 461-58-5
Group No.: 34-014
Molar Mass: 84.08

Table 34.14.1. Experimental heat capacities

Reference	Temp. range K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97ZHA/TAN	495.00	3.147	1.00	99.9	chrom	*p*	BDHT	96KAB/BLO

Name: Dimethoxymethane
Formula: $C_3H_8O_2$

CAS-RN: 109-87-5
Group No.: 41-002
Molar Mass: 76.10

Table 41.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		295.7–300.9	3 S	nosp	not specified		avg	DSIO	*81VON
64MCE/KIL	N	171.1–307.8	31	nosp	99.9	chrom	*p*	BSIO	55TAY/JOH
90TRE	N	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED

64MCE/KIL error below and above 250 K 0.03% and 0.3%, respectively
90TRE measured by D'Arcy P.Y. and Halpin C.Y. (personal communication)

Name: 1,2-Dimethoxyethane
Formula: $C_4H_{10}O_2$

CAS-RN: 110-71-4
Group No.: 41-007
Molar Mass: 90.12

Table 41.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
73KUS/SUU		298.1	1	0.10	not specified		*p*	DDCT	71KON/SUU
90TRE	N	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
96STE/CHI3	N	315.0–535.0	12	1.00	99.95	chrom	sat	BDHT	89KNI/ARC
99BUR/ZOC		298.1–323.1	2	2.00	99.5	chrom	*p*	FSIO	99BUR/ZOC

90TRE measured by D'Arcy P.Y. and Halpin C.Y. (personal communication)
96STE/CHI3 value at 535 K was not included in fit; heat capacity shows large drop on passing into the fluid phase

Table 41.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
73KUS/SUU	298.1	1	0.10	0.057	1.34–3	0.01	1.34–3	0
96STE/CHI3	315.0–515.0	11	1.00	1.482	4.51–1	1.48	2.39–3	−1
			Rejected data					
90TRE	(2.49–1,1.08,−2.49–1,−1)		91TRE/COS	(2.59–1,1.12,−2.59–1,−1)				
99BUR/ZOC	(6.64–1,2.88,−6.35–1,−2)							

Table 41.7.3. Parameters of regression polynomial

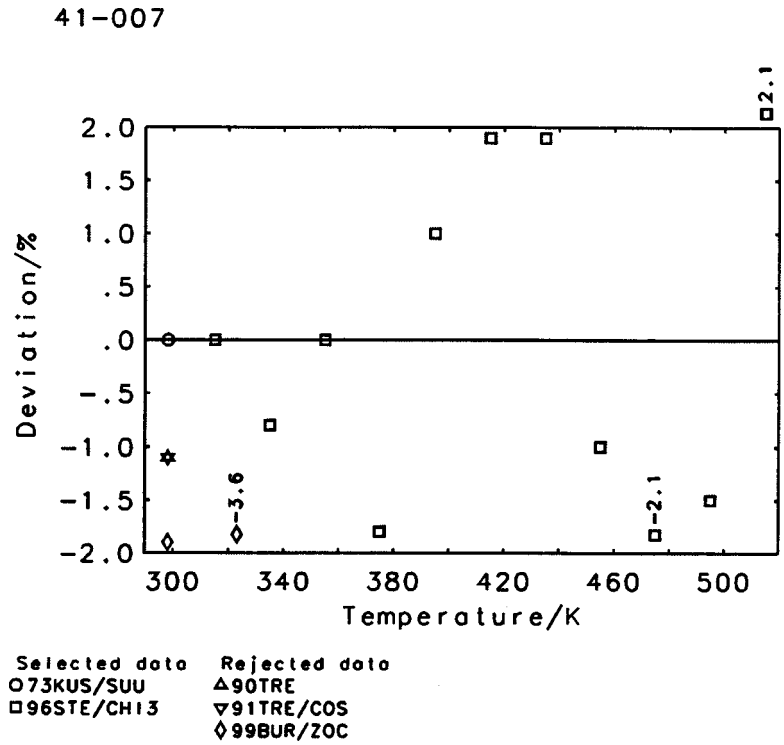
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	17	12	1.738	5.29–1	1.74	2.30–3	−1
sat	17	12	1.221	3.49–1	1.22	2.12–2	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
298.1–515.0	−3.21787+1	4.59037+1	−1.30685+1	1.31056	V
298.1–515.0	3.31684+1	−8.01721	1.57325	1.31056	V

Table 41.7.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	17	12	1.370	3.59–1	1.37	−4.61–2	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
298.1–515.0	537.00	−2.63759	2.24900−1	1.63059+1	7.73332	V



Name: 1-Methoxybutane
Formula: $C_5H_{12}O$

CAS-RN: 628-28-4
Group No.: 41-009
Molar Mass: 88.15

Table 41.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
75AND/MAR		160.2–315.7	52	nosp	99.98	melpt	*p*	BSAO	63AND/COU1
82VIL/CAS		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
90TRE	N	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED

90TRE measured by D'Arcy P.Y. and Halpin C.Y. (personal communication)

Name: 1-(Ethenyloxy)butane
Formula: $C_6H_{12}O$

CAS-RN: 111-34-2
Group No.: 41-013
Molar Mass: 100.16

Table 41.13.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
47SCH/ZOS		298.1	1	nosp	not specified		*p*	not specified	
96STE/CHI3	N	315.0–535.0	12	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

96STE/CHI3 value at 535 K was not included in fit; heat capacity shows large drop on passing into the fluid phase

Table 41.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
96STE/CHI2	315.0–515.0	11	1.00	0.812	2.70–1	0.81	4.77–3	−1

Table 41.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	13	11	1.017	3.38−1	1.02	4.77−3	−1
sat	13	11	0.857	2.53−1	0.86	2.64−3	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
315.0–515.0	−2.05604+2	1.70764+2	−4.20464+1	3.53885	V
315.0–515.0	−1.45476+2	1.22607+2	−2.92739+1	2.41580	V

Table 41.13.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	13	11	1.106	3.18−1	1.11	4.12−3	−3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
315.0–515.0	540.50	4.44252−1	4.48362−1	−2.76648+1	1.59346+2	−1.46859+2	5.03113+1	V

Name: 1,1′-Oxybispropane
Formula: $C_6H_{14}O$

CAS-RN: 111-43-3
Group No.: 41-017
Molar Mass: 102.18

Table 41.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
75AND/COU		160.6–322.7	66	nosp	99.97	melpt	*p*	BSAO	63AND/COU1
83KIM/TRE		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
90TRE	N	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED

90TRE measured by D'Arcy P.Y. and Halpin C.Y. (personal communication)

Name: 2,2′-Oxybispropane
Formula: $C_6H_{14}O$

CAS-RN: 108-20-3
Group No.: 41-018
Molar Mass: 102.18

Table 41.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
33PAR/HUF		194.5–293.1	8	1.00	not specified		*p*	BSIO	25PAR
61ROU	N	296.1–318.1	2	nosp	not specified		*p*	BSAO	61ROU
74AND/COU		187.8–340.0	19 S	nosp	99.86	melpt	*p*	BSAO	63AND/COU1
90TRE	N	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91GRO/ROU		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
93GRO/ROU		298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED
94GRO/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED

61ROU constant value in temperature range 296–318 K obtained by the author
90TRE measured by D'Arcy P.Y. and Halpin C.Y. (personal communication)

Name: 1,1′-Oxybis(2-methoxyethane) CAS-RN: 111-96-6
Formula: $C_6H_{14}O_3$ Group No.: 41-022
Molar Mass: 134.18

Table 41.22.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
66BEA/CLE		210.0–350.0	16	nosp	99.62	melpt	*p*	BSAO	33SOU/BRI
82VIL/CAS		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
83KIM/DAR		298.1	1	0.30	99.	chrom	*p*	FSIT	71PIC/LED
90TRE	N	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91NAK/SOE		298.1	1	nosp	99.9	chrom	*p*	FSIO	85OGA/MUR
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
97TOV/CAR3		298.1	1	nosp	99.5	anal	*p*	BDCT	83ROU/ROU
99BUR/ZOC		298.1–323.1	2	2.00	99.5	chrom	*p*	FSIO	99BUR/ZOC

90TRE measured by D'Arcy P.Y. and Halpin C.Y. (personal communication)

Name: 1,1′-Oxybisbutane CAS-RN: 142-96-1
Formula: $C_8H_{18}O$ Group No.: 41-034
Molar Mass: 130.23

Table 41.34.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
38PAN/DUD	N	298.0–363.0	eqn	nosp	not specified		*p*	not specified	
87COB/CAS		298.1–298.1	2	nosp	99.	anal	*p*	FSIT	71PIC/LED
96TAN/TOY1		298.1	1	nosp	99.9	chrom	*p*	FSIT	71PIC/LED
97TOV/CAR3		298.1	1	nosp	99.0	anal	*p*	BDCT	83ROU/ROU

38PAN/DUD temperature range of parameters validity estimated by the compilers

Table 41.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
87COB/CAS	298.1	2	0.50 #	0.466	7.80–2	0.23	−7.78–2	−2
96TAN/TOY1	298.1	1	0.50 #	0.467	7.85–2	0.23	7.85–2	1
97TOV/CAR3	298.1	1	0.50 #	0.467	7.85–2	0.23	7.85–2	1

Table 41.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	9	4	0.539	9.04–2	0.27	3.65–4	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	3.35326+1	III

Name: 2,5,8,11-Tetraoxadodecane
Formula: $C_8H_{18}O_4$

CAS-RN: 112-49-2
Group No.: 41-037
Molar Mass: 178.23

Table 41.37.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
66BEA/CLE		230.0–350.0	14	nosp	99.44	melpt	*p*	BSAO	33SOU/BRI
85BEN/KUM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
90TRE	N	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
97TOV/CAR1	N	288.1–308.1	3	nosp	99.0	anal	*p*	BDCT	83ROU/ROU
99BUR/ZOC		298.1–323.1	2	2.00	99.5	chrom	*p*	FSIO	99BUR/ZOC

90TRE measured by D'Arcy P.Y. and Halpin C.J. (personal communication)
97TOV/CAR1 same data for temperatures 288.15 K and 298.15 K in 97TOV/CAR2

Table 41.37.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
66BEA/CLE	230.0–350.0	14	1.50 #	0.089	5.87–2	0.13	−3.91–2	−9
85BEN/KUM	298.1	1	0.50 #	0.749	1.66–1	0.37	−1.66–1	−1
91TRE/COS	298.1	1	0.50 #	0.487	1.08–1	0.24	−1.08–1	−1
97TOV/CAR1	288.1–308.1	3	0.50 #	0.518	1.15–1	0.26	1.13–1	3
Rejected data								
90TRE	(2.52–1,0.57,−2.52–1,−1)		99BUR/ZOC	(3.16–1,0.70,2.75–1,2)				

Table 41.37.3. Parameters of regression polynomial

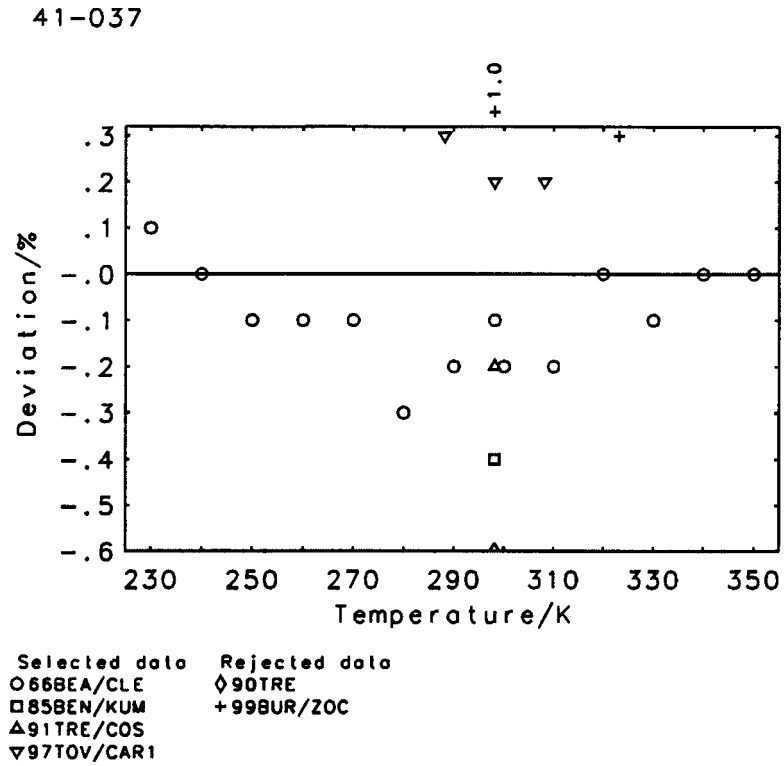
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	22	19	0.338	9.20–2	0.21	−2.54–2	−8

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
230.0–350.0	8.04670+1	−3.56519+1	1.11721+1	−1.09955	V

Table 41.37.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	22	19	0.358	1.34–1	0.30	−1.77–2	−3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
230.0–350.0	651.00	7.98194+1	3.00805+1	1.34937+1	5.29507+1	V



Name: 2,5,8,11,14-Pentaoxapentadecane
Formula: $C_{10}H_{22}O_5$

CAS-RN: 143-24-8
Group No.: 41-044
Molar Mass: 222.28

Table 41.44.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
65KRI/LOE		293.0–426.1	13	nosp	99.5	chrom	*p*	not specified	
91TRE/COS		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
97TOV/CAR2	N	288.1–308.1	3	nosp	98.0	anal	*p*	BDCT	83ROU/ROU
97TOV/CAR3		298.1	1	nosp	98.0	anal	*p*	BDCT	83ROU/ROU
99BUR/ZOC		298.1–323.1	2	2.00	99.5	chrom	*p*	FSIO	99BUR/ZOC

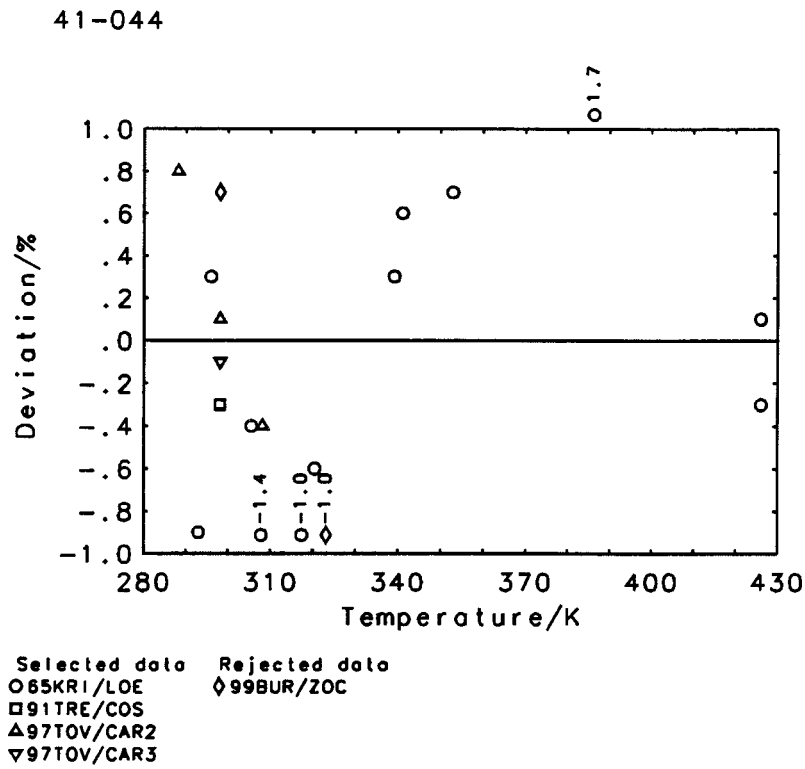
97TOV/CAR2 same data in 97TOV/CAR1

Table 41.44.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
65KRI/LOE	293.0–426.1	13	2.00 #	0.410	4.69–1	0.82	1.04–2	1
91TRE/COS	298.1	1	0.50 #	0.683	1.88–1	0.34	−1.88–1	−1
97TOV/CAR2	288.1–308.1	3	0.50 #	1.008	2.78–1	0.50	7.49–2	1
97TOV/CAR3	298.1	1	0.50 #	0.105	2.90–2	0.05	−2.90–2	−1
Rejected data								
99BUR/ZOC	(4.81–1,0.86,−1.06–1,0)							

Table 41.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	18	0.597	4.42−1	0.77	7.93−3	0
Temp. range K		A_1	A_2				Level of uncertainty
288.1–426.1		4.20772+1	4.38930				V



Name: 1,1′-[Oxybis(2,1-ethanediyloxy)]bisbutane
Formula: $C_{12}H_{26}O_3$

CAS-RN: 112-73-2
Group No.: 41-047
Molar Mass: 218.34

Table 41.47.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		p	not specified	
99BUR/ZOC		298.1–323.1	2	2.00	96.5	chrom	p	FSIO	99BUR/ZOC

52CUR/JOH technical product, purity in question

Table 41.47.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
52CUR/JOH	293.1	1	3.00 #	2.931	4.16	8.79	−4.16	−1
99BUR/ZOC	298.1–323.1	2	2.00	1.969	2.18	3.94	1.26	0

Table 41.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	3	4.043	5.17	10.41	−5.46−1	−1

Temp. range K	A_1	A_2	Level of uncertainty
293.1–323.1	8.54901−3	1.75305+1	VI

Name: 1,1′-[Methylenebis(oxy)]bisethane
Formula: $C_5H_{12}O_2$

CAS-RN: 462-95-3
Group No.: 41-049
Molar Mass: 104.15

Table 41.49.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
90TRE	N	298.15	1.814	nosp	not specified		p	FSIT	71PIC/LED
90TRE	measured by D'Arcy P.Y. and Halpin C.Y. (personal communication)								

Name: 1,1′-[Oxybis(methylene)]bisbenzene
Formula: $C_{14}H_{14}O$

CAS-RN: 103-50-4
Group No.: 41-050
Molar Mass: 198.26

Table 41.50.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00BEC/AUF	295.6–335.0	9	0.20	99.95	chrom	sat	BDCT	#00BEC/AUF

Table 41.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	9	9	0.324	2.59−2	0.06	2.50−5	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
295.6–335.0	1.29218	1.97460+1	−2.35823	III

Name: 1,1′-Oxybisoctane
Formula: $C_{16}H_{34}O$

CAS-RN: 629-82-3
Group No.: 41-051
Molar Mass: 242.45

Table 41.51.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86DJO/LAU	315.00	2.456	nosp	not specified		p	BDHT	69PER/COM

Name: Methanol-*d*
Formula: CH_3DO

CAS-RN: 1455-13-6
Group No.: 42-001
Molar Mass: 33.05

Table 42.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
49STA/GUP	180.0–270.0	10	0.50	not specified		*p*	BSAO	49STA/GUP
92FIL/AFA	298.1	1	nosp	not specified		*p*	BDCT	92FIL/AFA

Table 42.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
49STA/GUP	180.0–270.0	10	0.50	0.824	3.76–2	0.41	6.81–4	−2
92FIL/AFA	298.1	1	1.00 #	0.146	1.46–2	0.15	−1.46–2	−1

Table 42.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	11	11	0.923	4.24–2	0.46	−7.05–4	−3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
180.0–298.1	1.01695+1	−1.97701	6.43701−1	IV

Name: Methanol
Formula: CH_4O

CAS-RN: 67-56-1
Group No.: 42-002
Molar Mass: 32.04

Table 42.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
07WAL		292.1	1	nosp	not specified		avg	DSIO	07WAL
25DRU/WEI		293.1	1	nosp	not specified		*p*	BSIO	25DRU/WEI
25PAR		188.4–290.1	8	0.50	not specified		*p*	BSIO	25PAR
29KEL1		181.1–292.0	14	1.00	not specified		*p*	BSIO	29KEL1
29MIT/HAR1		190.5–264.8	18	nosp	not specified		*p*	BSIO	29MIT/HAR1
31FIO/GIN	N	318.1–378.1	7 S	0.10	99.97	estim	sat	BSIO	31FIO/GIN
39PHI		300.8	1	nosp	not specified		*p*	BSIO	49WEI
49STA/GUP		180.0–270.0	10 S	0.50	not specified		*p*	BSAO	49STA/GUP
49TSC/RIC2		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
50HOU/MAS2		323.1–353.1	4 S	0.40	99.8	estim	*p*	BSAO	50SAG/HOU
60SWI/ZIE	N	311.6	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
62KAT		283.1–333.1	4	nosp	not specified		*p*	BSIO	62KAT
66DRA/LAN	N	298.1	1	nosp	not specified		*p*	BSIO	66DRA/LAN
68PAZ/REC	N	313.1	1	nosp	not specified		*p*	BDCT	70PAZ/PAZ
71CAR/WES		180.0–320.0	17 S	nosp	99.975	melpt	*p*	BSAO	68WES/FUR
71DES/BHA		298.1–318.1	3 S	1.00	not specified		*p*	BSIO	58MUR/VAN
71GOP/GAM		308.0–333.0	eqn	1.00	not specified		*p*	BSAO	71GOP/GAM
81ATA/ELS		293.1	1	2.50	not specified		*p*	BDHO	81ATA/ELS
82BEN/DAR		288.1–308.1	2	nosp	not specified		*p*	FSIT	71PIC/LED
82VIL/CAS		298.1	1	0.30	99.8	chrom	*p*	FSIT	71PIC/LED
84ZEG/SOM2		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
85COS/PAT8		298.1–313.1	2	nosp	not specified		*p*	FSIT	71PIC/LED
86KOR/KUK		278.0–298.0	2	0.20	not specified		*p*	BSAO	83KUK/KOR
86OGA/MUR		298.1	1	0.10	not specified		*p*	FSIO	85OGA/MUR
86TAN/TOY		298.1	1	0.30	99.96	anal	*p*	FSIT	71PIC/LED
87LAN/CRI	N	298.1–313.1	2	nosp	not specified		*p*	FSIO	87LAN/CRI
88AND/PAT		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
88BOY/CRI	N	393.1–503.1	5	nosp	not specified		*p*	FSIO	87LAN/CRI
88OKA/OGA	N	298.1–299.1	2	nosp	not specified		*p*	FSIO	85OGA/MUR
89DOU/KHA		298.1	1	nosp	99.8	estim	*p*	FSIT	71PIC/LED
92FIL/AFA		298.1	1	nosp	not specified		*p*	BDCT	92FIL/AFA
93CON/GIR1		298.0–343.0	eqn	5.00	not specified		sat	BDHT	93CON/GIR1
93NAZ/BAS		298.1–325.5	2	2.20	99.5	anal	*p*	BDHO	86NAZ/BAS1
97RIG/COM		308.1	1	1.00	not specified		*p*	BDHT	95DIO/MAN

31FIO/GIN	data calculated using procedure by 85WIL/CHA
60SWI/ZIE	average value in temperature range 294–329 K
66DRA/LAN	grade: pure, water content 0.08%
68PAZ/REC	same datum in 70PAZ/PAZ
87LAN/CRI	C_p at 298.15 K measured by Picker calorimeter (71PIC/LED)
88BOY/CRI	original data measured at 8.3 MPa converted to vapor pressure
88OKA/OGA	water content below 0.083 mol.%

Name: Ethanol
Formula: C_2H_6O

CAS-RN: 64-17-5
Group No.: 42-005
Molar Mass: 46.07

Table 42.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
07WAL		291.6	1	nosp	not specified		avg	DSIO	07WAL
20GIB/PAR		196.2–271.4	11	nosp	not specified		*p*	BSIO	20GIB/LAT
24WIL/DAN		300.0–332.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
25PAR	N	160.0–298.0	7 S	0.50	not specified		*p*	BSIO	25PAR
29KEL2		163.5–294.3	20	1.00	99.96	estim	*p*	BSIO	29KEL1
29MIT/HAR1		184.4–268.8	25	nosp	not specified		*p*	BSIO	29MIT/HAR1
31BLA/LEI		303.1–343.1	9	3.00	not specified		*p*	BSIO	31BLA/LEI
31FIO/GIN	N	318.1–378.1	7 S	0.10	not specified		sat	BSIO	31FIO/GIN
36ERN/WAT		298.1	1	nosp	not specified		*p*	BSIO	49WEI
39BYK		298.1	1	nosp	not specified		*p*	BSIT	39BYK
40MAZ		174.1–297.8	46	nosp	not specified		*p*	BSIO	39MAZ3
49TSC/RIC2		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
60SWI/ZIE	N	316.5	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
62RAB/NIK		288.1–328.1	9 S	0.30	not specified		*p*	BSAO	47SKU
65KAU/BIT		293.1–349.1	11	1.00	not specified		*p*	FSIO	65KAU/BIT
66HWA/ZIE		165.3–304.2	41	nosp	99.95	chrom	*p*	BSAO	45SCO/MEY
66KLE		293.1–343.1	11 S	0.10	not specified		*p*	BSAO	66KLE
67GRA		308.1–338.1	6	1.00	not specified		*p*	BSIO	67GRA
67NIK/RAB2		160.0–250.0	19 S	0.20	not specified		*p*	BSAO	56POP/KOL
68PAZ/REC	N	313.1	1	nosp	not specified		*p*	BDCT	70PAZ/PAZ
75PED/KAY		300.8–344.2	16	nosp	not specified		*p*	BSIO	75PED/KAY
76FOR/BEN1		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
76FOR/BEN2		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
77HAI/SUG2		161.3–301.1	54	nosp	99.86	melpt	sat	BSAO	65SUG/SEK
78BYV/JAS		293.1–333.1	3	2.00	not specified		*p*	BDCT	78BYV/JAS
79BRO/ZIE		159.0–306.0	eqn	nosp	99.94	melpt	*p*	BSAO	45SCO/MEY
82BEN/DAR		288.1–308.1	2	0.30	not specified		*p*	FSIT	71PIC/LED
82VIL/CAS		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
84STE/OLS		266.1–318.1	11 S	nosp	not specified		*p*	BDHT	69PER/COM
84ZEG/SOM2		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
85OGA		298.1	1	0.20	not specified		*p*	FSIO	85OGA/MUR
86KOR/KUK		298.0	1	0.20	not specified		*p*	BSAO	83KUK/KOR
86OGA/MUR		298.1	1	0.10	not specified		*p*	FSIO	85OGA/MUR
86TAN/TOY		298.1	1	0.30	99.96	anal	*p*	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
89PET/PES1	N	258.1–318.1	4	0.20	not specified		*p*	BSAO	83KUK/KOR
94CON/GIA2		298.1	1	nosp	99.9	anal	*p*	FSIT	88CON/GIA
95CON/GIA		298.1	1	nosp	99.9	anal	*p*	FSIT	88CON/GIA
95LOW/PEU		298.2	1	1.00	not specified		*p*	BDCO	95LOW/PEU
96TAN/TOY1		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED

25PAR	same data in 27PAR/HUF
31FIO/GIN	data calculated using procedure by 85WIL/CHA
60SWI/ZIE	average value in temperature range 294–339 K
68PAZ/REC	same datum in 70PAZ/PAZ
89PET/PES1	same data in 90ALP/PES

Name: 1,2-Ethanediol
Formula: $C_2H_6O_2$

CAS-RN: 107-21-1
Group No.: 42-006
Molar Mass: 62.07

Table 42.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*98LOU	N	378.1–382.1	2	nosp	not specified		avg	DSIO	*98LOU
01DEF	N	309.4–349.1	2	nosp	not specified		avg	not specified	
02LOU1	N	380.6	1	nosp	not specified		avg	DSIO	*98LOU
09SCH		295.1–308.1	2	nosp	not specified		*p*	BSIO	09SCH
25PAR/KEL	N	262.0–293.0	6	nosp	99.	estim	*p*	BSIO	25PAR
32NEU/KUR		293.4–351.5	3	nosp	not specified		*p*	BSIO	32NEU
57CRU/JOS		293.1–338.1	2	2.00	not specified		*p*	BSIO	57CRU/JOS
62RAB/NIK		283.1–328.1	10 S	0.30	not specified		*p*	BSAO	47SKU
65TUN/MIS		298.1	1	nosp	not specified		*p*	BSIO	49WEI
67NIK/RAB1		265.0–310.0	10 S	nosp	not specified		*p*	BSAO	56POP/KOL
68PAZ/REC	N	301.1–313.1	2	nosp	not specified		*p*	BDCT	70PAZ/PAZ
72KAW/OTA		303.1	1	1.00	not specified		*p*	BSIO	49WEI
77MUR/SUB		298.1	1	0.30	not specified		*p*	BSIO	64MOE/THO
79STE/TAM		273.1–493.1	15 S	nosp	99.9	chrom	sat	BDHT	69PER/COM
82ZAR		298.0–363.0	3	0.60	99.7	chrom	*p*	BDCT	82ZAR
88MUK/ZAR		298.7–433.3	6	nosp	not specified		*p*	BDCT	82ZAR
91DOU/PAL		298.1	1	nosp	99.5	estim	*p*	FSIT	71PIC/LED

*98LOU average values in temperature ranges 295–461 K and 296–468 K
01DEF average values in temperature ranges 286–412 K and 286–333 K; calorimeter not identified, probably drop
02LOU1 average value in temperature range 293–468 K
25PAR/KEL original values decreased by 1.5%—correction for water content, recommendation given in 85WIL/CHA
68PAZ/REC same data in 70PAZ/PAZ

Table 42.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
25PAR/KEL	262.0–293.0	6	1.00 #	0.590	1.00–1	0.59	−9.34–2	−6
62RAB/NIK	283.1–328.1	10	0.30	1.129	6.31–2	0.34	−1.31–2	−5
67NIK/RAB1	265.0–310.0	10	0.50 #	1.168	1.07–1	0.58	8.69–2	10
68PAZ/REC	301.1–313.1	2	0.70 #	1.099	1.41–1	0.77	−8.42–2	0
77MUR/SUB	298.1	1	0.30	0.420	2.27–2	0.13	2.27–2	1
79STE/TAM	273.1–493.1	15	1.00 #	0.239	4.98–2	0.24	2.40–2	9
82ZAR	298.0–363.0	3	0.60	1.418	1.70–1	0.85	−7.64–2	1
88MUK/ZAR	298.7–433.3	6	1.00 #	1.157	2.26–1	1.16	−1.53–1	−4

Rejected data

*98LOU	(3.56–1,1.73,−3.56–1,−2)	01DEF	(2.07–1,1.07,−1.95–1,−2)
02LOU1	(2.93–1,1.38,2.93–1,1)	09SCH	(1.71–1,0.96,−4.66–2,0)
32NEU/KUR	(3.14–1,1.68,−3.08–1,−3)	57CRU/JOS	(4.94,18.70,3.35,0)
65TUN/MIS	(2.60–1,1.47,−2.60–1,−1)	72KAW/OTA	(7.03–1,4.03,−7.03–1,−1)
91DOU/PAL	(2.31–1,1.30,−2.31–1,−1)		

Table 42.6.3. Parameters of regression polynomial

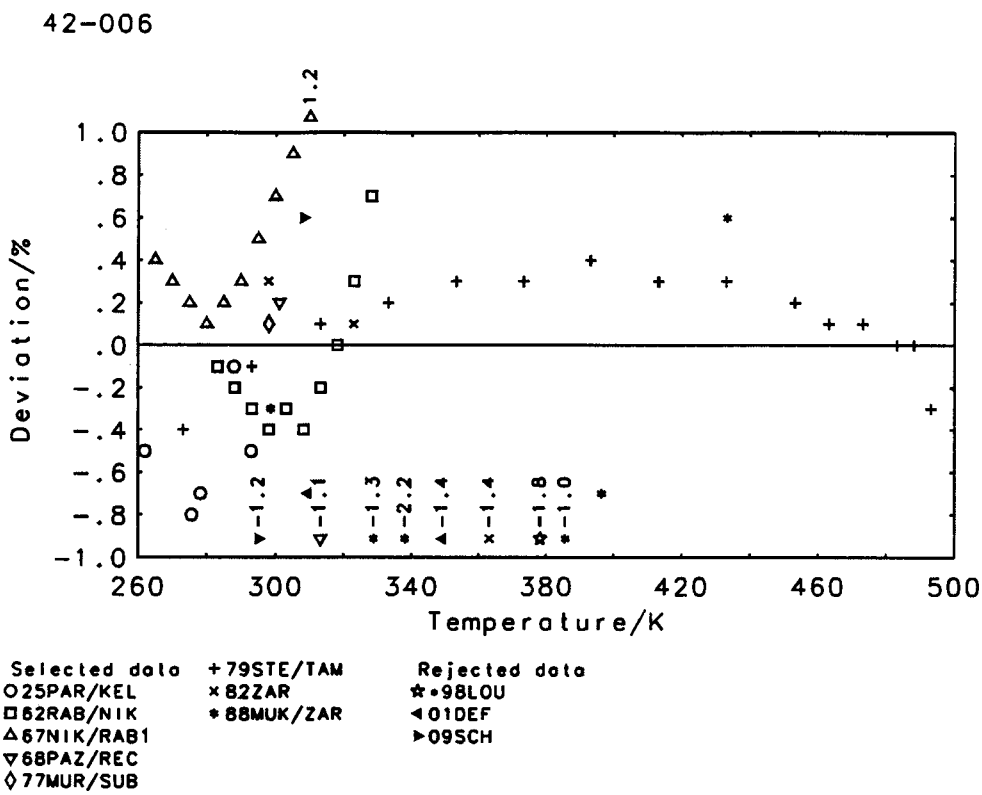
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	68	53	0.959	1.17−1	0.61	−1.43−2	6
sat	68	53	0.959	1.17−1	0.62	−1.40−2	5

Temp. range K	A_1	A_2	A_3	Level of uncertainty
262.0–493.1	5.88415	4.37971	−1.09376−1	IV
262.0–493.1	5.83706	4.40987	−1.14176−1	IV

Table 42.6.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	68	53	1.004	1.22−1	0.64	−1.33−2	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
262.0–493.1	790.00	−2.21957	1.54794−1	4.16324	4.02706+1	−2.03507+1	3.66559	IV



Name: 1-Propanol
Formula: C_3H_8O

CAS-RN: 71-23-8
Group No.: 42-009
Molar Mass: 60.10

Table 42.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
20GIB/PAR		165.7–274.6	29	nosp	not specified		*p*	BSIO	20GIB/LAT
26PAR/HUF	N	152.1–275.0	7	nosp	not specified		*p*	BSIO	25PAR
27PAR/HUF		169.1–275.3	7	nosp	not specified		*p*	BSIO	25PAR
29MIT/HAR1		162.8–274.4	35	nosp	not specified		*p*	BSIO	29MIT/HAR1
39PHI		301.1	1	nosp	not specified		*p*	BSIO	49WEI
41ZHD		279.6–318.8	5	nosp	not specified		*p*	BSIT	34KOL/UDO
49TSC/RIC2		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
51EUC/EIG		273.0–393.0	12 S	nosp	not specified		sat	BSAO	51EUC/EIG
60SWI/ZIE	N	320.9	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
68COU/LEE		153.9–361.5	47	0.10	99.75	melpt	*p*	BSAO	63AND/COU1
68PAZ/REC	N	313.1	1	nosp	not specified		*p*	BDCT	70PAZ/PAZ
68REC1	N	298.0–313.0	eqn	nosp	not specified		*p*	BSAO	68REC1
76FOR/BEN1		298.1–298.1	2	0.30	not specified		*p*	FSIT	71PIC/LED
76FOR/BEN2		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
77MUR/SUB		298.1	1	0.30	not specified		*p*	BSIO	64MOE/THO
79GRI/YAN	N	303.4–463.0	11	0.90	not specified		*p*	BDAO	75RAS/GRI
80KAL/JED		181.8–303.1	66	0.20	99.95	chrom	*p*	BSAO	80KAL/JED
81ARU/BAG		293.1–353.1	4 S	1.50	99.0	melpt	*p*	BDHT	81ARU
82BEN/DAR		288.1–308.1	2 S	0.30	not specified		*p*	FSIT	71PIC/LED
82VIL/CAS		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
84ZEG/SOM2		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
86KOR/KUK		278.0–298.0	2	0.20	not specified		*p*	BSAO	83KUK/KOR
86TAN/TOY		298.1	1	0.30	99.9	anal	*p*	FSIT	71PIC/LED
91OGA/MIT		298.1	1	nosp	not specified		*p*	FSIO	85OGA/MUR
95LOW/PEU		298.2	1	1.00	not specified		*p*	BDCO	95LOW/PEU
97HOV/ROU		298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED
99CER/TOV		288.1–308.1	4	nosp	99.5	chrom	*p*	BDCT	83ROU/ROU
#00BEC/AUF	N	307.0–337.0	7	0.30	99.95	chrom	sat	BDCT	#00BEC/AUF
#00BEC/AUF	N	330.1–354.9	6	0.20	99.95	chrom	sat	BDCT	#00BEC/AUF

26PAR/HUF	high sample purity
60SWI/ZIE	average value in temperature range 294–347 K
68PAZ/REC	same datum in 70PAZ/PAZ
68REC1	same data in 68REC2 and 68REC3
79GRI/YAN	data above 343.28 K measured at elevated pressures up to 1.52 MPa
#00BEC/AUF	‘‘step by step’’ method was used
#00BEC/AUF	‘‘three-step’’ method was used

Table 42.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
68COU/LEE	153.9–361.5	47	0.10	1.236	2.21–2	0.12	3.96–3	6
76FOR/BEN1	298.1	2	0.30	0.388	2.02–2	0.12	1.86–2	2
76FOR/BEN2	298.1	1	0.30	0.063	3.26–3	0.02	3.26–3	1
79GRI/YAN	303.4–463.0	11	0.90	0.842	2.08–1	0.76	−3.85–2	−5
80KAL/JED	181.8–303.1	64	0.20	0.608	1.80–2	0.12	−5.89–3	−16
86TAN/TOY	298.1	1	0.30	0.271	1.41–2	0.08	1.41–2	1
91OGA/MIT	298.1	1	0.30 #	0.448	2.32–2	0.13	−2.32–2	−1
97HOV/ROU	298.1	1	0.50 #	0.032	2.75–3	0.02	−2.75–3	−1
#00BEC/AUF	307.0–337.0	7	0.30	0.722	4.18–2	0.22	−2.48–2	−3
#00BEC/AUF	330.1–354.9	6	0.20	1.152	4.72–2	0.23	−4.44–2	−6
			Rejected data					
20GIB/PAR	(1.04–1,0.75,2.13–2,7)		26PAR/HUF	(1.26–1,0.83,1.17–1,5)				
27PAR/HUF	(1.22–1,0.84,1.17–1,7)		29MIT/HAR1	(7.88–1,5.22,7.30–1,31)				
39PHI	(2.30,11.62,2.30,1)		41ZHD	(4.11–1,2.18,3.51–1,5)				
49TSC/RIC2	(5.72–1,3.20,5.72–1,1)		51EUC/EIG	(4.56–1,2.48,−3.95–1,−10)				
60SWI/ZIE	(2.82–1,1.50,−2.82–1,−1)		68PAZ/REC	(6.99–1,3.66,6.99–1,1)				
68REC1	(2.37–1,1.33,4.73–2,0)		77MUR/SUB	(6.20–1,3.46,6.20–1,1)				
81ARU/BAG	(2.71–1,1.37,−2.08–1,−2)		82BEN/DAR	(1.87–1,1.02,1.29–1,0)				
82VIL/CAS	(3.65–1,2.07,3.65–1,1)		84ZEG/SOM2	(7.18–2,0.41,7.18–2,1)				
86KOR/KUK	(8.90–2,0.53,8.80–2,2)		95LOW/PEU	(6.96–1,3.87,6.96–1,1)				
99CER/TOV	(1.55–1,0.88,1.52–1,4)							

Table 42.9.3. Parameters of cubic spline polynomials

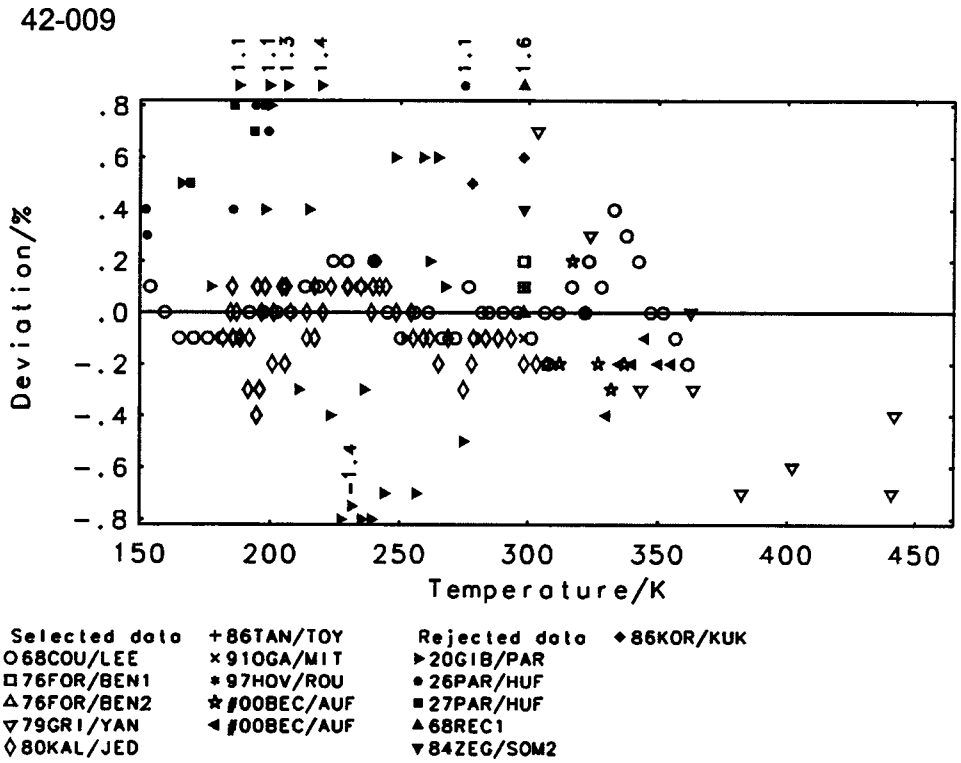
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	260	141	0.925	6.38–2	0.25	−7.28–3	−22
sat	260	141	0.926	5.91–2	0.24	−7.01–3	−23

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
153.9–260.0	9.65084	5.18303	−3.28012	8.07501−1	II
260.0–330.0	2.46530+1	−1.21271+1	3.37763	−4.60571−2	II
330.0–463.0	1.32404+2	−1.10083+2	3.30611+1	−3.04439	IV
153.9–260.0	9.61862	5.23067	−3.30315	8.11145−1	II
260.0–330.0	2.49840+1	−1.24986+1	3.51580	−6.30804−2	II
330.0–463.0	1.37215+2	−1.14527+2	3.44334+1	−3.18607	IV

Table 42.9.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	260	141	2.237	7.04–2	0.34	6.65–3	11

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
153.9–463.0	536.78	9.82362+1	5.06087	6.22306	1.14912+2	−5.84971+1	1.95962+2	IV



Name: 2-Propanol
Formula: C_3H_8O

CAS-RN: 67-63-0
Group No.: 42-010
Molar Mass: 60.10

Table 42.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
24WIL/DAN		303.0–328.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
25PAR/KEL		195.4–293.1	9	nosp	not specified		*p*	BSIO	25PAR
28PAR/KEL	N	195.4–293.1	11	1.00	99.96	estim	*p*	BSIO	25PAR
29KEL3		188.4–292.8	12	1.00	99.95	estim	*p*	BSIO	29KEL1
33TRE/WAT		298.1	1	nosp	not specified		*p*	BSIO	49WEI
39PHI		303.1	1	nosp	not specified		*p*	BSIO	49WEI
45ZHD		280.0–320.0	4	nosp	not specified		*p*	BSIT	34KOL/UDO
48GIN/COR		273.1–473.1	11 S	nosp	not specified		sat	DSTO	50GIN/DOU
58SWI/ZIE2	N	324.0	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
62KAT		293.1–343.1	3	nosp	not specified		*p*	BSIO	62KAT
63AND/COU2		188.3–327.1	60	nosp	not specified		*p*	BSAO	63AND/COU1
77HOF/SAN	N	353.1–463.1	12 S	1.00	not specified		*p*	FSIO	75SAN
79BRO/ZIE		185.0–304.0	eqn	nosp	99.84	melpt	*p*	BSAO	45SCO/MEY
79GRI/YAN		329.3–341.5	2	0.90	not specified		*p*	BDAO	75RAS/GRI
80ROU/ROB		283.1–298.1	2	0.30	not specified		*p*	FSIT	71PIC/LED
86KOR/KUK		298.0	1	0.20	not specified		*p*	BSAO	83KUK/KOR
93CON/GIR1		298.0–363.0	eqn	5.00	not specified		sat	BDHT	93CON/GIR1
93NAZ/BAS		302.4–349.0	3	2.20	99.6	anal	*p*	BDHO	86NAZ/BAS1
95LOW/PEU		298.2	1	1.00	not specified		*p*	BDCO	95LOW/PEU
96TAN/TOY2		298.1	1	nosp	99.98	chrom	*p*	FSIT	71PIC/LED
99CER/TOV		288.1–308.1	4	nosp	99.9	chrom	*p*	BDCT	83ROU/ROU

28PAR/KEL similar data in 25PAR/KEL
58SWI/ZIE2 average value in temperature range 294–354 K
77HOF/SAN C_p at saturation curve extrapolated from high pressure measurements

Name: 1,2-Propanediol
Formula: C_3H_8O

CAS-RN: 57-55-6
Group No.: 42-011
Molar Mass: 76.10

Table 42.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
27PAR/HUF		194.3–276.6	7	nosp	not specified		*p*	BSIO	25PAR
52CUR/JOH	N	213.1–460.5	26 S	nosp	not specified		sat	not specified	
72KAW/OTA		303.1	1	1.00	not specified		*p*	BSIO	49WEI
82ZAR		298.0–363.0	3	0.60	99.87	chrom	*p*	BDCT	82ZAR

52CUR/JOH correlated data (sources: Dow Chemical Co.(technical product) and 27PAR/HUF)

Table 42.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
27PAR/HUF	194.3–276.6	7	1.00 #	0.278	5.20–2	0.28	2.82–2	2
52CUR/JOH	213.1–460.5	26	1.50 #	0.351	1.13–1	0.53	−9.63–3	2
82ZAR	298.0–363.0	3	0.60	0.374	5.62–2	0.22	−8.43–3	−1
Rejected data								
72KAW/OTA	(1.54, 7.13, −1.54, −1)							

Table 42.11.3. Parameters of regression polynomial

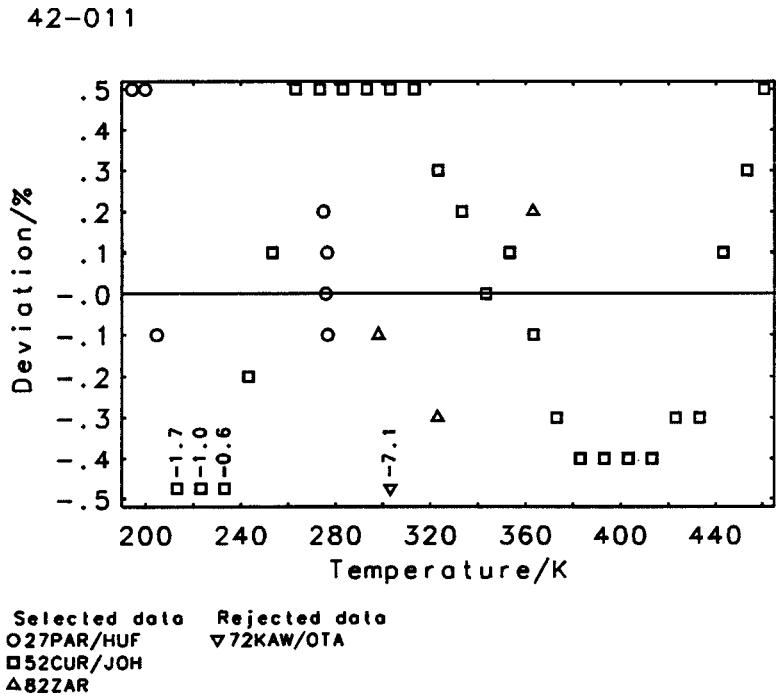
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	37	36	0.361	1.06–1	0.50	−2.17–3	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
194.3–460.5	1.97532+1	−6.36155	3.48862	−3.37136−1	IV

Table 42.11.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	37	36	0.688	1.67–1	0.77	2.96–2	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
194.3–460.5	688.00	−4.52356	1.96542−1	8.73240	2.60282+1	V



Name: 1,2,3-Propanetriol
Formula: $C_3H_8O_3$

CAS-RN: 56-81-5
Group No.: 42-012
Molar Mass: 92.09

Table 42.12.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*79BER	N	330.1–380.6	3	nosp	not specified		avg	DSIO	*79BER
22SIM		294.4	1	nosp	not specified		*p*	BSIO	23SIM/LAN
23GIB/GIA		299.4	1	nosp	99.67	melpt	*p*	BSIO	20GIB/LAT
27PAR/HUF		299.4	1	nosp	not specified		*p*	BSIO	25PAR
36ERN/WAT		298.1	1	nosp	not specified		*p*	BSIO	49WEI
62OMEI	N	293.1–453.1	6 S	nosp	not specified		*p*	not specified	
62RAB/NIK		293.1–328.1	8 S	0.30	not specified		*p*	BSAO	47SKU
68PAZ/REC	N	301.1–313.1	2	nosp	not specified		*p*	BDCT	70PAZ/PAZ
77MUR/SUB		298.1	1	0.30	not specified		*p*	BSIO	64MOE/THO
81ATA/ELS		293.1	1	2.50	not specified		*p*	BDHO	81ATA/ELS
82CHE/GE		313.1	1	3.00	not specified		*p*	BDHO	82CHE/GE
88BAS/NIL		298.1	1	nosp	not specified		*p*	DDCT	74SUU/WAD
98RIG/SAL		298.0–383.0	eqn	nosp	99.5	anal	*p*	BDHT	98SAL/FER

*79BER average values in temperature ranges 287–373 K, 289–452 K and 293–468 K
62OME1 the first 3 data points from Nevolin F.V.:Chim.i Tekhn.Proizv.Glicerina, 1954; the other from Zozulya N.V.:Teploper.i Tepl.Model.,AN SSSR 1959
68PAZ/REC same data in 70PAZ/PAZ

Table 42.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
62OME1	293.1–353.1	4	3.00 #	0.339	2.75–1	1.02	9.73–2	0
62RAB/NIK	293.1–328.1	8	0.30	0.579	4.78–2	0.17	−6.10–3	−4
88BAS/NIL	298.1	1	0.30 #	0.670	5.29–2	0.20	5.29–2	1
98RIG/SAL	298.0–382.7	8	1.00 #	0.507	1.45–1	0.51	−7.92–3	0
			Rejected data					
*79BER	(5.17–1,1.83,−4.69–1,−3)		22SIM	(8.99–1,3.33,8.99–1,1)				
23GIB/GIA	(5.10–1,1.90,5.10–1,1)		27PAR/HUF	(5.10–1,1.90,5.10–1,1)				
36ERN/WAT	(5.54–1,2.15,−5.54–1,−1)		68PAZ/REC	(2.09,6.94,1.57,2)				
77MUR/SUB	(4.14–1,1.55,4.14–1,1)		81ATA/ELS	(3.74–1,1.42,3.74–1,1)				
82CHE/GE	(4.45–1,1.61,4.45–1,1)							

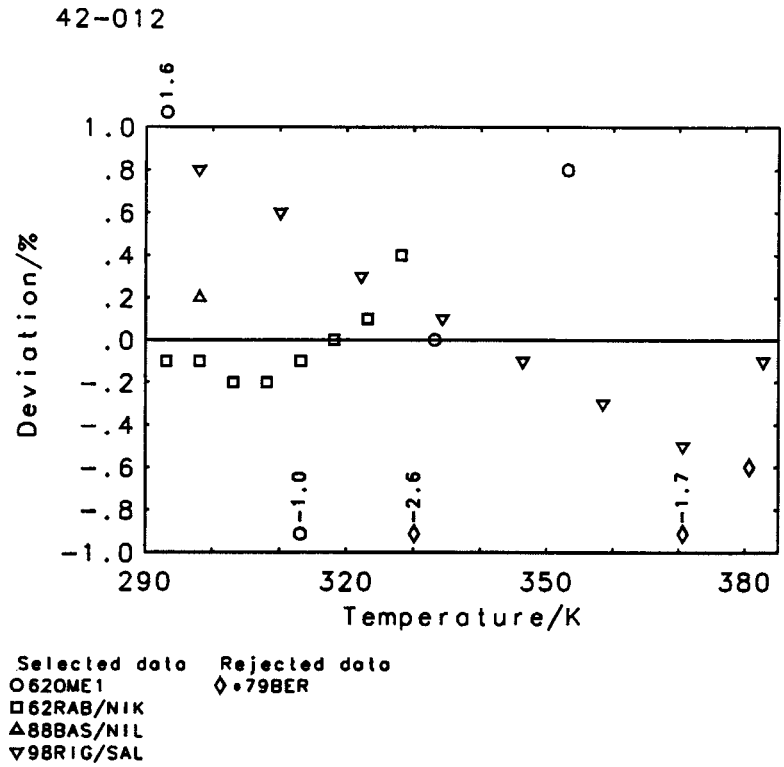
Table 42.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	35	21	0.545	1.61–1	0.58	1.57–2	−3
Temp. range K		A_1	A_2				Level of uncertainty
293.1–382.7		9.16889	5.73727				V

Table 42.12.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	35	21	0.527	1.60–1	0.59	3.71–2	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
293.1–382.7	800.00	1.87190+1	1.18708	5.59442	7.37947+1	V



Name: 1-Butanol
Formula: $C_4H_{10}O$

CAS-RN: 71-36-3
Group No.: 42-013
Molar Mass: 74.12

Table 42.13.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
24WIL/DAN		303.0–348.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
25PAR		194.6–294.0	12	0.50	not specified		*p*	BSIO	25PAR
33TRE/WAT		298.1	1	nosp	not specified		*p*	BSIO	49WEI
38PAN/DUD	N	298.0–363.0	eqn	nosp	not specified		*p*	not specified	
39PHI		302.5	1	nosp	not specified		*p*	BSIO	49WEI
49TSC/RIC2		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
60SWI/ZIE	N	322.4	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
65COU/HAL		188.2–322.3	25	0.20	99.94	melpt	*p*	BSAO	63AND/COU1
67GRA		308.1–338.1	4	1.00	not specified		*p*	BSIO	67GRA
68PAZ/REC	N	301.1–313.1	2	nosp	not specified		*p*	BDCT	70PAZ/PAZ
75SAN	N	295.9–466.6	20	0.90	not specified		*p*	FSIO	75SAN
78BYV/JAS		293.1–333.1	3	2.00	not specified		*p*	BDCT	78BYV/JAS
79GRI/YAN	N	324.0–462.5	8 S	0.90	not specified		*p*	BDAO	75RAS/GRI
81ARU/BAG		293.1–373.1	5 S	1.50	not specified		*p*	BDHT	81ARU
86GAT/WOO		298.1–368.1	4	nosp	99.	anal	*p*	BDCT	83ROU/ROU
86KOR/KUK		278.0–298.0	2	0.20	not specified		*p*	BSAO	83KUK/KOR
86NAZ/BAS1		321.0–373.4	3	2.00	not specified		*p*	BDHO	86NAZ/BAS1
86OGA/MUR		298.1	1	0.10	not specified		*p*	FSIO	85OGA/MUR
86ROU/GRO		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
86TAN/TOY		298.1	1	0.30	99.9	anal	*p*	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
88PIE/SOM2		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
89COB/GAR		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
97HOV/ROU		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
99CAL/BRO		298.1	1	nosp	99.8	chrom	*p*	FSIT	71PIC/LED

38PAN/DUD	temperature range of parameters validity estimated by the compilers
60SWI/ZIE	average value in temperature range 294–350 K
68PAZ/REC	same data in 70PAZ/PAZ; apparently wrong value at 313.15 K
75SAN	C_p at pressure near 1.4 MPa
79GRI/YAN	data above 363.61 K measured at elevated pressures up to 0.92 MPa

Name: 2-Methyl-1-propanol
Formula: $C_4H_{10}O$

CAS-RN: 78-83-1
Group No.: 42-017
Molar Mass: 74.12

Table 42.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH		308.6–328.1	9 S	nosp	not specified		avg	DSIO	*86SCH
*98LOU	N	337.9	1	nosp	not specified		avg	DSIO	*98LOU
24WIL/DAN		303.0–353.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
41ZHD		278.3–319.0	3	nosp	not specified		*p*	BSIT	34KOL/UDO
58SWI/ZIE2	N	333.6–336.7	2	nosp	not specified		avg	DSIO	58SWI/ZIE1
60SWI/ZIE	N	322.6	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
68COU/LEE		180.0–355.0	65	0.15	99.96	melpt	*p*	BSAO	63AND/COU1
68PAZ/REC	N	301.1–313.1	2	nosp	not specified		*p*	BDCT	70PAZ/PAZ
77HOF/SAN	N	383.1–493.1	12 S	1.00	not specified		*p*	FSIO	75SAN
78RYB/EME		293.1–353.1	7 S	nosp	not specified		*p*	BSIO	78RYB/EME
86KOR/KUK		298.0	1	0.20	not specified		*p*	BSAO	83KUK/KOR
88OKA/OGA	N	298.1	1	nosp	not specified		*p*	FSIO	85OGA/MUR
88PIE/SOM1		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
92NAZ/BAS		300.6–396.1	5	2.20	99.8	chrom	*p*	BDHO	86NAZ/BAS1
97HOV/ROU		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
#00BEC/AUF	N	307.0–332.0	6	0.30	99.95	chrom	sat	BDCT	#00BEC/AUF
#00BEC/AUF	N	323.2–363.2	9	0.20	99.95	chrom	sat	BDCT	#00BEC/AUF

*98LOU	average value in temperature range 294–382 K
58SWI/ZIE2	average values in temperature ranges 295–372 K and 295–379 K
60SWI/ZIE	average value in temperature range 294–351 K
68PAZ/REC	same data in 70PAZ/PAZ
77HOF/SAN	C_p at saturation curve extrapolated from high pressure measurements
88OKA/OGA	water content below 0.083 mol.%
#00BEC/AUF	‘‘step by step’’ method was used
#00BEC/AUF	‘‘three-step’’ method was used

Table 42.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
68COU/LEE	180.0–355.0	65	0.15	0.858	2.82–2	0.13	6.29–4	−10
77HOF/SAN	383.1–493.1	12	1.00	0.424	1.45–1	0.42	−4.92–2	−2
88OKA/OGA	298.1	1	0.40 #	0.159	1.38–2	0.06	1.38–2	1
97HOV/ROU	298.1	1	0.50 #	0.227	2.47–2	0.11	−2.47–2	−1
#00BEC/AUF	307.0–332.0	6	0.30	0.727	5.45–2	0.22	4.36–2	5
#00BEC/AUF	323.2–363.2	9	0.20	1.643	8.63–2	0.33	−1.65–2	−3

Rejected data

*86SCH	(1.94–1,0.78,1.72–1,9)	*98LOU	(4.70–1,1.76,4.70–1,1)
24WIL/DAN	(6.47–1,2.30,5.19–1,3)	41ZHD	(4.40–1,1.88,3.30–1,1)
58SWI/ZIE2	(1.40–1,0.54,1.38–1,2)	60SWI/ZIE	(2.59–1,1.07,−2.59–1,−1)
68PAZ/REC	(8.37–1,3.43,6.97–1,2)	78RYB/EME	(5.37–1,2.06,−3.72–1,−3)
86KOR/KUK	(5.93–2,0.27,5.93–2,1)	88PIE/SOM1	(1.29–1,0.59,1.29–1,1)
92NAZ/BAS	(1.67,6.05,−1.43,−5)		

Table 42.17.3. Parameters of cubic spline polynomials

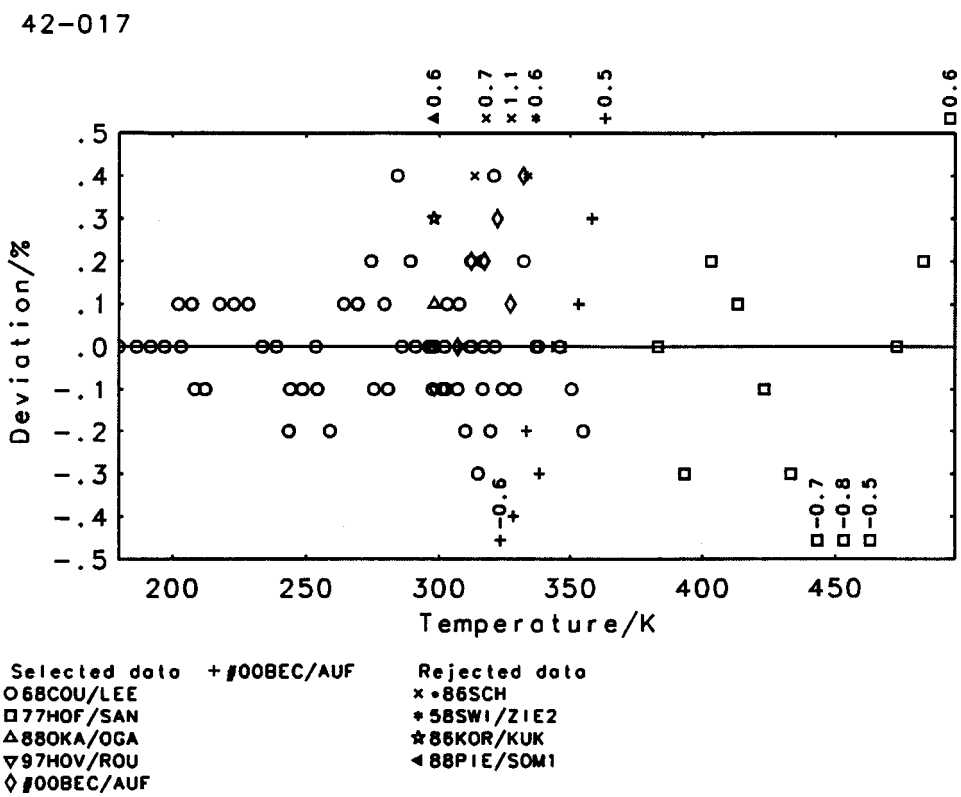
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	129	94	0.939	6.67−2	0.23	−4.76−3	−10
sat	129	94	0.933	6.08−2	0.21	−4.55−3	−10

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
180.0–290.0	7.12445	1.16833+1	−6.37295	1.37558	II
290.0–370.0	1.57026+2	−1.43387+2	4.70995+1	−4.77068	II
370.0–493.1	−1.87142+2	1.35668+2	−2.83206+1	2.02393	V
180.0–290.0	7.15990	1.16394+1	−6.35520	1.37324	II
290.0–370.0	1.57459+2	−1.43843+2	4.72593+1	−4.78935	II
370.0–493.1	−1.66412+2	1.18755+2	−2.37131+1	1.60456	V

Table 42.17.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	129	94	5.760	3.01−1	1.09	8.03−2	18

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
180.0–493.1	547.78	2.44985+2	1.64826+1	−3.12684	2.53998+2	−3.08315+1	3.23667+2	V



Name: 1,3-Butanediol
Formula: $C_4H_{10}O_2$

CAS-RN: 107-88-0
Group No.: 42-019
Molar Mass: 90.12

Table 42.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
72KAW/OTA	303.1	1	nosp	not specified		*p*	BSIO	49WEI
96STE/CHI1	300.0–670.0	20 S	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 42.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
96STE/CHI1	300.0–670.0	20	1.00	1.093	5.93–1	1.09	1.97–2	−2
Rejected data								
72KAW/OTA	(1.52,5.55,1.52,1)							

Table 42.19.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	21	20	1.306	7.08–1	1.31	1.97–2	−2
sat	21	20	0.770	3.62–1	0.77	5.42–3	−3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–450.0	−1.39795+1	1.44997+1	1.58472−1	−2.00697−1	IV
450.0–635.0	−1.58301+2	1.10714+2	−2.12226+1	1.38308	IV
635.0–670.0	−1.80115+5	8.51298+4	−1.34100+4	7.04209+2	V
300.0–450.0	−1.63262+1	1.63820+1	−3.36847−1	−1.57979−1	IV
450.0–635.0	−1.32524+2	9.38470+1	−1.75513+1	1.11716	IV
635.0–670.0	−1.06396+5	5.02970+4	−7.92356+3	4.16131+2	V

Table 42.19.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	21	20	1.393	6.96–1	1.39	3.41–3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
300.0–670.0	676.00	2.44199	4.08726−1	−3.42028+1	2.20389+2	−2.26871+2	8.58396+1	V

Name: Cyclopentanol
Formula: $C_5H_{10}O$

CAS-RN: 96-41-3
Group No.: 42-023
Molar Mass: 86.13

Table 42.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
56PAR/KEN	260.0–300.0	5 S	1.00	99.8	melpt	*p*	BSIO	25PAR
76CON/GIA	298.1	1	nosp	not specified		*p*	BDCT	76CON/GIA
86BEN/DAR2	298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
95KAB/DIK	256.3–302.9	12	0.40	99.8	chrom	*p*	BSAO	93DIK/KAB
97HOV/ROU	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

Table 42.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
			Selected data					
56PAR/KEN	260.0–300.0	5	1.00	0.736	1.57–1	0.74	1.43–1	5
86BEN/DAR2	298.1	1	0.30	1.184	7.76–2	0.36	−7.76–2	−1
95KAB/DIK	256.3–302.9	12	0.40	0.369	2.94–2	0.15	6.27–3	4
97HOV/ROU	298.1	1	0.50 #	0.678	7.40–2	0.34	−7.40–2	−1
			Rejected data					
76CON/GIA	(3.77–1,1.69,3.77–1,1)							

Table 42.23.3. Parameters of regression polynomial

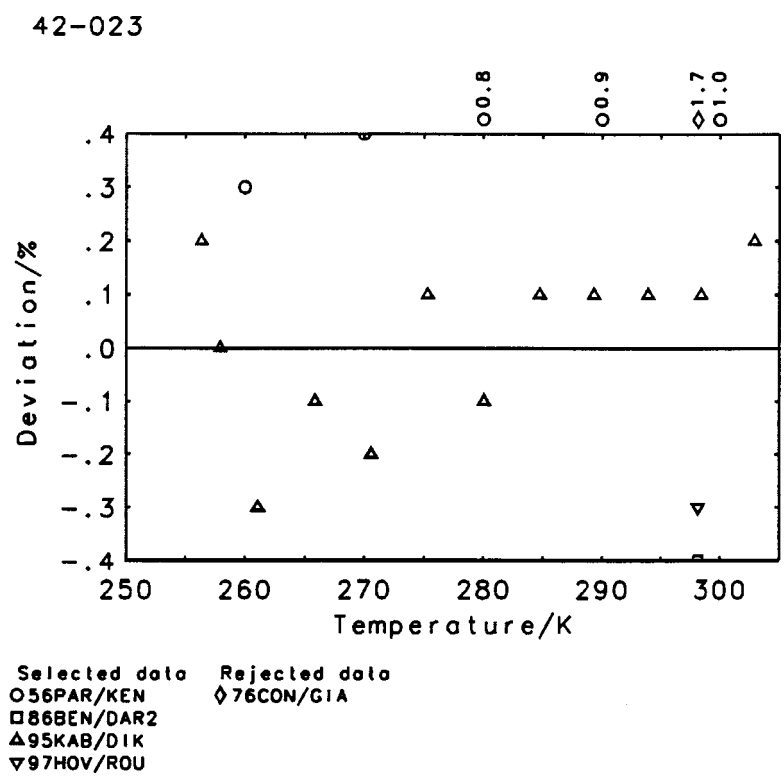
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	19	0.623	9.51–2	0.45	3.35–2	7

Temp. range K	A_1	A_2	A_3	Level of uncertainty
256.3–302.9	2.44422+1	−1.17152+1	3.64505	III

Table 42.23.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	19	0.769	8.69–2	0.41	6.60–4	−3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
256.3–302.9	619.50	8.37285	2.06103+1	−1.26902+1	8.50360−1	III



Name: 2-Methyl-1-butanol
Formula: $C_5H_{12}O$

CAS-RN: 137-32-6
Group No.: 42-025
Molar Mass: 88.15

Table 42.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*98LOU	N	347.1	1	nosp	not specified		avg	DSIO	*98LOU
49LEE		313.0–343.0	eqn	nosp	not specified		*p*	BDHO	33FER/MIL
94SVO/CEJ		303.0–326.2	6	0.50	99.8	chrom	*p*	BSAO	91SVO/ZAB1
97CEN/RUZ		307.8–337.6	12	1.00	99.92	chrom	*p*	BDCT	91BAN/GAR

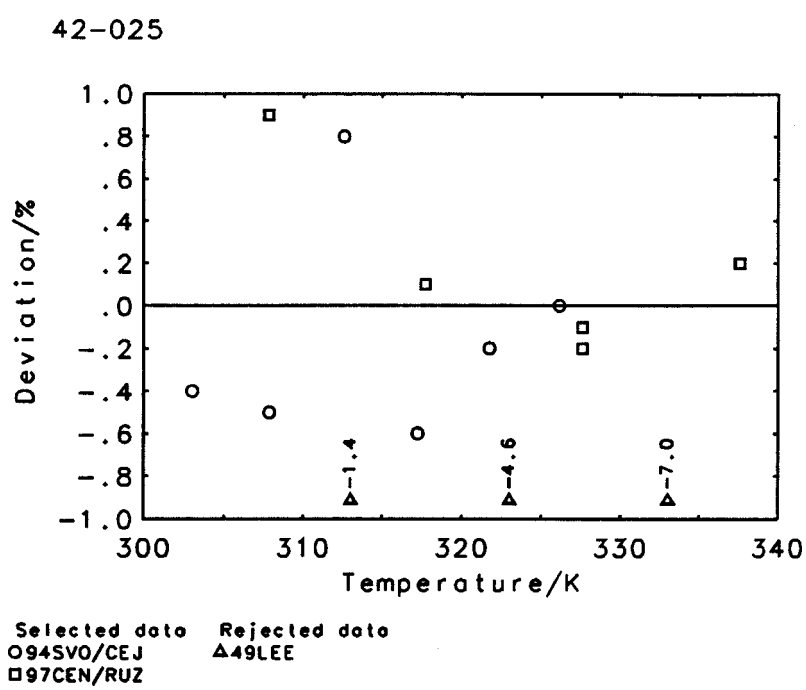
*98LOU average value in temperature range 295–400 K

Table 42.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94SVO/CEJ	303.0–326.2	6	0.50	0.989	1.37–1	0.49	−3.57–2	−4
97CEN/RUZ	307.8–337.6	12	1.00	0.473	1.29–1	0.47	7.52–2	6
Rejected data								
49LEE	(1.39,4.92,−1.22,−3)							

Table 42.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	23	18	0.755	1.44–1	0.53	3.83–2	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
303.0–337.6		−1.20252+2	7.90093+1	−1.01423+1			IV



Name: 2-Methyl-2-butanol
Formula: $C_5H_{12}O$

CAS-RN: 75-85-4
Group No.: 42-026
Molar Mass: 88.15

Table 42.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*98LOU	N	332.4	1	nosp	not specified		avg	DSIO	*98LOU
33PAR/HUF		275.0–294.4	4	1.00	not specified		*p*	BSIO	25PAR
49LEE		313.0–343.0	eqn	nosp	not specified		*p*	BDHO	33FER/MIL
83DAP/DEL		288.1–298.1	2	0.30	not specified		*p*	FSIT	71PIC/LED
86BEN/DAR2		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
88PIE/SOM1		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
94SVO/CEJ		303.0–326.2	6	0.50	98.8	chrom	*p*	BSAO	91SVO/ZAB1
96TAN/TOY2		298.1	1	nosp	99.99	chrom	*p*	FSIT	71PIC/LED
97CEN/RUZ		307.9–347.5	10	1.00	99.91	chrom	*p*	BDCT	91BAN/GAR

*98LOU average value in temperature range 293–372 K

Table 42.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R	d_r %	d_b/R	±
Selected data								
33PAR/HUF	275.0–294.4	4	1.00	0.141	4.03–2	0.14	−3.77–5	0
83DAP/DEL	288.1–298.1	2	0.30	0.240	2.09–2	0.07	−2.07–2	−2
86BEN/DAR2	298.1	1	0.30	1.618	1.45–1	0.49	1.45–1	1
88PIE/SOM1	298.1	1	0.50 #	0.407	6.04–2	0.20	−6.04–2	−1
94SVO/CEJ	303.0–326.2	6	0.50	1.826	2.80–1	0.91	−9.77–2	−1
96TAN/TOY2	298.1	1	0.50 #	1.465	2.20–1	0.73	2.20–1	1
97CEN/RUZ	307.9–347.5	10	1.00	0.374	1.19–1	0.37	7.26–2	4
Rejected data								
*98LOU	(7.24–1,2.16,−7.24–1,−1)		49LEE	(4.89–1,1.46,−4.61–1,−4)				

Table 42.26.3. Parameters of regression polynomial

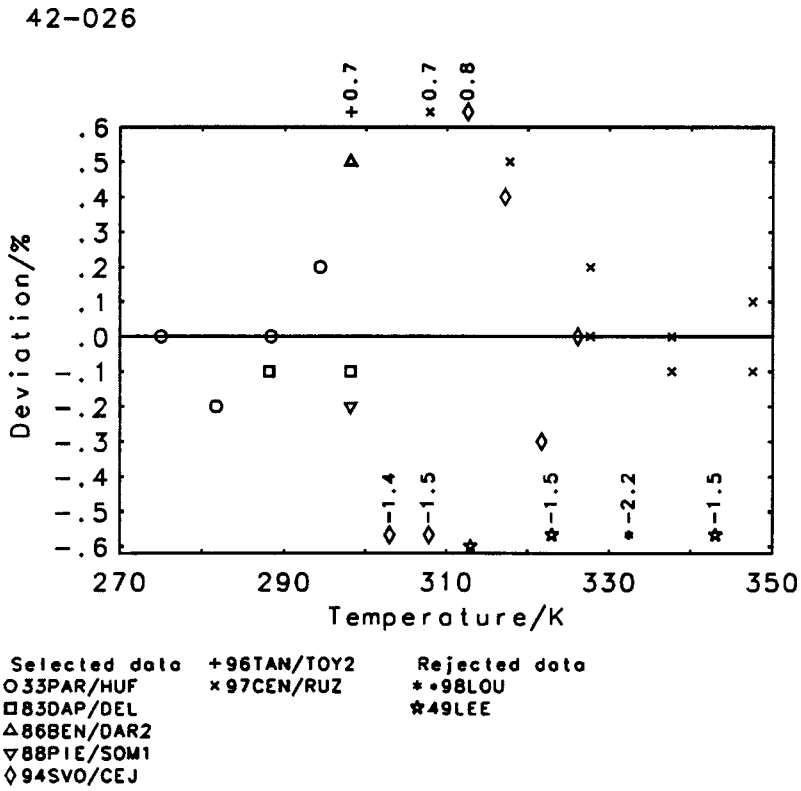
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	30	25	1.124	1.82–1	0.59	1.61–2	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
275.0–347.5	5.25848+2	−5.09372+2	1.69896+2	−1.83990+1	IV

Table 42.26.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	30	25	1.342	2.61–1	0.85	8.52–2	7

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
275.0–347.5	543.70	5.16990+1	4.07265	−2.80229+1	1.64069+2	IV



Name: 3-Methyl-1-butanol
Formula: $C_5H_{12}O$

CAS-RN: 123-51-3
Group No.: 42-027
Molar Mass: 88.15

Table 42.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH		309.7–337.4	10 S	nosp	not specified		avg	DSIO	*86SCH
*98LOU	N	348.6	1	nosp	not specified		avg	DSIO	*98LOU
07BAT		224.0–263.6	6	nosp	not specified		*p*	BSIO	07BAT
12LUS	N	321.0	1	nosp	not specified		avg	DSIO	12LUS
24WIL/DAN		303.0–353.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
45ZHD		280.5–319.9	3	nosp	not specified		*p*	BSIT	34KOL/UDO
49LEE		313.0–343.0	eqn	nosp	not specified		*p*	BDHO	33FER/MIL
58SWI/ZIE2	N	347.5	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
90RAO/RAJ		318.1–333.1	4	4.00	not specified		*p*	BDHT	89PRA/RAJ
92NAZ/BAS		302.0–368.3	4	2.20	98.3	chrom	*p*	BDHO	86NAZ/BAS1
94SVO/CEJ		303.0–326.2	6	0.50	100.0	chrom	*p*	BSAO	91SVO/ZAB1
97CEN/RUZ		307.7–357.4	11	1.00	99.72	chrom	*p*	BDCT	91BAN/GAR

*98LOU average value in temperature range 294–403 K
12LUS average value in temperature range 287–355 K
58SW1/ZIE2 average value in temperature range 295–400 K

Table 42.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
07BAT	224.0–263.6	6	3.00 #	0.341	2.15–1	1.02	−2.58–3	0
58SWI/ZIE2	347.5	1	1.00 #	0.419	1.30–1	0.42	1.30–1	1
94SVO/CEJ	303.0–326.2	6	0.50	1.071	1.42–1	0.54	−1.73–2	−2
97CEN/RUZ	307.7–357.4	11	1.00	0.437	1.30–1	0.44	3.03–2	5
Rejected data								
*86SCH	(4.24–1,1.48,4.20–1,10)		*98LOU	(1.68–1,0.54,−1.68–1,−1)				
12LUS	(1.86,6.31,1.86,1)		24WIL/DAN	(4.50–1,1.59,−4.38–1,−5)				
45ZHD	(2.45–1,0.95,2.23–1,3)		49LEE	(3.77–1,1.30,−1.27–1,0)				
90RAO/RAJ	(1.13,4.30,−9.81–1,−4)		92NAZ/BAS	(1.73,5.68,1.70,3)				

Table 42.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r	s_b/R	±
			%				
p	56	24	0.596	1.16–1	0.46	2.73–2	6
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
224.0–357.4		1.07722+2	−9.35318+1	3.12230+1	−3.07206		IV

Table 42.27.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r	s_b/R	±
			%				
p	56	24	0.821	2.26–1	0.99	−9.45–3	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
224.0–357.4	579.40	−1.34581	1.22299+1	−9.51783−1	3.70239−2		V

Name: 3-Methyl-2-butanol
Formula: $C_5H_{12}O$

CAS-RN: 598-75-4
Group No.: 42-028
Molar Mass: 88.15

Table 42.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91ATR/NES	218.4–370.7	29	nosp	99.9	anal	sat	BSAO	78ZHU/ATR
94SVO/CEJ	303.0–326.2	6	0.50	99.6	chrom	p	BSAO	91SVO/ZAB1
97CEN/RUZ	304.2–347.4	16	1.00	99.99	chrom	p	BDCT	91BAN/GAR

Table 42.28.2. Correlated heat capacities

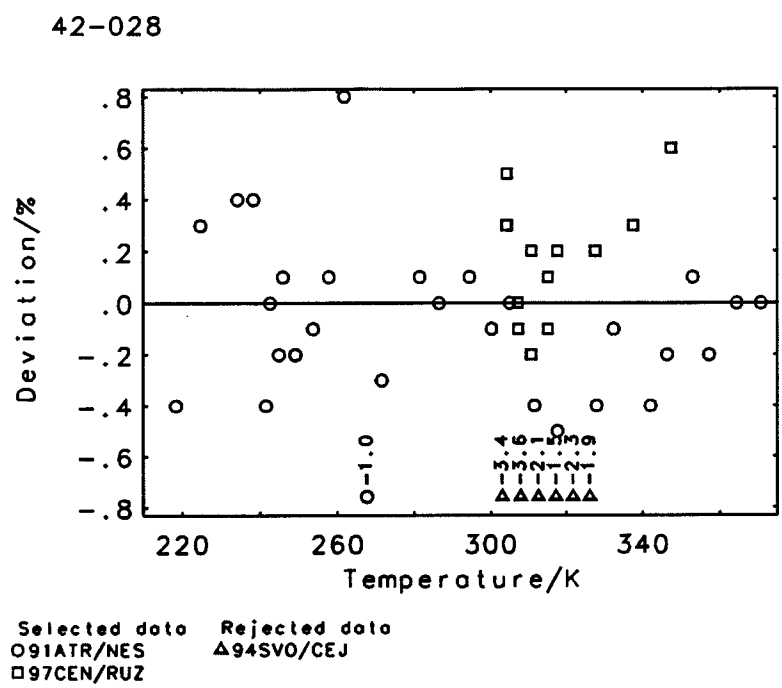
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
91ATR/NES	218.4–370.7	29	1.00 #	0.338	8.90–2	0.34	−2.64–2	−3
97CEN/RUZ	304.2–347.4	16	1.00	0.275	8.90–2	0.27	4.96–2	6
Rejected data								
94SVO/CEJ	(7.86–1,2.57,−7.57–1,−6)							

Table 42.28.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	51	45	0.336	9.44−2	0.34	5.99−4	3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
218.4–310.0		1.95360+2	−2.14072+2	8.32014+1	−1.00688+1		IV
310.0–370.7		−2.13907+2	1.81992+2	−4.45613+1	3.66917		IV

Table 42.28.4. Parameters of quasipolynomial equation

Heat capacity type		No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
				%				
C		51	45	1.033	1.71−1	0.54	−1.41−2	−4
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
218.4–370.7	556.10	8.29530+3	9.55136+2	−9.83528+2	7.88195+3	9.65637+2	5.34052+3	IV



Name: 1-Pentanol
Formula: $C_5H_{12}O$

CAS-RN: 71-41-0
Group No.: 42-029
Molar Mass: 88.15

Table 42.29.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
33PAR/HUF		204.1–298.0	6	1.00	not specified		*p*	BSIO	25PAR
39PHI	N	302.4	1	nosp	not specified		*p*	BSIO	49WEI
49LEE		313.0–343.0	eqn	nosp	not specified		*p*	BDHO	33FER/MIL
49TSC/RIC2		298.1	1	nosp	not specified		*p*	BSIO	49TSC/RIC1
68COU/LEE		205.1–389.1	53	0.15	99.87	melpt	*p*	BSAO	63AND/COU1
68PAZ/REC	N	313.1	1	nosp	not specified		*p*	BDCT	70PAZ/PAZ
76SKO/SUU		298.1	1	0.10	not specified		*p*	DDCT	71KON/SUU
79GRI/YAN	N	301.3–463.4	9	0.90	not specified		*p*	BDAO	75RAS/GRI
81ARU/BAG		293.1–393.1	6 S	1.50	not specified		*p*	BDHT	81ARU
83DAP/DEL		288.1–298.1	2	0.30	not specified		*p*	FSIT	71PIC/LED
83PFE/SCH		298.1	1	nosp	not specified		*p*	BDCT	68WAD
84ZEG/SOM2		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
86BEN/DAR2		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
86TAN/TOY		298.1	1	0.30	98.	anal	*p*	FSIT	71PIC/LED
99CAL/BRO		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED

39PHI isomer not specified, 1-alkanol assumed
68PAZ/REC same datum in 70PAZ/PAZ
79GRI/YAN data above 382.68 K were measured at elevated pressures up to 0.81 MPa

Name: 2-Pentanol
Formula: $C_5H_{12}O$

CAS-RN: 6032-29-7
Group No.: 42-030
Molar Mass: 88.15

Table 42.30.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
38PAN/DUD	N	298.0–363.0	eqn	nosp	not specified		*p*	not specified	
94SVO/CEJ		303.0–326.2	6	0.50	99.6	chrom	*p*	BSAO	91SVO/ZAB1
96TAN/TOY2		298.1	1	nosp	99.8	chrom	*p*	FSIT	71PIC/LED
97CEN/RUZ		307.8–367.4	20	1.00	99.93	chrom	*p*	BDCT	91BAN/GAR

38PAN/DUD temperature range of parameters validity estimated by the compilers

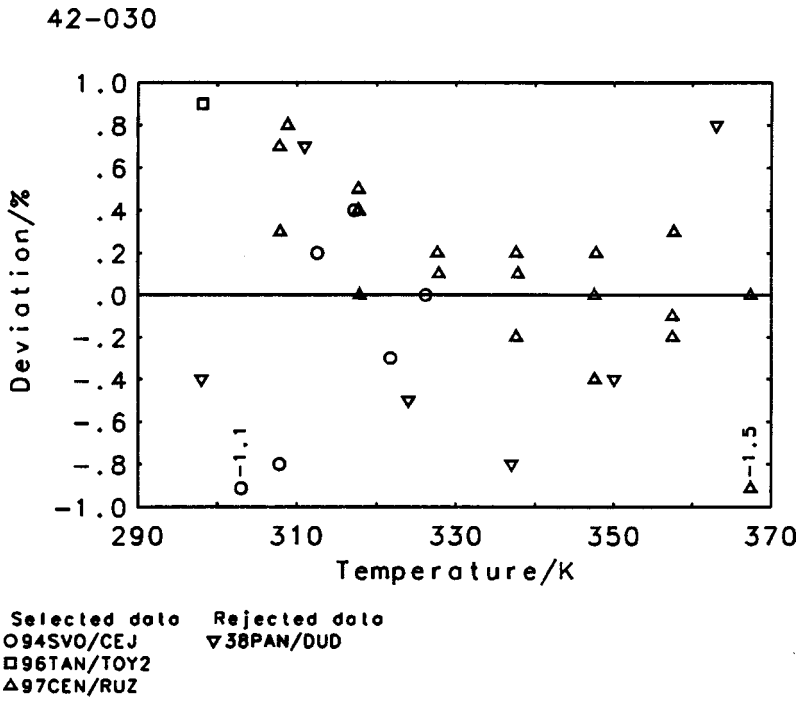
Table 42.30.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
			Selected data					
94SVO/CEJ	303.0–326.2	6	0.50	1.232	1.79–1	0.62	−7.57–2	−2
96TAN/TOY2	298.1	1	0.50 #	1.752	2.47–1	0.88	2.47–1	1
97CEN/RUZ	307.8–367.4	20	1.00	0.324	1.01–1	0.32	4.57–2	8
			Rejected data					
38PAN/DUD	(2.21–1,0.67,−5.51–3,−1)							

Table 42.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	33	27	0.771	1.38–1	0.46	2.62–2	7

Temp. range K	A_1	A_2	A_3	Level of uncertainty
298.1–367.4	−8.46311+1	5.92957+1	−7.22361	IV



Name: 3-Pentanol
Formula: $C_5H_{12}O$

CAS-RN: 584-02-1
Group No.: 42-031
Molar Mass: 88.15

Table 42.31.1. Experimental heat capacities

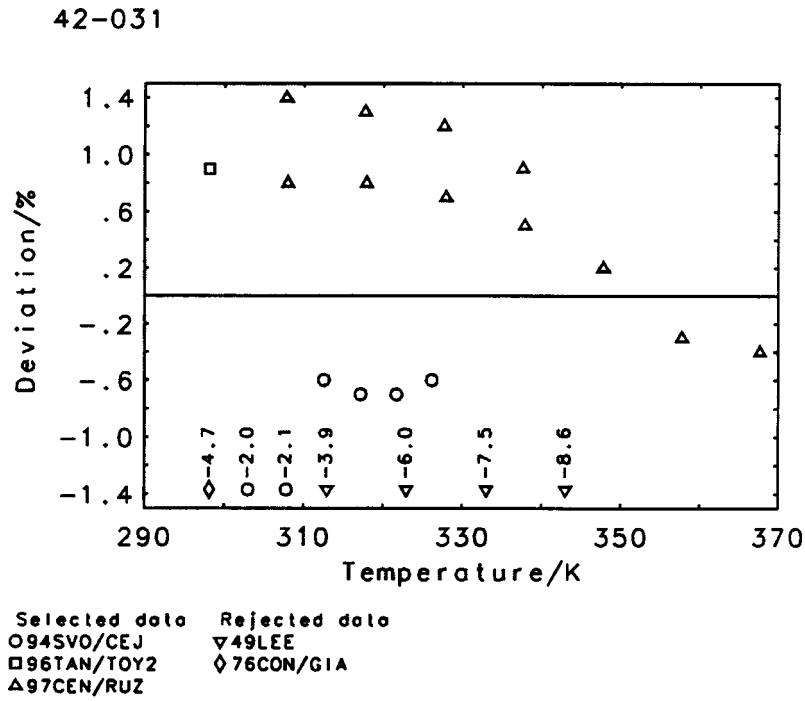
Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
49LEE	313.0–343.0	eqn	nosp	not specified		*p*	BDHO	33FER/MIL
76CON/GIA	298.1	1	nosp	not specified		*p*	BDCT	76CON/GIA
94SVO/CEJ	303.0–326.2	6	0.50	99.6	chrom	*p*	BSAO	91SVO/ZAB1
96TAN/TOY2	298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
97CEN/RUZ	307.8–367.7	11	1.00	99.90	chrom	*p*	BDCT	91BAN/GAR

Table 42.31.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94SVO/CEJ	303.0–326.2	6	0.80 #	1.637	4.04–1	1.31	−3.51–1	−6
96TAN/TOY2	298.1	1	0.50 #	1.812	2.76–1	0.91	2.76–1	1
97CEN/RUZ	307.8–367.7	11	1.00	0.872	2.90–1	0.87	2.15–1	7
Rejected data								
49LEE	(2.14,6.74,−2.06,−4)		76CON/GIA	(1.37,4.74,−1.37,−1)				

Table 42.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	23	18	1.359	3.63–1	1.14	2.96–2	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.1–367.7		−6.88783+1	5.28468+1	−6.57922			V



Name: Cyclohexanol
Formula: $C_6H_{12}O$

CAS-RN: 108-93-0
Group No.: 42-038
Molar Mass: 100.16

Table 42.38.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
24HER/BLO	289.6	1	nosp	not specified		*p*	DSIO	22HER/SCH
29KEL4	298.1–298.7	2	0.50	not specified		*p*	BSIO	29KEL1
39PHI	305.0	1	nosp	not specified		*p*	BSIO	49WEI
68ADA/SUG	300.1–316.5	9	nosp	99.975	melpt	*p*	BSAO	65SUG/SEK
74PET/TER	298.0–427.7	13	1.00	99.	chrom	*p*	BDCT	74PET/TER
76CON/GIA	298.1	1	nosp	not specified		*p*	BDCT	76CON/GIA
88CAC/COS	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
90MAY/RAC	298.0–312.0	eqn	nosp	99.91	melpt	*p*	BSAO	90MAY/RAC
97HOV/ROU	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
97STE/CHI2	300.0–620.0	17	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 42.38.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
68ADA/SUG	300.1–316.5	9	0.20 #	0.931	4.98–2	0.19	3.12–3	1
88CAC/COS	298.1	1	0.50 #	1.369	1.73–1	0.68	−1.73–1	−1
97STE/CHI2	300.0–620.0	17	1.00	0.842	3.18–1	0.84	8.41–3	−1
			Rejected data					
29KEL4	(3.39–1,1.35,−3.36–1,−2)		39PHI	(1.93,7.95,−1.93,−1)				
74PET/TER	(7.70–1,2.36,1.84–1,4)		76CON/GIA	(1.04,3.93,1.04,1)				
90MAY/RAC	(2.90–1,1.08,2.87–1,4)		97HOV/ROU	(3.71–1,1.48,−3.71–1,−1)				

Table 42.38.3. Parameters of cubic spline polynomials

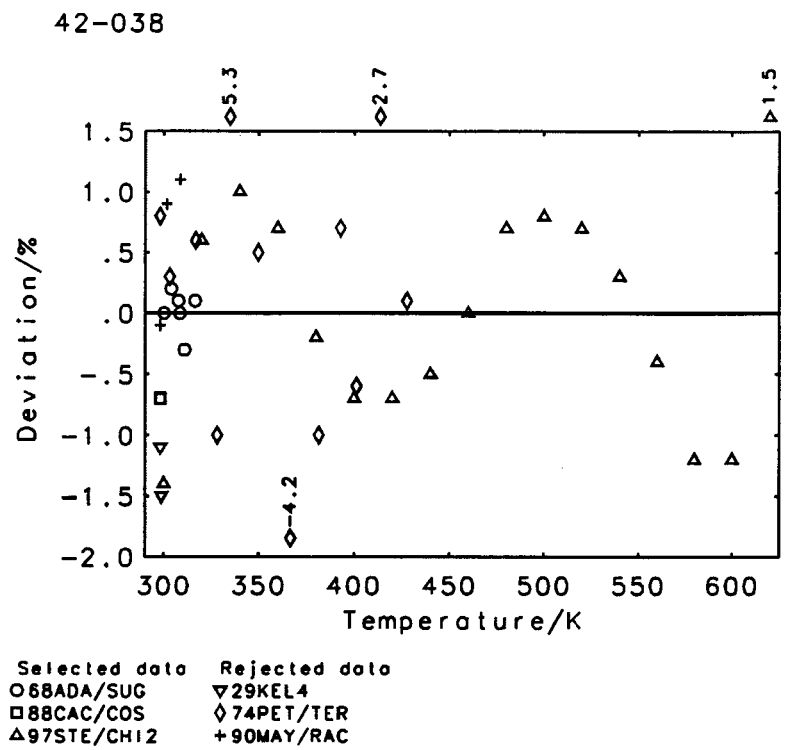
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	51	27	0.994	2.83−1	0.76	−6.92−5	−1
sat	51	27	0.870	1.94−1	0.59	2.25−3	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
298.1–410.0	7.00487+1	−6.56122+1	2.48446+1	−2.63546	III
410.0–620.0	−3.41109+2	2.35235+2	−4.85328+1	3.33019	IV
298.1–410.0	5.77126+1	−5.49632+1	2.18183+1	−2.35317	III
410.0–620.0	−3.01412+2	2.07811+2	−4.22730+1	2.85750	IV

Table 42.38.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	51	27	1.907	3.95−1	1.08	5.88−2	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
298.1–620.0	650.00	2.31147+1	1.44563	−1.16120+2	5.99048+2	−7.40458+2	3.50757+2	V



Name: 1-Hexanol
Formula: $C_6H_{14}O$

CAS-RN: 111-27-3
Group No.: 42-041
Molar Mass: 102.18

Table 42.41.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
29KEL2		229.6–290.0	7	1.00	not specified		*p*	BSIO	29KEL1
59HUT/BAI		298.1	1	nosp	not specified		*p*	BSIO	55HUT/MAN
73KAL/WOY		303.1	1	nosp	not specified		*p*	BSIO	70REC
79GRI/YAN	N	303.7–462.0	9	0.90	not specified		*p*	BDAO	75RAS/GRI
81ARU		293.1–393.1	6 S	1.50	not specified		*p*	BDHT	81ARU
83BEN/DAR		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
84BRA/PIN		298.1	1	nosp	99.	melpt	*p*	FSIT	71PIC/LED
84KAL/WOY		229.1–300.6	35	nosp	99.9	chrom	*p*	BSAO	80KAL/JED
84ZEG/SOM2		298.1	1	nosp	99.	chrom	*p*	FSIT	71PIC/LED
85COS/PAT8		283.1–313.1	3	0.30	98.	estim	*p*	FSIT	71PIC/LED
86ORT		298.1	1	1.00	99.	anal	*p*	BDCT	70PAZ/PAZ
86TAN/TOY		298.1	1	0.30	98.	anal	*p*	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
89VES/BAR	N	298.1–318.1	5	0.50	not specified		*p*	BSAO	79VES/ZAB
91ATR/NES		227.3–362.6	20	nosp	99.9	anal	sat	BSAO	78ZHU/ATR
98RUZ/MAJ		304.2–349.9	25	1.00	99.60	chrom	*p*	BDCT	91BAN/GAR
99CAL/BRO		298.1	1	nosp	99.0	chrom	*p*	FSIT	71PIC/LED

79GRI/YAN data above 385.43 K measured at elevated pressures up to 0.74 MPa
89VES/BAR water content 0.04 mass %

Table 42.41.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
79GRI/YAN	303.7–462.0	9	0.90	1.271	4.40–1	1.14	1.23–2	2
83BEN/DAR	298.1	1	0.30	1.381	1.20–1	0.41	−1.20–1	−1
84ZEG/SOM2	298.1	1	0.50 #	0.271	3.93–2	0.14	−3.93–2	−1
86TAN/TOY	298.1	1	0.30	1.492	1.30–1	0.45	−1.30–1	−1
88AND/PAT	298.1	1	0.50 #	0.271	3.93–2	0.14	−3.93–2	−1
89VES/BAR	298.1–318.1	5	0.50	0.905	1.38–1	0.45	1.35–1	5
91ATR/NES	227.3–362.6	20	0.50 #	0.703	1.04–1	0.35	1.48–2	6
98RUZ/MAJ	304.2–349.9	25	1.00	0.239	7.33–2	0.24	−2.23–2	−6
99CAL/BRO	298.1	1	0.50 #	1.037	1.50–1	0.52	−1.50–1	−1
Rejected data								
29KEL2	(7.05–1,2.87,−6.08–1,−5)		59HUT/BAI	(1.74–1,0.59,1.74–1,1)				
73KAL/WOY	(2.92–1,0.98,2.92–1,1)		81ARU	(2.57–1,0.69,−4.29–2,−4)				
84BRA/PIN	(2.44–1,0.85,−2.44–1,−1)		84KAL/WOY	(5.44–1,1.97,4.92–1,35)				
85COS/PAT8	(2.77–1,01.00,−2.50–1,−3)		86ORT	(4.57–1,1.60,−4.57–1,−1)				

Table 42.41.3. Parameters of cubic spline polynomials

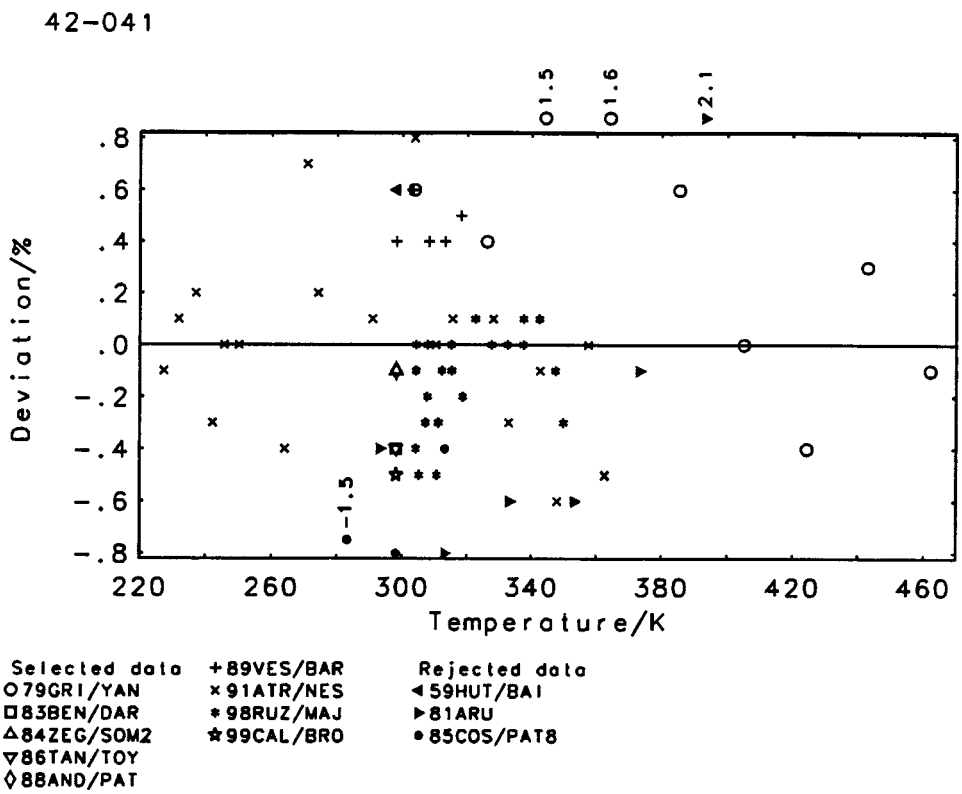
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	119	64	0.665	1.46–1	0.43	1.17–2	−7
sat	119	64	0.665	1.47–1	0.43	1.17–2	−7

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
227.3–300.0	1.35937+1	1.23650+1	−6.39986	1.33886	III
300.0–400.0	1.82261+2	−1.56302+2	4.98225+1	−4.90808	III
400.0–462.0	−6.45593+2	4.64588+2	−1.05400+2	8.02714	IV
227.3–300.0	1.33883+1	1.25956+1	−6.48563	1.34942	III
300.0–400.0	1.82897+2	−1.56913+2	5.00172+1	−4.92867	III
400.0–462.0	−6.38849+2	4.59396+2	−1.04060+2	7.91111	IV

Table 42.41.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	119	64	0.772	1.97−1	0.55	1.50−3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
227.3–462.0	610.70	1.89364+3	1.79686+2	−1.73541+2	1.92042+3	−6.90434+1	1.70875+3	IV



Name: 1-Methylcyclohexanol
Formula: $C_7H_{14}O$

CAS-RN: 590-67-0
Group No.: 42-056
Molar Mass: 114.19

Table 42.56.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
88CAC/COS	298.1	1	nosp	not specified		p	FSIT	71PIC/LED
98KAB/BLO	299.4–320.0	4 S	0.40	99.95	chrom	p	BSAO	93DIK/KAB

Table 42.56.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
98KAB/BLO	299.4–320.0	4	0.40	0.016	2.15−3	0.01	0.00	0

Table 42.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	5	4	0.023	3.04−3	0.01	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
299.4–320.0	−4.10425	1.22453+1	IV

Name: 1-Heptanol
Formula: $C_7H_{16}O$

CAS-RN: 111-70-6
Group No.: 42-063
Molar Mass: 116.20

Table 42.63.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
56PAR/KEN		240.0–300.0	7 S	1.00	98.2	melpt	*p*	BSIO	25PAR
59HUT/BAI		298.1	1	nosp	not specified		*p*	BSIO	55HUT/MAN
67GRA		308.1–338.1	4	1.00	not specified		*p*	BSIO	67GRA
79GRI/YAN	N	303.0–462.3	9	0.90	not specified		*p*	BDAO	75RAS/GRI
80VAS/TRE		323.0–453.0	eqn	2.00	99.8	anal	sat	BSAO	80VAS/TRE
84ZEG/SOM2		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
88ARU/MOV		293.1–433.1	8	3.00	not specified		*p*	BDHT	81ARU
88NAZ/BAS		303.4–447.1	7	2.20	99.2	anal	*p*	BDHO	86NAZ/BASI
89VES/BAR	N	298.1–318.1	5	0.50	not specified		*p*	BSAO	79VES/ZAB
98RUZ/MAJ		304.3–406.0	34	1.00	99.34	chrom	*p*	BDCT	91BAN/GAR
99CAL/BRO		298.1	1	nosp	99.0	chrom	*p*	FSIT	71PIC/LED
#00FUL/RUZ		330.6–570.7	13	2.00	99.94	chrom	sat	BDCT	91BAN/GAR

79GRI/YAN data above 425.19 K were measured at elevated pressures up to 0.27 MPa
89VES/BAR water content 0.007 mass %

Table 42.63.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
56PAR/KEN	240.0–300.0	7	1.00	1.281	4.11–1	1.28	2.91–1	5
59HUT/BAI	298.1	1	1.00 #	0.090	2.96–2	0.09	2.96–2	1
79GRI/YAN	303.0–462.3	9	1.50 #	0.782	4.98–1	1.17	3.15–1	5
84ZEG/SOM2	298.1	1	0.50 #	0.512	8.43–2	0.26	8.43–2	1
88AND/PAT	298.1	1	0.50 #	0.499	8.17–2	0.25	−8.17–2	−1
89VES/BAR	298.1–318.1	5	0.50	1.504	2.55–1	0.75	−2.53–1	−5
98RUZ/MAJ	304.3–406.0	34	1.00	0.425	1.69–1	0.42	7.54–2	23
99CAL/BRO	298.1	1	0.50 #	0.322	5.28–2	0.16	−5.28–2	−1
#00FUL/RUZ	330.6–570.7	13	2.00	0.500	4.58–1	01.00	−1.09–1	−3
Rejected data								
67GRA	(8.52–1,2.49,−8.01–1,−4)		80VAS/TRE	(6.78–1,1.69,−6.52–1,−9)				
88ARU/MOV	(1.70,3.44,7.99–1,0)		88NAZ/BAS	(1.29,3.38,3.82–1,1)				

Table 42.63.3. Parameters of cubic spline polynomials

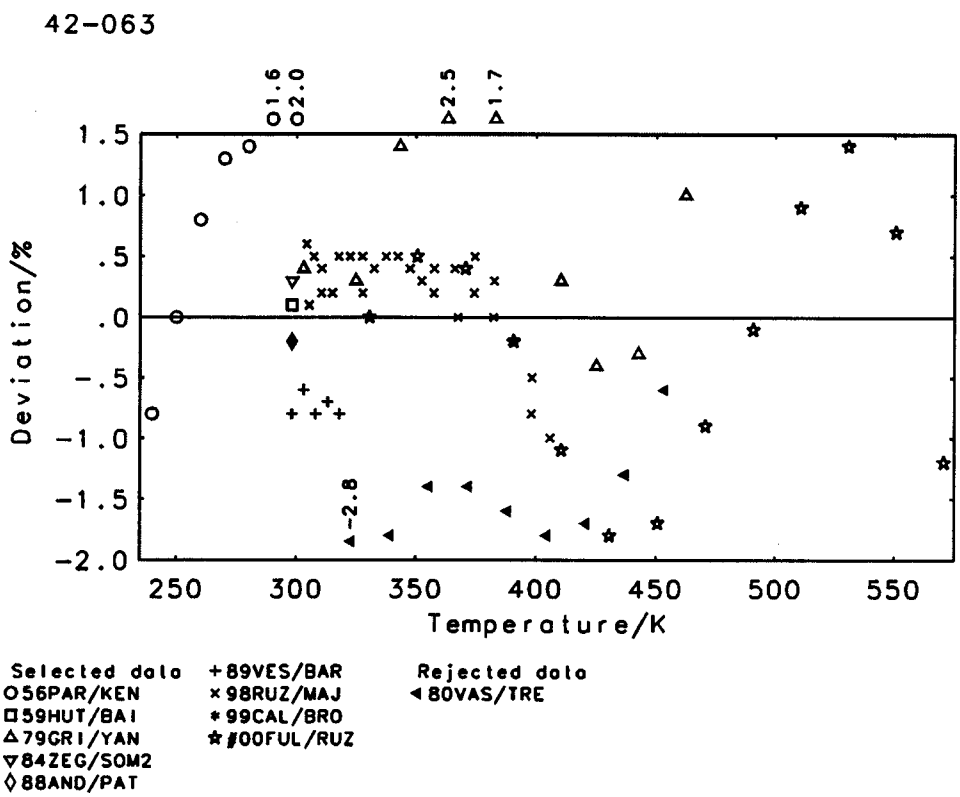
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	100	72	0.762	3.36−1	0.83	6.58−2	25
sat	100	72	0.765	3.40−1	0.84	6.54−2	25

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
240.0–320.0	1.94648+2	−1.73962+2	5.80936+1	−6.02041	IV
320.0–430.0	9.42920+1	−7.98788+1	2.86925+1	−2.95780	V
430.0–570.7	−6.49211+2	4.38844+2	−9.19408+1	6.39362	V
240.0–320.0	1.95524+2	−1.74861+2	5.83977+1	−6.05440	IV
320.0–430.0	9.38215+1	−7.95146+1	2.86020+1	−2.95068	V
430.0–570.7	−6.20167+2	4.18617+2	−8.72426+1	6.02952	V

Table 42.63.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	100	72	2.250	9.87−1	2.44	−7.13−2	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
240.0–570.7	632.50	4.42346+1	3.32760	−1.40039+1	1.47005+2	V



Name: 2-Ethyl-1-hexanol
Formula: $C_8H_{18}O$

CAS-RN: 104-76-7
Group No.: 42-067
Molar Mass: 130.23

Table 42.67.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
58ANO	298.1	1	nosp	not specified		*p*	not specified	
78RYB/EME	293.1–353.1	7 S	nosp	not specified		*p*	BSIO	78RYB/EME
87BUS/MAS	153.3–322.0	34	0.20	not specified		*p*	BSAO	76LEB/LIT
87BUS/MAS	327.6–349.1	5	1.00	not specified		*p*	BSAO	68LEA

Table 42.67.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
78RYB/EME	293.1–353.1	7	2.00 #	0.658	5.46–1	1.32	5.19–1	7
87BUS/MAS	153.3–322.0	33	0.20	1.188	7.75–2	0.24	3.04–3	1
87BUS/MAS	327.6–349.1	5	1.00	1.554	6.87–1	1.55	−6.08–1	−5
Rejected data								
58ANO	(1.13,3.05,−1.13,−1)							

Table 42.67.3. Parameters of regression polynomial

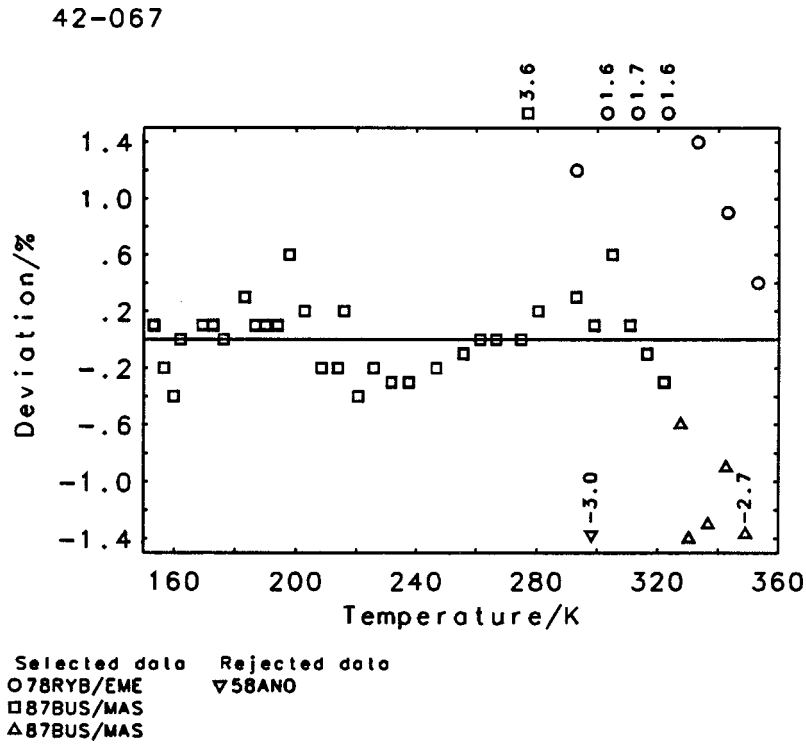
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	47	45	1.212	3.33–1	0.79	1.54–2	3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
153.3–353.1	3.35616+1	−1.06242+1	4.07540	IV

Table 42.67.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	47	45	2.384	3.24–1	0.82	−3.92–2	−21

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
153.3–353.1	640.20	2.65359+3	2.85265+2	−2.62291+2	2.44082+3	5.87758+2	1.64179+3	V



Name: 1-Octanol
Formula: $C_8H_{18}O$

CAS-RN: 111-87-5
Group No.: 42-079
Molar Mass: 130.23

Table 42.79.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		314.2–384.8	5 S	nosp	not specified		avg	DSIO	*81VON
31CLI/AND		246.0–286.0	4	nosp	not specified		sat	DSIO	26AND/LYN
59HUT/BAI		298.1	1	nosp	not specified		*p*	BSIO	55HUT/MAN
61ROU		298.9–311.3	5	nosp	not specified		*p*	BSAO	61ROU
79GRI/YAN		310.7–452.3	8	0.90	not specified		*p*	BDAO	75RAS/GRI
80VAS/TRE		313.0–468.0	eqn	2.00	99.6	anal	sat	BSAO	80VAS/TRE
83PFE/SCH		298.1	1	nosp	not specified		*p*	BDCT	68WAD
84ZEG/SOM2		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
86NAZ/BAS2		303.2–448.6	7	2.00	99.6	estim	*p*	BDHO	86NAZ/BAS1
89VES/BAR	N	298.1–318.1	5	0.50	not specified		*p*	BSAO	79VES/ZAB
92PFE/SCH		298.1–313.1	2	nosp	not specified		*p*	BDCT	68WAD
98RUZ/MAJ		304.3–367.4	32	1.00	99.90	chrom	*p*	BDCT	91BAN/GAR
99CAL/BRO		298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED
#00FUL/RUZ		330.6–550.7	12	2.00	99.94	chrom	sat	BDCT	91BAN/GAR

89VES/BAR water content 0.039 mass %

Table 42.79.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
31CLI/AND	246.0–286.0	4	2.00 #	0.877	5.65–1	1.75	−1.22–3	0
79GRI/YAN	310.7–452.3	8	0.90	0.859	3.61–1	0.77	1.87–1	2
89VES/BAR	298.1–318.1	5	0.50	0.959	1.85–1	0.48	−1.35–1	−3
92PFE/SCH	298.1–313.1	2	0.50 #	1.407	2.71–1	0.70	9.32–2	0
98RUZ/MAJ	304.3–367.4	32	1.00	0.259	1.06–1	0.26	−1.98–2	−12
99CAL/BRO	298.1	1	0.50 #	1.163	2.13–1	0.58	2.13–1	1
#00FUL/RUZ	330.6–550.7	12	2.00	0.209	1.90–1	0.42	2.07–2	0
Rejected data								
*81VON	(2.71,6.15,−2.09,−3)		59HUT/BAI	(1.14,3.03,1.14,1)				
61ROU	(2.80–1,0.75,2.08–1,3)		80VAS/TRE	(5.02–1,1.14,−4.29–1,−6)				
83PFE/SCH	(2.04,5.92,−2.04,−1)		84ZEG/SOM2	(2.50–1,0.68,2.50–1,1)				
86NAZ/BAS2	(1.38,3.17,2.30–1,−1)							

Table 42.79.3. Parameters of cubic spline polynomials

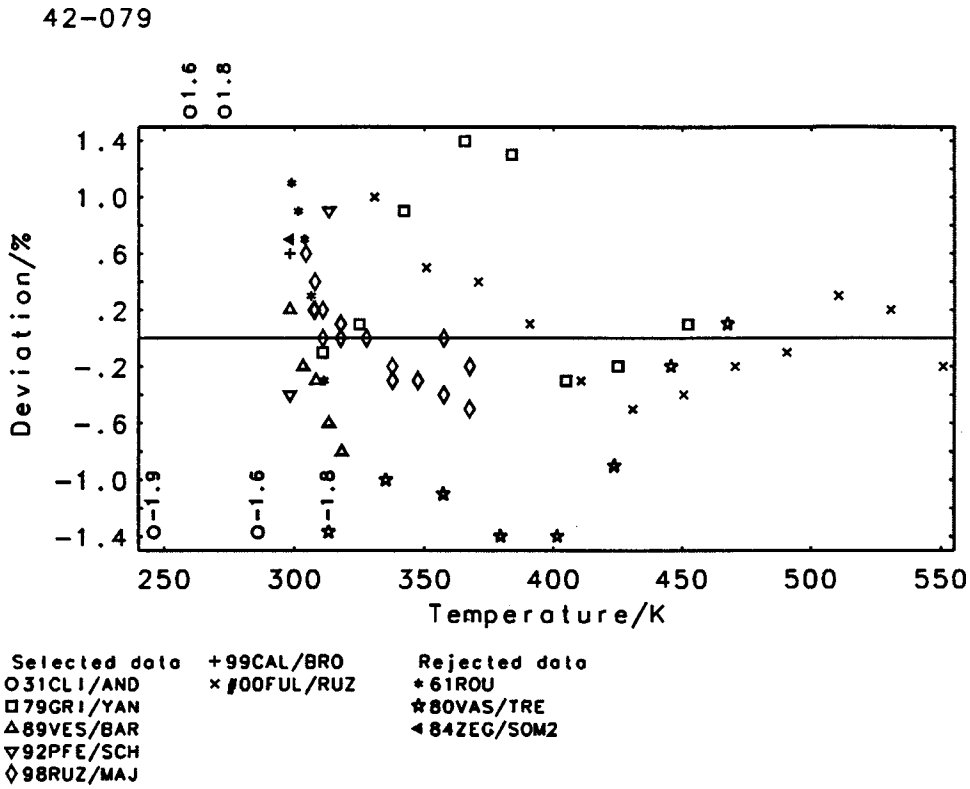
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	92	64	0.604	2.43–1	0.64	1.30–2	−12
sat	92	64	0.605	2.43–1	0.64	1.32–2	−12

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
246.0–400.0	9.92272+1	−8.72102+1	3.24986+1	−3.45623	IV
400.0–550.6	−3.55479+2	2.53819+2	−5.27587+1	3.64855	V
246.0–400.0	9.92973+1	−8.72838+1	3.25241+1	−3.45911	IV
400.0–550.6	−3.50081+2	2.49750+2	−5.17344+1	3.56243	V

Table 42.79.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	92	64	1.119	7.16–1	1.76	−1.14–1	−20

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
246.0–550.7	652.50	1.42900+2	1.63632+1	−4.89180+1	3.11989+2	V



Name: 1-Nonanol
Formula: $C_9H_{20}O$

CAS-RN: 143-08-8
Group No.: 42-084
Molar Mass: 144.26

Table 42.84.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
79GRI/YAN	304.2–464.2	10	0.90	not specified		*p*	BDAO	75RAS/GRI
82VAS/PET	303.0–423.0	eqn	nosp	99.2	anal	sat	BSAO	80VAS/TRE
82VAS/PET	423.0–483.0	eqn	nosp	99.2	anal	sat	BSAO	80VAS/TRE
86NAZ/BAS2	303.1–474.1	8	2.00	99.4	estim	*p*	BDHO	86NAZ/BAS1
99CAL/BRO	298.1	1	nosp	98.0	anal	*p*	FSIT	71PIC/LED

Table 42.84.2. Correlated heat capacities

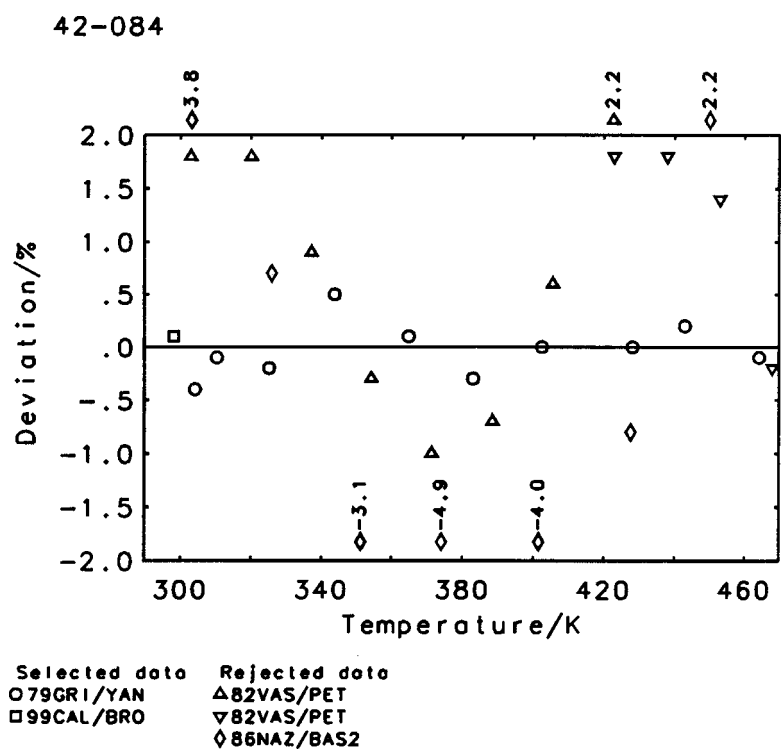
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
79GRI/YAN	304.2–464.2	10	0.90	0.289	1.24–1	0.26	−1.56–2	−3
99CAL/BRO	298.1	1	0.50 #	0.245	4.98–2	0.12	4.98–2	1
			Rejected data					
82VAS/PET	(6.63–1,1.34,3.25–1,2)		82VAS/PET	(9.30–1,1.66,9.24–1,3)				
86NAZ/BAS2	(1.55,3.16,−4.53–1,−1)							

Table 42.84.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	32	11	0.387	1.62−1	0.34	−9.62−3	−2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
298.1–380.0		4.10123+2	−3.59596+2	1.12447+2	−1.12048+1		IV
380.0–464.2		−7.72208+2	5.73824+2	−1.33190+2	1.03423+1		IV

Table 42.84.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	32	11	1.087	4.10−1	0.84	−5.08−2	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
298.1–464.2	671.50	1.07089+3	1.35144+2	−1.47287+2	1.01526+3	5.24175+2	2.17044+2	V



Name: 1-Decanol
Formula: $C_{10}H_{22}O$

CAS-RN: 112-30-1
Group No.: 42-090
Molar Mass: 158.28

Table 42.90.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
67GRA	308.1–338.1	4	1.00	not specified		*p*	BSIO	67GRA
75WOY/KAL	303.1	1	nosp	not specified		*p*	BSIO	70REC
79GRI/YAN	305.8–463.3	9	0.90	not specified		*p*	BDAO	75RAS/GRI
79SVE	301.0–461.0	33 S	nosp	99.80	chrom	sat	BDHT	69PER/COM
80VAS/TRE	323.0–403.0	eqn	2.00	99.2	anal	sat	BSAO	80VAS/TRE
80VAS/TRE	403.0–503.0	eqn	2.00	99.2	anal	sat	BSAO	80VAS/TRE
85COS/PAT8	283.1–313.1	3	nosp	99.	estim	*p*	FSIT	71PIC/LED
88AND/PAT	298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
88NAZ/BAS	304.0–523.0	9	2.20	99.1	anal	*p*	BDHO	86NAZ/BAS1
92PFE/SCH	298.1–313.1	2	nosp	not specified		*p*	BDCT	68WAD
98RUZ/MAJ	304.4–404.7	38	1.00	99.70	chrom	*p*	BDCT	91BAN/GAR
99CAL/BRO	298.1	1	nosp	99.0	chrom	*p*	FSIT	71PIC/LED
#00FUL/RUZ	330.6–570.7	13	2.00	99.87	chrom	sat	BDCT	91BAN/GAR

Table 42.90.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
75WOY/KAL	303.1	1	0.50 #	0.421	9.55–2	0.21	9.55–2	1
79GRI/YAN	305.8–463.3	9	0.90	1.297	6.69–1	1.17	5.24–1	5
79SVE	301.0–461.0	33	1.50 #	0.247	2.05–1	0.37	−1.08–1	−17
85COS/PAT8	283.1–313.1	3	0.50 #	0.561	1.25–1	0.28	−1.17–1	−3
88AND/PAT	298.1	1	0.50 #	1.375	3.08–1	0.69	3.08–1	1
98RUZ/MAJ	304.4–404.7	38	1.00	0.259	1.41–1	0.26	−9.58–2	−30
99CAL/BRO	298.1	1	0.50 #	0.412	9.19–2	0.21	9.19–2	1
#00FUL/RUZ	330.6–570.7	13	2.00	0.397	4.68–1	0.79	−2.78–1	−3
Rejected data								
67GRA	(1.62,3.59,−1.50,−4)		80VAS/TRE	(5.39–1,1.05,−4.81–1,−6)				
80VAS/TRE	(3.26–1,0.54,1.50–1,0)		88NAZ/BAS	(3.12,4.84,1.11,1)				
92PFE/SCH	(2.31,4.84,2.31,2)							

Table 42.90.3. Parameters of cubic spline polynomials

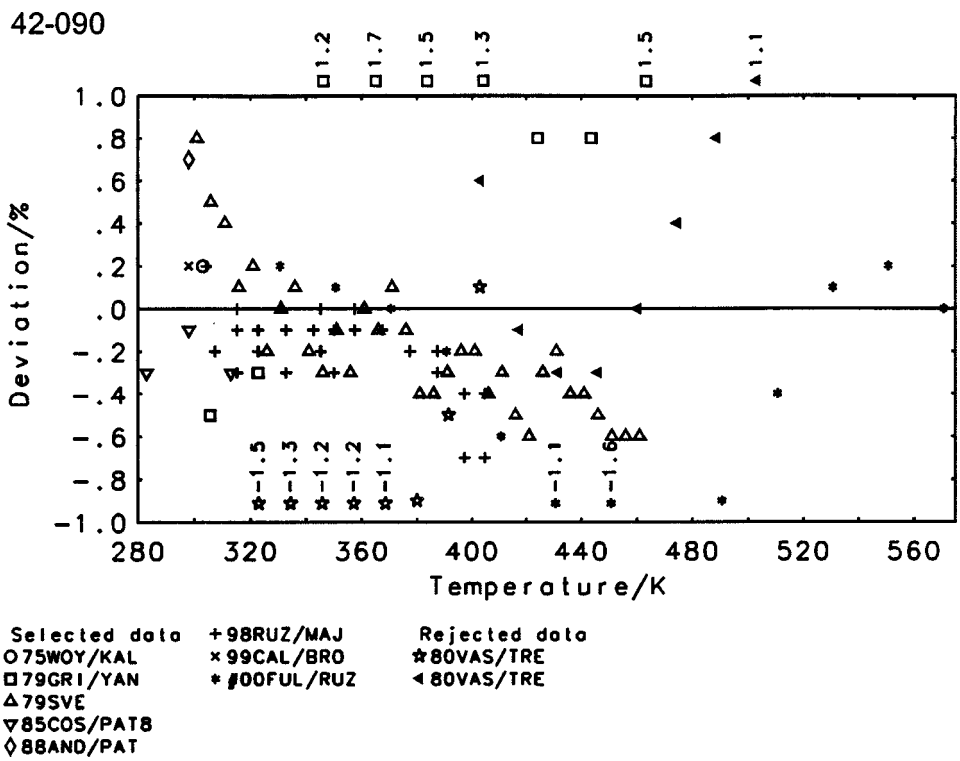
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	130	99	0.518	3.14–1	0.55	−6.02–2	−45
sat	130	99	0.518	3.14–1	0.55	−6.01–2	−44

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
283.1–380.0	1.86081+2	−1.58308+2	5.35843+1	−5.50357	IV
380.0–450.0	−2.30199+2	1.70334+2	−3.29005+1	2.08282	V
450.0–570.7	−4.22670+2	2.98648+2	−6.14146+1	4.19497	V
283.1–380.0	1.85933+2	−1.58172+2	5.35429+1	−5.49939	IV
380.0–450.0	−2.28489+2	1.69003+2	−3.25557+1	2.05313	V
450.0–570.7	−4.18164+2	2.95453+2	−6.06558+1	4.13461	V

Table 42.90.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	130	99	0.899	6.84−1	1.19	−1.88−1	−27

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
283.1–570.7	689.00	2.49141+2	3.43524+1	−7.01076+1	4.51726+2	V



Name: 1-Dodecanol
Formula: $C_{12}H_{26}O$

CAS-RN: 112-53-8
Group No.: 42-095
Molar Mass: 186.34

Table 42.95.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
79SVE	316.0–486.0	35 S	nosp	99.98	chrom	sat	BDHT	69PER/COM
82VAS/PET	303.0–423.0	eqn	nosp	99.9	anal	sat	BSAO	80VAS/TRE
82VAS/PET	423.0–533.0	eqn	nosp	99.9	anal	sat	BSAO	80VAS/TRE
88AND/PAT	298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
98RUZ/MAJ	307.2–357.6	24	1.00	99.00	chrom	*p*	BDCT	91BAN/GAR

Table 42.95.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
79SVE	316.0–486.0	35	1.50 #	0.138	1.32–1	0.21	1.05–2	2
88AND/PAT	298.1	1	0.50 #	0.296	7.80–2	0.15	7.80–2	1
98RUZ/MAJ	307.2–357.6	24	1.00	0.175	9.85–2	0.17	−1.91–2	0
Rejected data								
82VAS/PET	(2.60,4.03,2.58,8)		82VAS/PET	(2.61,3.68,2.61,5)				

Table 42.95.3. Parameters of cubic spline polynomials

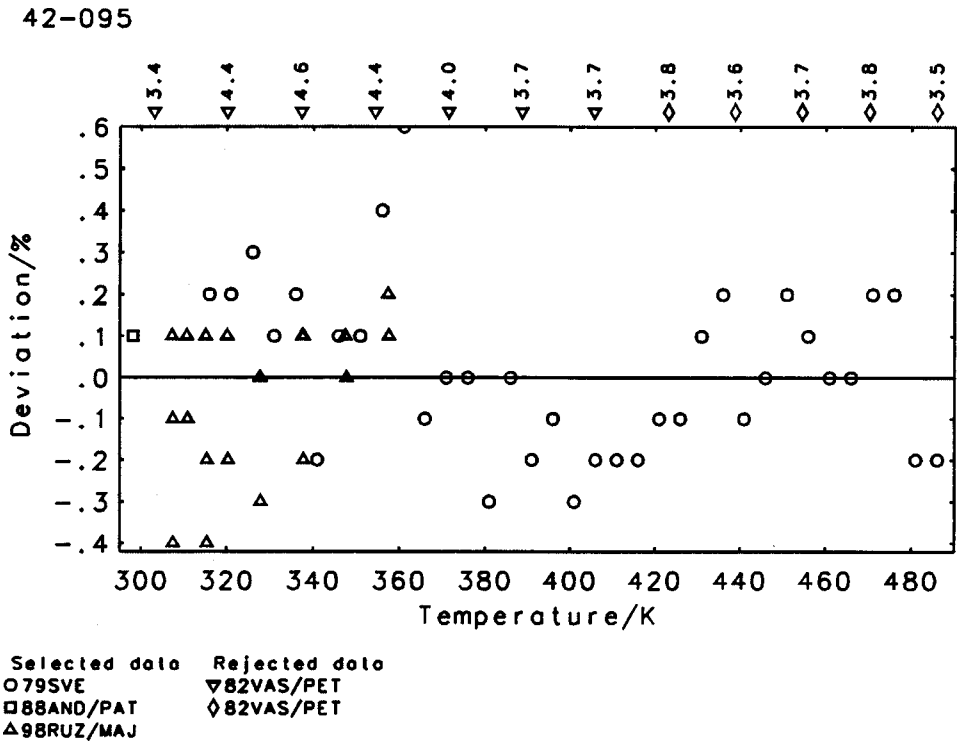
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	76	60	0.164	1.24–1	0.20	−2.41–4	3
sat	76	60	0.165	1.25–1	0.20	−2.53–4	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
298.1–400.0	1.85891+2	−1.52201+2	5.20271+1	−5.35551	IV
400.0–486.0	−6.73239+2	4.92147+2	−1.09060+2	8.06840	V
298.1–400.0	1.85618+2	−1.51964+2	5.19589+1	−5.34900	IV
400.0–486.0	−6.71366+2	4.90774+2	−1.08726+2	8.04138	V

Table 42.95.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	76	60	0.505	2.21–1	0.38	−3.12–2	−5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
298.1–486.0	720.00	5.64092+2	9.45197+1	−1.56372+2	8.41622+2	V



Name: 1-Tridecanol
Formula: $C_{13}H_{28}O$

CAS-RN: 112-70-9
Group No.: 42-097
Molar Mass: 200.36

Table 42.97.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
74MOS/MOU	305.0–346.0	eqn	nosp	99.97	chrom	*p*	BSAO	74MOS/MOU
77BEL/BUB	313.1	1	nosp	not specified		*p*	BDCT	68WAD
80VAS/TRE	323.0–423.0	eqn	2.00	99.2	anal	sat	BSAO	80VAS/TRE
80VAS/TRE	423.0–553.0	eqn	2.00	99.2	anal	sat	BSAO	80VAS/TRE

Name: 1-Tetradecanol
Formula: $C_{14}H_{30}O$

CAS-RN: 112-72-1
Group No.: 42-098
Molar Mass: 214.39

Table 42.98.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
74MOS/MOU	312.0–346.0	eqn	nosp	99.95	chrom	*p*	BSAO	74MOS/MOU
80VAS/TRE	333.0–413.0	eqn	2.00	99.2	anal	sat	BSAO	80VAS/TRE
80VAS/TRE	413.0–463.0	eqn	2.00	99.2	anal	sat	BSAO	80VAS/TRE
80VAS/TRE	463.0–573.0	eqn	2.00	99.2	anal	sat	BSAO	80VAS/TRE
91STE/CHI2	324.0–564.0	25	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 42.98.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
74MOS/MOU	312.0–346.0	5	0.50 #	0.320	1.08–1	0.16	−6.72–2	−2
80VAS/TRE	463.0–573.0	5	2.00	0.619	9.72–1	1.24	7.30–1	5
91STE/CHI2	324.0–564.0	25	1.00	0.316	2.34–1	0.32	2.01–2	1
			Rejected data					
80VAS/TRE	(9.50–1,1.35,1.16–1,1)		80VAS/TRE	(1.54,1.98,1.54,5)				

Table 42.98.3. Parameters of cubic spline polynomials

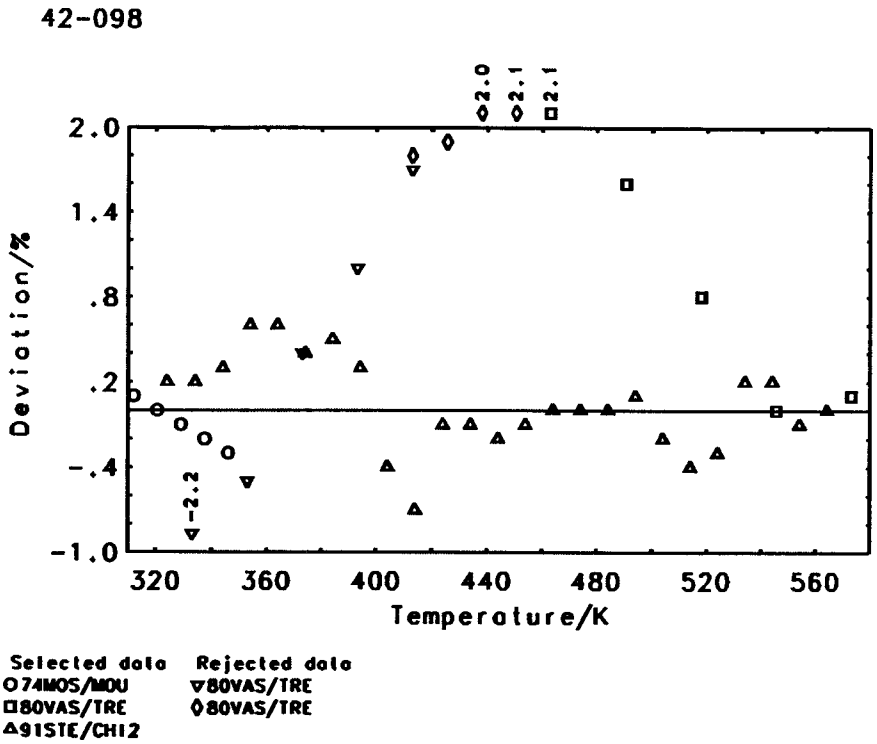
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	45	35	0.412	4.60–1	0.60	1.09–1	4
sat	45	35	0.412	4.60–1	0.60	1.09–1	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
312.0–400.0	2.22827+2	−1.76719+2	5.88986+1	−5.98507	IV
400.0–480.0	−6.88384+2	5.06690+2	−1.11954+2	8.25261	IV
480.0–573.0	6.59962+2	−3.36027+2	6.36124+1	−3.93947	IV
312.0–400.0	2.22104+2	−1.76109+2	5.87281+1	−5.96928	IV
400.0–480.0	−6.86307+2	5.05199+2	−1.11599+2	8.22464	IV
480.0–573.0	6.62392+2	−3.37737+2	6.40128+1	−3.97062	IV

Table 42.98.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	45	35	0.831	5.29–1	0.70	−7.44–3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
312.0–573.0	747.00	1.46925+3	1.37357+2	−4.44196+2	3.34208+3	−3.17233+3	3.05902+3	V



Name: 1-Hexadecanol
Formula: $C_{16}H_{34}O$

CAS-RN: 36653-82-4
Group No.: 42-102
Molar Mass: 242.45

Table 42.102.1. Experimental heat capacities

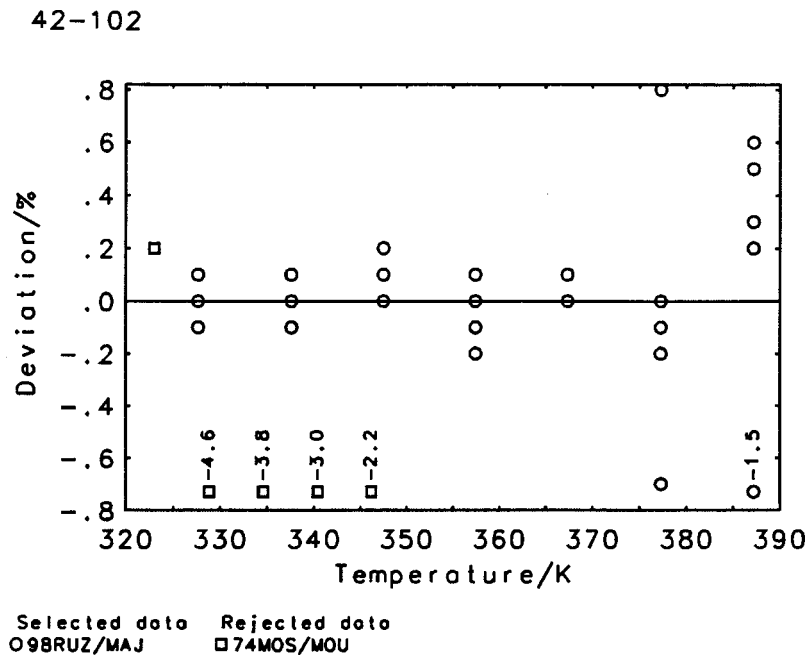
Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
74MOS/MOU	323.0–346.0	eqn	nosp	99.96	chrom	*p*	BSAO	74MOS/MOU
98RUZ/MAJ	327.6–387.2	35	1.00	99.60	chrom	*p*	BDCT	91BAN/GAR

Table 42.102.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
98RUZ/MAJ	327.6–387.2	35	1.00	0.351	2.89−1	0.35	2.09−3	5
Rejected data								
74MOS/MOU	(2.58,3.53,−2.51,−4)							

Table 42.102.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	40	35	0.373	3.07−1	0.37	2.09−3	5
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
327.6–387.2		8.90027+2	−7.55550+2	2.27949+2	−2.23720+1		IV



Name: 1-Octadecanol
Formula: $C_{18}H_{38}O$

CAS-RN: 112-92-5
Group No.: 42-103
Molar Mass: 270.50

Table 42.103.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
80VAS/TRE	353.0–413.0	eqn	2.00	99.8	anal	sat	BSAO	80VAS/TRE
80VAS/TRE	413.0–513.0	eqn	2.00	99.8	anal	sat	BSAO	80VAS/TRE
80VAS/TRE	513.0–623.0	eqn	2.00	99.8	anal	sat	BSAO	80VAS/TRE
98RUZ/MAJ	337.6–397.2	28	1.00	99.60	chrom	p	BDCT	91BAN/GAR
#01VAN/OON	332.6–358.7	18	0.20	98.0	anal	p	BSAO	87VAN/VAN

Table 42.103.2. Correlated heat capacities

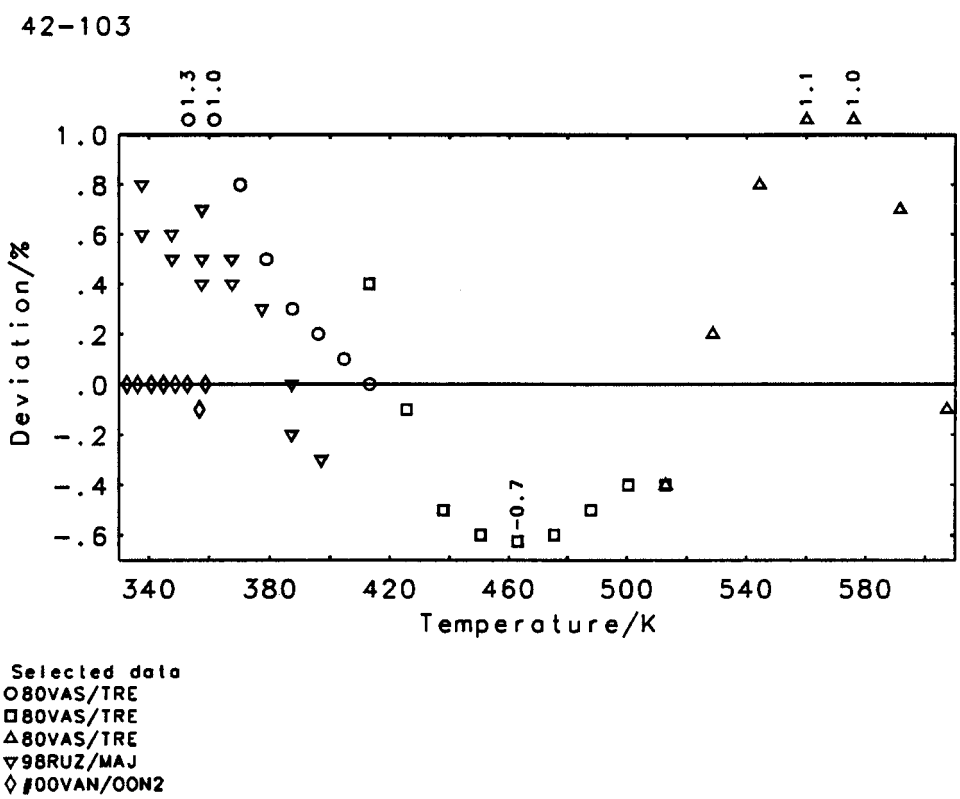
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
80VAS/TRE	353.0–413.2	8	2.00	0.336	6.03−1	0.67	4.72−1	7
80VAS/TRE	413.0–513.0	9	2.00	0.255	4.94−1	0.51	−3.76−1	−7
80VAS/TRE	513.0–622.9	8	2.00	0.409	8.46−1	0.82	2.36−1	2
98RUZ/MAJ	337.5–397.2	28	1.00	0.458	4.04−1	0.46	2.82−1	18
#01VAN/OON	332.6–358.7	18	0.20	0.212	3.67−2	0.04	−1.84−2	−10

Table 42.103.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	71	71	0.379	4.83−1	0.51	1.39−1	10
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
332.6–380.0		3.01548+2	−2.35565+2	7.68013+1	−7.71879		III
380.0–622.9		−3.09133+2	2.46551+2	−5.00713+1	3.41038		V

Table 42.103.4. Parameters of quasipolynomial equation

Heat capacity type		No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
				%				
C		71	71	6.674	1.35	1.57	−7.74−1	−28
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
332.6–622.9	790.00	9.41086+2	9.43427+1	−2.39952+2	2.07451+3	−1.86836+3	1.81406+3	V



Name: Methanol-d_4
Formula: CD_4O

CAS-RN: 811-98-3
Group No.: 42-106
Molar Mass: 36.07

Table 42.106.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92FIL/AFA	298.15	2.437	nosp	not specified		p	BDCT	92FIL/AFA

Name: Methan-d_3-ol
Formula: CHD_3O

CAS-RN: 1849-29-2
Group No.: 42-107
Molar Mass: 35.06

Table 42.107.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92FIL/AFA	298.15	2.419	nosp	not specified		*p*	BDCT	92FIL/AFA

Name: (±)-1,2-Butanediol
Formula: $C_4H_{10}O_2$

CAS-RN: 26171-83-5
Group No.: 42-108
Molar Mass: 90.12

Table 42.108.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96STE/CHI1	300.0–670.0	20 S	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 42.108.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	20	1.232	5.52–1	1.23	1.32–2	−2
sat	20	20	0.877	3.59–1	0.88	5.73–3	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–630.0	−6.17930+1	5.70467+1	−1.14939+1	8.08269−1	IV
630.0–670.0	−1.03147+5	4.91452+4	−7.80327+3	4.13072+2	V
300.0–630.0	−5.11918+1	4.90150+1	−9.50337	6.46675−1	IV
630.0–670.0	−6.60403+4	3.14724+4	−4.99734+3	2.64553+2	V

Table 42.108.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	20	1.088	5.51–1	1.09	1.81–3	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
300.0–670.0	680.00	3.45963	6.59495−1	−1.39157+1	1.54628+2	−1.56991+2	6.20148+1	V

Name: 2,2-Dimethyl-1-propanol
Formula: $C_5H_{12}O$

CAS-RN: 75-84-3
Group No.: 42-109
Molar Mass: 88.15

Table 42.109.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97CEN/RUZ	335.4–362.6	10	1.00	99.79	chrom	*p*	BDCT	91BAN/GAR

Table 42.109.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	10	10	0.049	1.70−2	0.05	1.22−5	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
335.4−362.6	−8.86868+1	6.24793+1	−7.80887	IV

Name: 1-Methylcyclopentanol
Formula: $C_6H_{12}O$

CAS-RN: 1462-03-9
Group No.: 42-110
Molar Mass: 100.16

Table 42.110.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96KAB/BLO	308.6−315.3	5	0.40	99.96	chrom	sat	BDHT	92KAB/KOZ

Table 42.110.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	5	5	0.760	9.18−2	0.30	3.39−4	3

Temp. range K	A_1	A_2	Level of uncertainty
308.6−315.3	−1.04834+1	1.30929+1	III

Name: 1,6-Hexanediol
Formula: $C_6H_{14}O_2$

CAS-RN: 629-11-8
Group No.: 42-111
Molar Mass: 118.18

Table 42.111.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91STE/CHI2	333.0−513.0	10	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 42.111.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	10	10	0.334	1.42−1	0.33	8.52−4	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
333.0−513.0	−5.02700+1	3.73095+1	−3.49400	IV

Table 42.111.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	10	10	0.301	1.33−1	0.30	6.32−4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
333.0−513.0	700.00	1.24910+2	1.37833+1	−4.49922+1	2.82995+2	IV

Name: 2-(1,1-Dimethylethyl)phenol
Formula: $C_{10}H_{14}O$

CAS-RN: 88-18-6
Group No.: 42-112
Molar Mass: 150.22

Table 42.112.1. Experimental heat capacities

Reference	Temp. range K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER3	298.15	2.050	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 4-(1,1-Dimethylethyl)-1,2-benzenediol
Formula: $C_{10}H_{14}O_2$

CAS-RN: 98-29-3
Group No.: 42-113
Molar Mass: 166.22

Table 42.113.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI3	350.0–610.0	14	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 42.113.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	14	14	0.415	2.10–1	0.42	1.16–3	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
350.0–550.0	4.48875+1	−7.50802	3.11615	−2.65596−1	IV
550.0–610.0	−3.53761+3	1.94658+3	−3.52173+2	2.12671+1	V

Table 42.113.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	14	14	0.835	4.51–1	0.84	5.61–3	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
350.0–610.0	775.00	3.64775+2	4.06004+1	−9.61481+1	8.17937+2	−7.04847+2	6.59279+2	V

Name: (1α,2β,5α)-5-Methyl-2-(1-methylethyl)cyclohexanol
Formula: $C_{10}H_{20}O$

CAS-RN: 89-78-1
Group No.: 42-114
Molar Mass: 156.27

Table 42.114.1. Experimental heat capacities

Reference		Temp. range K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	333.65	2.356	nosp	not specified		avg	DSIO	*94BRU

*94BRU average value in temperature range 325–342 K

Name: 1,10-Decanediol
Formula: $C_{10}H_{22}O_2$

CAS-RN: 112-47-0
Group No.: 42-115
Molar Mass: 174.28

Table 42.115.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99LI/TAN	353.8–369.9	7	0.50	98.69	melpt	*p*	BSAO	95TAN/SUN

Table 42.115.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	7	7	0.563	1.66–1	0.28	4.58–4	−1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
353.8–369.9	−1.01039+3	5.77009+2	−7.77750+1	V

Name: 2-(1,1-Dimethylethyl)-5-methylphenol
Formula: $C_{11}H_{16}O$

CAS-RN: 88-60-8
Group No.: 42-116
Molar Mass: 164.25

Table 42.116.1. Experimental heat capacities

Reference	Temp. range K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER3	298.15	1.640	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 2,6-Bis(1-methylethyl)phenol
Formula: $C_{12}H_{18}O$

CAS-RN: 2078-54-8
Group No.: 42-117
Molar Mass: 178.27

Table 42.117.1. Experimental heat capacities

Reference	Temp. range K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER4	298.15	2.090	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 2-(1,1-Dimethylethyl)-4,6-dimethylphenol
Formula: $C_{12}H_{18}O$

CAS-RN: 1879-09-0
Group No.: 42-118
Molar Mass: 178.27

Table 42.118.1. Experimental heat capacities

Reference	Temp. range K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99VER4	298.15	1.450	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: *trans*-[1,1′-Bicyclohexyl]-2-ol
Formula: $C_{12}H_{22}O$

CAS-RN: 58879-21-3
Group No.: 42-119
Molar Mass: 182.31

Table 42.119.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97MAK/KAB	328.3–337.7	5	0.40	99.48	chrom	sat	BSAO	93DIK/KAB

Table 42.119.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	5	5	0.002	3.57−4	0.00	−1.53−6	0

Temp. range K	A_1	A_2	Level of uncertainty
328.3–337.7	−1.00473+1	1.85635+1	III

Name: (*Z*)-9-Octadecen-1-ol
Formula: $C_{18}H_{36}O$

CAS-RN: 143-28-2
Group No.: 42-120
Molar Mass: 268.48

Table 42.120.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93CON/GIR2	299.0–370.0	eqn	nosp	not specified		sat	BDHT	93CON/GIR1

Table 42.120.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	17	17	0.000	7.06−6	0.00	5.38−6	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
299.0–369.4	9.98758+1	−3.12770+1	6.89411	VI

Name: 1-Nonadecanol
Formula: $C_{19}H_{40}O$

CAS-RN: 1454-84-8
Group No.: 42-121
Molar Mass: 284.53

Table 42.121.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#01VAN/OON	336.8–359.1	23	0.20	98.0	anal	*p*	BSAO	87VAN/VAN

Table 42.121.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	23	23	0.303	5.48−2	0.06	6.17−5	0

Temp. range K	A_1	A_2	Level of uncertainty
336.8–359.1	2.73759+1	1.82529+1	III

Name: 1-Eicosanol
Formula: $C_{20}H_{42}O$

CAS-RN: 629-96-9
Group No.: 42-122
Molar Mass: 298.55

Table 42.122.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#01VAN/OON	339.0–371.3	26	0.20	98.0	anal	*p*	BSAO	87VAN/VAN

Table 42.122.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	26	26	0.385	7.45–2	0.08	9.39–5	−1
Temp. range K		A_1	A_2				Level of uncertainty
339.0–371.3		3.61958+1	1.69618+1				III

Name: 2-Octyl-1-dodecanol
Formula: $C_{20}H_{42}O$

CAS-RN: 5333-42-6
Group No.: 42-123
Molar Mass: 298.55

Table 42.123.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93CON/GIR2	299.0–441.0	eqn	nosp	not specified		sat	BDHT	93CON/GIR1

Table 42.123.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	14	14	0.000	1.78–5	0.00	9.81–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
299.0–440.7		−1.67688+2	1.25604+2	−1.51170+1			VI

Name: 1-Docosanol
Formula: $C_{22}H_{46}O$

CAS-RN: 661-19-8
Group No.: 42-124
Molar Mass: 326.61

Table 42.124.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#01VAN/OON	346.4–371.3	16	0.20	98.3	melpt	*p*	BSAO	87VAN/VAN

Table 42.124.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	16	16	0.337	7.11–2	0.07	8.35–5	−1
Temp. range K		A_1	A_2				Level of uncertainty
346.4–371.3		4.10801+1	1.80852+1				III

Name: Cholesterol
Formula: $C_{27}H_{46}O$

CAS-RN: 57-88-5
Group No.: 42-125
Molar Mass: 386.66

Table 42.125.1. Experimental heat capacities

Reference	Temp. range K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98VAN/VAN	424.44	2.423	0.20	98.8	melpt	*p*	BSAO	98VAN/VAN

Name: 2-Propanone
Formula: C_3H_6O

CAS-RN: 67-64-1
Group No.: 43-004
Molar Mass: 58.08

Table 43.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		307.5–321.9	4 S	nosp	not specified		avg	DSIO	*81VON
*98LOU	N	321.9	1	nosp	not specified		avg	DSIO	*98LOU
07WAL		291.6	1	nosp	not specified		*p*	DSIO	07WAL
12SCH1		233.1–308.1	4	nosp	not specified		*p*	BSIO	12SCH1
12SCH3		253.1–323.1	5	nosp	not specified		*p*	BSIO	12SCH1
16BRA		283.1	1	nosp	not specified		avg	DSTO	16BRA
21TRE		296.7–319.4	7	nosp	not specified		*p*	BSIO	49WEI
25PAR/KEL		193.2–289.4	10	nosp	not specified		*p*	BSIO	25PAR
25WIL/DAN		293.1–313.1	3 S	nosp	not specified		*p*	BSAO	24WIL/DAN
28PAR/KEL		193.2–289.4	10	1.00	not specified		*p*	BSIO	25PAR
29KEL3		180.3–297.0	14	1.00	not specified		*p*	BSIO	29KEL1
29MIT/HAR1		204.8–256.3	24	nosp	not specified		*p*	BSIO	29MIT/HAR1
32TRE	N	298.0	1	nosp	not specified		*p*	BSIO	49WEI
39PHI		302.4	1	nosp	not specified		*p*	BSIO	49WEI
47SKU		293.1	1	0.30	not specified		*p*	BSAO	47SKU
55STA/TUP		287.9–323.7	10	1.00	not specified		*p*	BSAO	55STA/TUP
62LOW/MOE		253.2–308.2	7 S	0.50	not specified		*p*	BSIO	57HAR/MOE
67RAS/GAN		293.1–333.1	3 S	0.50	not specified		*p*	BSAO	67RAS/GAN
71DES/BHA		298.1–318.1	3 S	1.00	not specified		*p*	BSIO	58MUR/VAN
79SAL/PEA		298.1–298.1	2	nosp	not specified		*p*	BSIO	80FUC
80FUC		298.2–298.2	2	0.50	99.	chrom	*p*	BSIO	80FUC
85COS/PAT9		283.1–313.1	3	nosp	99.	chrom	*p*	FSIT	71PIC/LED
86ALP/PES	N	258.1–318.1	4	0.20	not specified		*p*	BSAO	83KUK/KOR
89COS/YAO		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
90YAM/OGA	N	298.1	1	nosp	not specified		*p*	FSIO	85OGA/MUR
91GRO/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
94GRO/ROU		298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED

*98LOU average value in temperature range 293–351 K
32TRE same datum in 33TRE/WAT
86ALP/PES same data in 89PET/PES and 90ALP/PES
90YAM/OGA water content less than 0.02 mol %

Name: 2-Butanone
Formula: C_4H_8O

CAS-RN: 78-93-3
Group No.: 43-007
Molar Mass: 72.11

Table 43.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
33KOL/UDO	N	297.0	1	nosp	not specified		*p*	BSIT	34KOL/UDO2
38PAN/DUD	N	298.0–363.0	eqn	nosp	not specified		*p*	not specified	
56PAR/KEN		180.0–300.0	13 S	1.00	99.7	melpt	*p*	BSIO	25PAR
64SIN/OET		191.6–336.4	64	0.30	99.78	melpt	sat	BSAO	58HIL/KRA
67RAS/GAN		293.1–353.1	4 S	0.50	not specified		*p*	BSAO	67RAS/GAN
68AND/COU2		190.8–319.8	27	nosp	99.98	melpt	sat	BSAO	63AND/COU1
75GRO/BEN		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
78ROU/PER1		283.1–313.1	3 S	0.30	99.8	chrom	*p*	FSIT	71PIC/LED
80FUC		298.2	1	0.50	not specified		*p*	BSIO	80FUC
84GRO/BEN		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
85COS/PAT9		283.1–313.1	3	nosp	99.	chrom	*p*	FSIT	71PIC/LED
91KAL/KOH		293.1–313.1	2	1.00	99.89	anal	*p*	FSIT	71PIC/LED
97HOV/ROU		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED

33KOL/UDO same datum in 34KOL/UDO2
38PAN/DUD temperature range of parameters validity estimated by the compilers

Name: Cyclopentanone
Formula: C_5H_8O

CAS-RN: 120-92-3
Group No.: 43-008
Molar Mass: 84.12

Table 43.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
80FUC	298.2	1	0.50	not specified		*p*	BSIO	80FUC
87SHV/PES	217.8–327.5	29	nosp	not specified		*p*	BSAO	78ZHU/ATR
97HOV/ROU	298.1	1	nosp	99.	chrom	*p*	FSIT	71PIC/LED

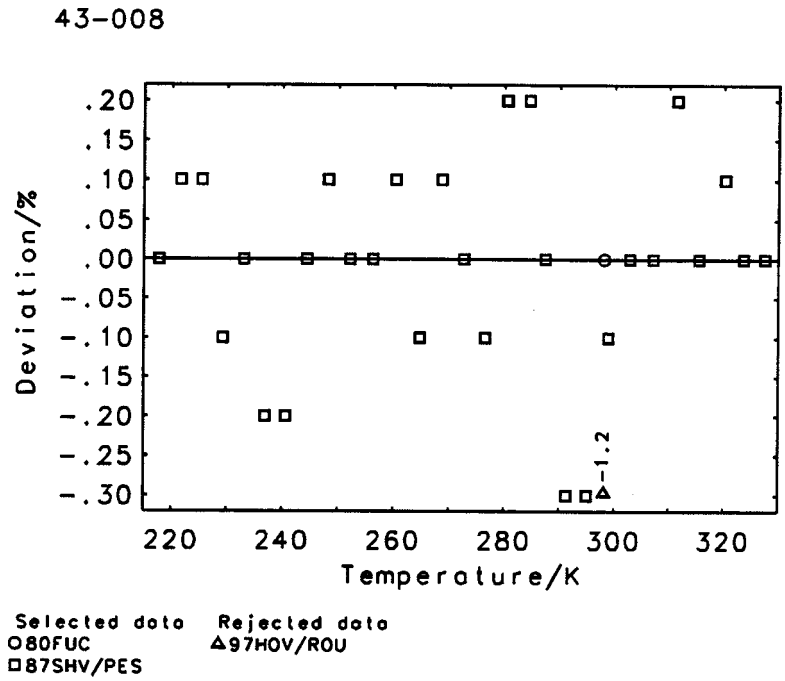
Table 43.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
			Selected data					
80FUC	298.2	1	0.50	0.056	5.16–3	0.03	−5.16–3	−1
87SHV/PES	217.8–327.5	29	1.00 #	0.124	2.22–2	0.12	7.68–4	2
			Rejected data					
97HOV/ROU	(2.18–1,1.18,−2.18–1,−1)							

Table 43.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	31	30	0.261	2.35–2	0.13	4.94–5	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
217.8–327.5	3.25531+1	−2.01713+1	7.79034	−8.70682−1	III



Name: 2,4-Pentanedione
Formula: $C_5H_8O_2$

CAS-RN: 123-54-6
Group No.: 43-009
Molar Mass: 100.12

Table 43.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
69MEL/MER	N	254.8–300.0	8 S	nosp	not specified		sat	BSAO	45SCO/MEY
97HOV/ROU		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
#00BEC/AUF		300.0–360.0	13	0.20	99.95	chrom	sat	BDCT	#00BEC/AUF

69MEL/MER predominately enol form

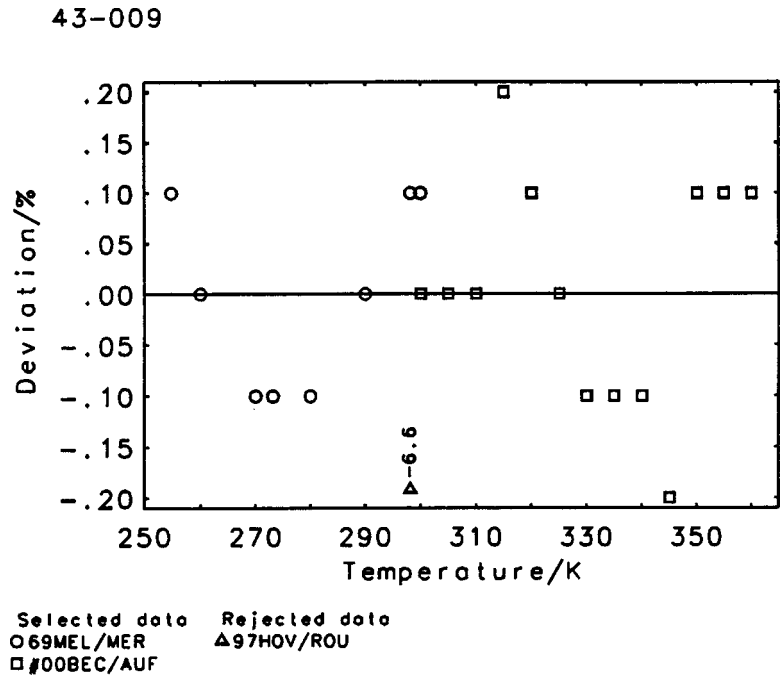
Table 43.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
				Selected data				
69MEL/MER	254.8–300.0	8	0.30 #	0.237	1.74–2	0.07	5.90–4	−2
#00BEC/AUF	300.0–360.0	13	0.20	0.545	2.88–2	0.11	−9.46–5	−1
				Rejected data				
97HOV/ROU	(1.55,6.59,−1.55,−1)							

Table 43.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
C	22	21	0.490	2.71–2	0.10	1.66–4	−3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
254.8–360.0	5.09972	8.93993	−7.57459−1	III



Name: 2,2-Dimethylpropanal
Formula: $C_5H_{10}O$

CAS-RN: 630-19-3
Group No.: 43-010
Molar Mass: 86.13

Table 43.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
80FUC		298.2	1	0.50	not specified		*p*	BSIO	80FUC
83KOR/DYA	N	274.1–350.0	18 S	nosp	not specified		*p*	BSAO	77KU/COM
88WHI/PER	N	272.2–298.4	8	0.50	95.	chrom	*p*	BSAO	87VAN/WHI
88WHI/PER	N	274.4–295.8	9	0.50	99.	chrom	*p*	BSAO	87VAN/WHI

83KOR/DYA error of 0.3%–1.0% reported in 84VAS/PET
88WHI/PER commercial sample
88WHI/PER commercial sample after destilation

Table 43.10.2. Correlated heat capacities

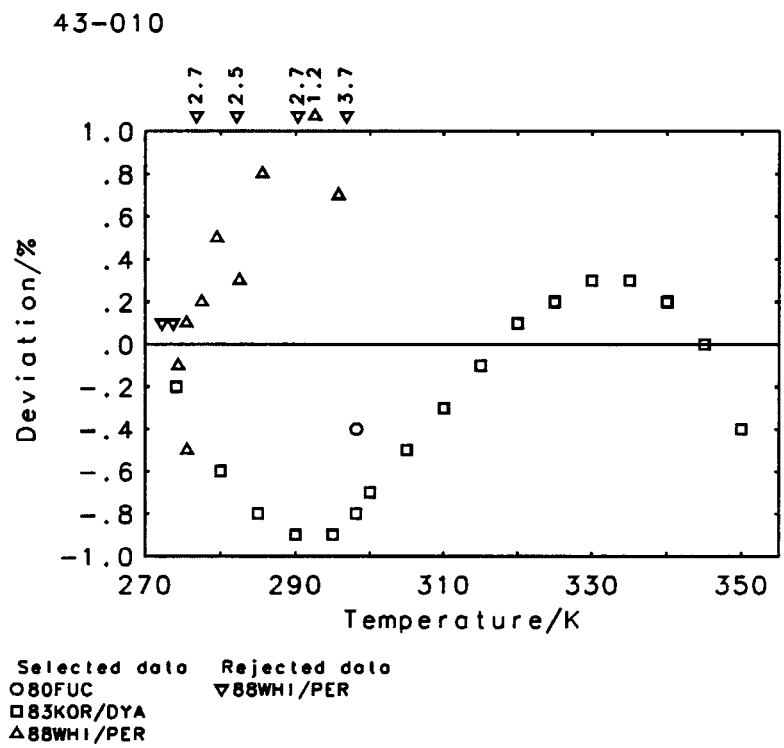
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
80FUC	298.2	1	0.50	0.897	1.01–1	0.45	−1.01–1	−1
83KOR/DYA	274.1–350.0	18	0.70 #	0.733	1.15–1	0.51	−6.57–2	−8
88WHI/PER	274.4–295.8	9	0.50	1.214	1.36–1	0.61	8.12–2	5
Rejected data								
88WHI/PER	(7.04–1,3.07,6.94–1,6)							

Table 43.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	36	28	0.994	1.31−1	0.59	−1.98−2	−4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
274.1–350.0		−1.99595+2	2.11728+2	−6.79337+1	7.34650		IV

Table 43.10.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	36	28	1.138	1.32−1	0.59	9.05−3	−7
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
274.1–350.0	525.00	−3.29246	4.99794−1	1.53932+1	5.42239		IV



Name: Cyclohexanone
Formula: $C_6H_{10}O$

CAS-RN: 108-94-1
Group No.: 43-017
Molar Mass: 98.14

Table 43.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
24HER/BLO	289.6	1	nosp	not specified		*p*	DSIO	22HER/SCH
39PHI	303.9	1	nosp	not specified		*p*	BSIO	49WEI
71VAN	250.0–280.0	7 S	nosp	99.95	melpt	sat	BSAO	72VAN
80FUC	298.2–298.2	2	0.50	not specified		*p*	BSIO	80FUC
80NAK/SUG	244.8–301.4	25	0.30	99.92	melpt	sat	BSAO	65SUG/SEK
97HOV/ROU	298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED

Name: 4-Methyl-3-penten-2-one
Formula: $C_6H_{10}O$

CAS-RN: 141-79-7
Group No.: 43-018
Molar Mass: 98.14

Table 43.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		317.2–354.7	6 S	nosp	not specified		avg	DSIO	*81VON
*98LOU	N	344.1	1	nosp	not specified		avg	DSIO	*98LOU
97STE/CHI1		290.0–580.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

*98LOU average value in temperature range 294–394 K

Table 43.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
				Selected data				
*81VON	317.2–354.7	6	1.50 #	0.323	1.20–1	0.49	−3.50–3	0
97STE/CHI1	290.0–580.0	59	1.00	0.502	1.76–1	0.50	2.24–3	−1
				Rejected data				
*98LOU	(5.02–1,1.95,5.02–1,1)							

Table 43.18.3. Parameters of regression polynomial

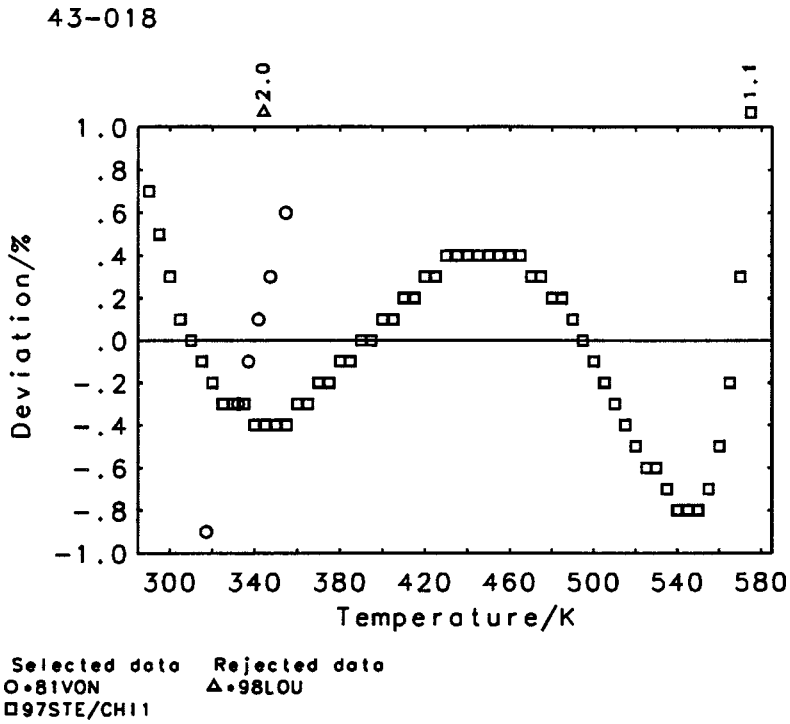
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	66	65	0.504	1.78–1	0.52	1.70–3	−1
sat	66	65	0.129	4.84–2	0.19	3.72–3	−31

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
290.0–580.0	−6.86124	2.01043+1	−4.60678	4.28806−1	IV
290.0–580.0	1.76123+1	7.78581−1	4.10714−1	4.28806−1	IV

Table 43.18.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	66	65	0.204	6.11–2	0.23	4.80–3	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
290.0–580.0	605.00	−2.43279	8.82752−2	1.33967+1	1.67614+1	IV



Name: 1-Phenylethanone
Formula: C_8H_8O

CAS-RN: 98-86-2
Group No.: 43-036
Molar Mass: 120.15

Table 43.36.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
00LOU	N	381.1	1	nosp	not specified		avg	DSIO	*98LOU
39PHI		303.1	1	nosp	not specified		*p*	BSIO	49WEI
80FUC		298.2–298.2	2	0.50	not specified		*p*	BSIO	80FUC
96STE/CHI1		300.0–700.0	21 S	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

00LOU average value in temperature range 293–469 K

Table 43.36.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
80FUC	298.2	2	0.50	0.470	5.80–2	0.23	2.08–2	0
96STE/CHI1	300.0–700.0	21	1.00	0.474	1.80–1	0.47	−5.99–3	−5
Rejected data								
00LOU	(8.42–1,2.94,8.42–1,1)		39PHI	(2.55,9.32,2.55,1)				

Table 43.36.3. Parameters of cubic spline polynomials

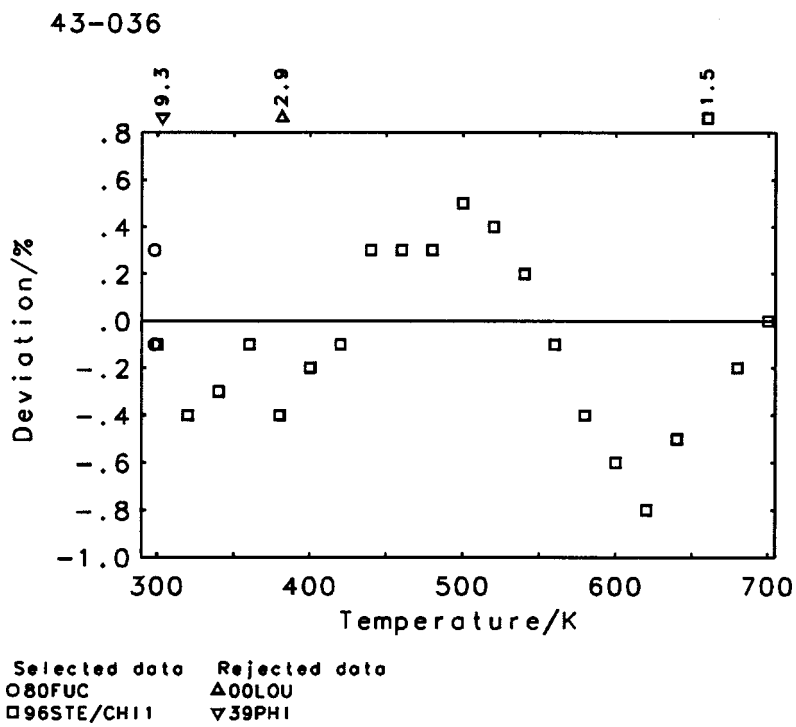
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	25	23	0.535	1.96−1	0.52	−3.66−3	−5
sat	25	23	0.355	1.20−1	0.33	−2.67−3	−4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
298.2–650.0	8.70588	7.53489	−1.00472	9.05180−2	IV
650.0–700.0	−3.92064+4	1.81068+4	−2.78551+3	1.42886+2	IV
298.2–650.0	1.45507+1	3.03448	1.23033−1	−1.68711−3	IV
650.0–700.0	−2.40602+4	1.11145+4	−1.70933+3	8.76624+1	IV

Table 43.36.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	25	23	0.832	2.89−1	0.81	−1.32−2	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
298.2–700.0	713.00	−1.95831	3.74450−1	6.78376	5.13324+1	−3.43313+1	8.71629	IV



Name: 2-Cyclohexen-1-one
Formula: C_6H_8O

CAS-RN: 930-68-7
Group No.: 43-065
Molar Mass: 96.13

Table 43.65.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI2	310.0–530.0	12	nosp	99.95	chrom	sat	BDHT	89KNI/ARC

Table 43.65.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	12	12	0.420	1.17−1	0.42	7.16−4	0
sat	12	12	0.500	1.50−1	0.50	1.34−3	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
310.0–530.0	−3.18233	1.40493+1	−2.99223	3.05804−1	IV
310.0–530.0	1.71016+1	−1.20558	7.75060−1	3.05804−1	IV

Table 43.65.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	12	12	0.345	9.81−2	0.35	4.91−4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
310.0–530.0	685.00	−6.50162	8.17739−1	9.49746	1.29231+1	IV

Name: 3,4-Dihydro-1(2*H*)-naphthalenone
Formula: $C_{10}H_{10}O$

CAS-RN: 529-34-0
Group No.: 43-066
Molar Mass: 146.19

Table 43.66.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g) %	Error %	Purity method	Purity Type	Type capac	Calorimeter Type	Calorimeter Reference
98VER1	298.15	1.590	nosp	99.88	chrom	p	BDHT	69PER/COM

Name: (±)-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one
Formula: $C_{10}H_{14}O$

CAS-RN: 22327-39-5
Group No.: 43-067
Molar Mass: 150.22

Table 43.67.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96GAL/VAN2	241.1–270.0	4	0.20	not specified		p	BSAO	87VAN/VAN

Table 43.67.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	4	4	0.008	4.95−4	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
241.1–270.0	2.14089+1	3.80928	III

Name: (*R*)-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one
Formula: $C_{10}H_{14}O$

CAS-RN: 6485-40-1
Group No.: 43-068
Molar Mass: 150.22

Table 43.68.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96GAL/VAN3	249.5–290.0	6 S	0.20	99.0	chrom	*p*	BSAO	87VAN/VAN

Table 43.68.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	6	6	0.532	3.38–2	0.11	3.56–5	−2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
249.5–290.0		3.39892+1	−6.32546	2.03943			III

Name: 1,1′-(1,4-Phenylene)bis[2-phenylethanedione]
Formula: $C_{22}H_{14}O_4$

CAS-RN: 3363-97-1
Group No.: 43-069
Molar Mass: 342.35

Table 43.69.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
77KAR/RAB	N	415.2–518.1	9	1.50	99.01	melpt	*p*	BDAO	51POP/GAL
77KAR/RAB	data from a graph only								

Table 43.69.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	9	9	0.209	2.44–1	0.31	1.20–3	−1
Temp. range K		A_1	A_2				Level of uncertainty
415.2–518.1		4.93982+1	6.25584				V

Name: 16-Hentriacontanone
Formula: $C_{31}H_{62}O$

CAS-RN: 502-73-8
Group No.: 43-070
Molar Mass: 450.83

Table 43.70.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94NAK/TAK	380.0–380.0	2	nosp	99.9	anal	*p*	BDHT	94NAK/TAK

Table 43.70.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	2	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
380.0–380.0		1.31096+2					VI

Name: 20-Nonatriacontanone
Formula: $C_{39}H_{78}O$

CAS-RN: 22986-70-5
Group No.: 43-071
Molar Mass: 563.05

Table 43.71.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94NAK/TAK	380.0–380.0	2	nosp	99.7	anal	*p*	BDHT	94NAK/TAK

Table 43.71.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	2	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
380.0–380.0		1.75597+2					VI

Name: Formic acid
Formula: CH_2O_2

CAS-RN: 64-18-6
Group No.: 44-001
Molar Mass: 46.03

Table 44.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		313.2–341.7	4 S	nosp	not specified		avg	DSIO	*81VON
*86LUD	N	306.1	1	nosp	not specified		avg	DSIO	*86LUD
*86SCH		309.8–322.7	6 S	nosp	not specified		avg	DSIO	*86SCH
*95MAS/GUI	N	323.1	1	nosp	not specified		avg	not specified	
20GIB/LAT		286.0–291.5	3	nosp	not specified		*p*	BSIO	20GIB/LAT
34RAD/JUL		290.1	1	nosp	not specified		*p*	BSIO	49WEI
36GLA/CHE		298.1	1	0.50	not specified		*p*	BSIO	32NEU
41STO/FIS	N	275.3–299.8	9	0.20	99.994	melpt	*p*	BSIO	28GIA/WIE1
81CAS/WIL		298.1	1	nosp	99.	melpt	*p*	FSIT	71PIC/LED
93NAN/BHA		303.1	1	nosp	not specified		*p*	BSIO	93NAN/BHA

*86LUD average value in temperature range 289–323 K
*95MAS/GUI average value in temperature range 293–353 K; calorimeter not identified, probably drop
41STO/FIS experimental temperature multiplied by the factor 273.15/273.10

Name: Acetic acid
Formula: $C_2H_4O_2$

CAS-RN: 64-19-7
Group No.: 44-002
Molar Mass: 60.05

Table 44.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		313.5–325.1	3 S	nosp	not specified		avg	DSIO	*81VON
*86LUD	N	308.1	1	nosp	not specified		avg	DSIO	*86LUD
*86SCH		312.9–337.4	8 S	nosp	not specified		avg	DSIO	*86SCH
*95PIC	N	314.1	1	3.70	not specified		avg	BDHO	*90PIC
00LOU	N	340.1	1	nosp	not specified		avg	DSIO	*98LOU
12BAU		290.1	1	nosp	not specified		*p*	not specified	
13NAS/BRE2		291.3–293.2	4	nosp	not specified		*p*	BSIO	49WEI
25PAR/KEL		292.6–294.7	2	nosp	99.9	estim	*p*	BSIO	25PAR
32NEU	N	297.0–353.6	4	nosp	not specified		*p*	BSIO	32NEU
34RAD/JUL		289.6	1	nosp	not specified		*p*	BSIO	49WEI
47PUS/FED		296.4–309.6	6	nosp	not specified		*p*	DSIO	47PUS/FED
58SWI/ZIE1	N	332.3–348.8	2	nosp	not specified		avg	DSIO	58SWI/ZIE1
65CAM/GIE		298.6	1	0.50	not specified		*p*	DSIO	64CAM/NAG
81CAS/WIL		298.1	1	nosp	99.8	melpt	*p*	FSIT	71PIC/LED
82MAR/AND		293.2–350.8	30	nosp	99.95	melpt	*p*	BSAO	68WES/FUR
82MAR/AND		315.1–400.2	18	nosp	99.95	melpt	*p*	BSAO	68WES/FUR

*86LUD average value in temperature range 293–323 K
*95PIC average value in temperature range 290–339 K
00LOU average value in temperature range 296–385 K
32NEU same data in 32NEI
58SWI/ZIE1 average values in temperature ranges 295–369 K and 295–402 K

Name: 2-Propenoic acid
Formula: $C_3H_4O_2$

CAS-RN: 79-10-7
Group No.: 44-003
Molar Mass: 72.06

Table 44.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
83KAR/ABD2		289.3–342.9	21	0.50	not specified		*p*	BSAO	82KAR/IGA
85KAR/ABD1	N	286.0–333.0	eqn	0.50	not specified		*p*	BSAO	82KAR/IGA
99LEB/KUL3		293.5–329.1	14	0.20	99.89	melpt	*p*	BSAO	97VAR/DRU1

85KAR/ABD1 same data in 85KAR/SAI

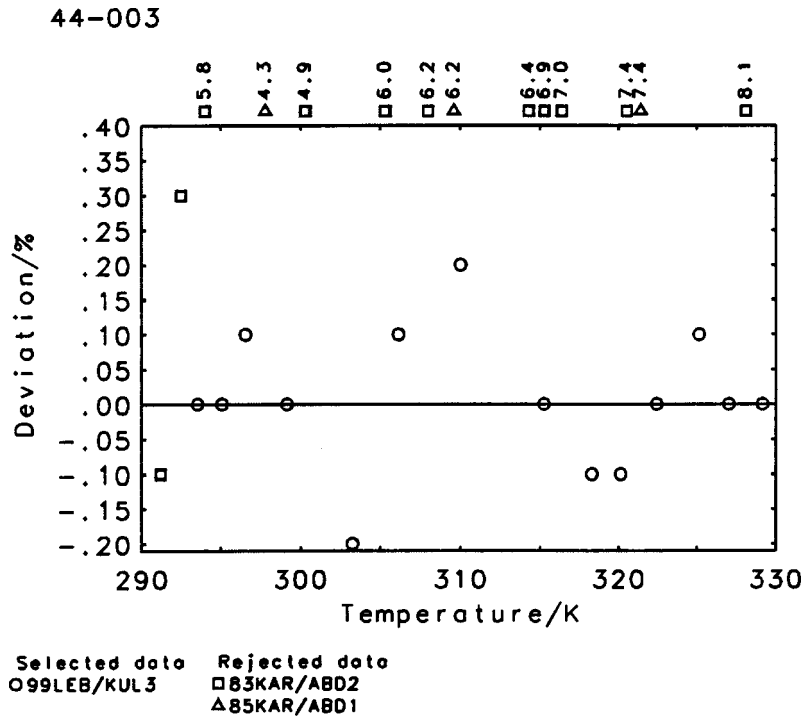
Table 44.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
			Selected data					
99LEB/KUL3	293.5–329.1	14	0.20	0.469	1.57–2	0.09	2.78–5	1
			Rejected data					
83KAR/ABD2	(1.22,6.74,1.20,11)		85KAR/ABD1	(1.09,6.11,1.07,3)				

Table 44.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	40	14	0.529	1.77–2	0.11	2.78–5	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
293.5–329.1	2.81387+1	−8.82167	1.65470	III



Name: Propanoic acid
Formula: $C_3H_6O_2$

CAS-RN: 79-09-4
Group No.: 44-004
Molar Mass: 74.08

Table 44.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86LUD	N	309.1	1	nosp	not specified		avg	DSIO	*86LUD
02LOU2	N	351.7	1	nosp	not specified		avg	DSIO	*98LOU
34RAD/JUL		289.1	1	nosp	not specified		*p*	BSIO	49WEI
71KON/WAD		298.1	1	nosp	99.80	melpt	*p*	BSIO	70LKB/COM
78WOY/KAL		303.1	1	nosp	not specified		*p*	BSIO	70REC
81CAS/WIL		298.1	1	nosp	99.5	melpt	*p*	FSIT	71PIC/LED
82BIR/SIK		270.0–370.0	eqn	1.00	not specified		*p*	BDHT	69PER/COM
82MAR/AND		254.8–353.1	49	nosp	99.93	melpt	*p*	BSAO	68WES/FUR
82MAR/AND		303.4–447.1	25	nosp	99.93	melpt	*p*	BSAO	68WES/FUR

*86LUD average value in temperature range 295–323 K
02LOU2 average value in temperature range 294–410 K

Name: 2,5-Furandione
Formula: $C_4H_2O_3$

CAS-RN: 108-31-6
Group No.: 44-005
Molar Mass: 98.06

Table 44.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78MAR/CIO2	N	330.0–480.0	2	nosp	not specified		*p*	DSIO	71MAR/CIO
83DEW/DEK		327.7–357.5	13	nosp	99.87	melpt	*p*	BSAO	79SCH/OFF
83DEW/OFF		335.0–355.0	5 S	nosp	not specified		*p*	BDHT	69PER/COM
96LEB/KUL2	N	331.3–350.0	3 S	2.50	99.49	melpt	*p*	BDHT	69YAG

78 MAR/CIO2 constant value calculated from temperature dependence of enthalpy by the authors
96LEB/KUL2 value C_p at 340 K provided by the authors

Name: (*E*)-2-Butenoic acid
Formula: $C_4H_6O_2$

CAS-RN: 107-93-7
Group No.: 44-006
Molar Mass: 86.09

Table 44.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	314.6	1	nosp	not specified		avg	DSIO	*94BRU
25LYN		344.5	1	1.00	not specified		*p*	not specified	

*94BRU average value in temperature range 353–368 K

Table 44.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*94BRU	314.6	1	3.00 #	0.000	0.00	0.00	0.00	0
25LYN	344.5	1	1.00	0.000	0.00	0.00	0.00	0

Table 44.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
314.6–344.5	1.90560+1	7.59080−1	VI

Name: 2-Methylpropanoic acid
Formula: $C_4H_8O_2$

CAS-RN: 79-31-2
Group No.: 44-010
Molar Mass: 88.11

Table 44.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON	316.0–374.3	5 S	nosp	not specified		avg	DSIO	*81VON
*86SCH	322.5–350.3	7 S	nosp	not specified		avg	DSIO	*86SCH
67RAB/LEB	227.2–300.0	3 S	0.50	99.43	melpt	*p*	BSAO	66NIK/LEB
71KON/WAD	298.1	1	nosp	99.8	chrom	*p*	BSIO	70LKB/COM
82BIR/SIK	270.0–370.0	eqn	1.00	not specified		*p*	BDHT	69PER/COM

Table 44.10.2. Correlated heat capacities

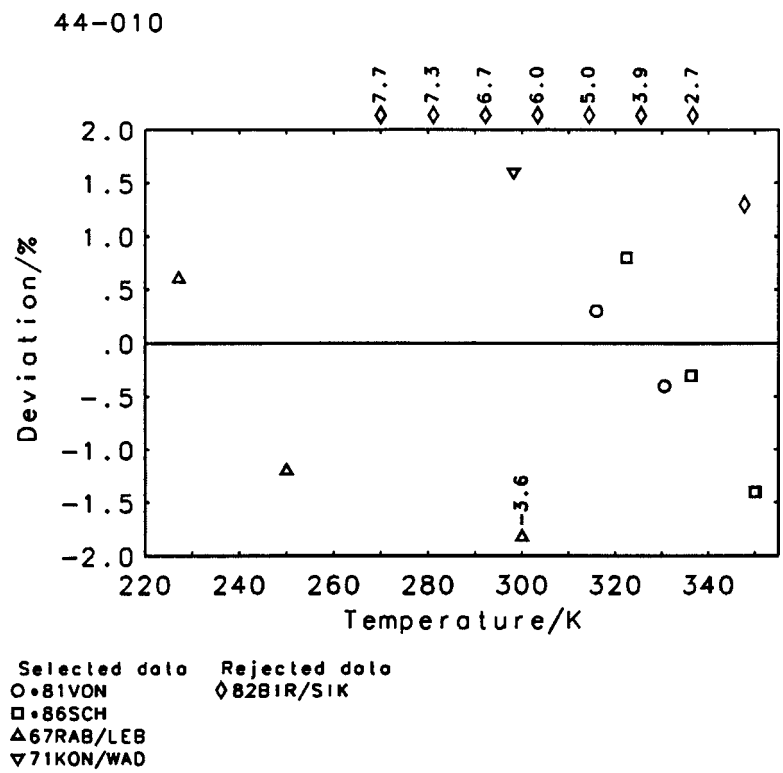
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*81VON	316.0–330.5	2	2.00 #	0.189	8.49–2	0.38	−1.70–2	0
*86SCH	322.5–350.3	7	2.00 #	0.432	2.05–1	0.86	−7.54–2	−3
67RAB/LEB	227.2–300.0	3	0.50	4.403	4.32–1	2.20	−2.72–1	−1
71KON/WAD	298.1	1	0.30 #	5.409	3.38–1	1.62	3.38–1	1
Rejected data								
82BIR/SIK	(1.19,5.51,1.11,8)							

Table 44.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	26	13	2.980	3.14−1	1.51	−7.99−2	−3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
227.2–350.3		2.71367+1	−1.08361+1	2.88441			V

Table 44.10.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	26	13	3.516	3.45−1	1.77	−5.02−2	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
227.2–350.3	609.00	−6.35928	5.60688	4.57896	1.80316		V



Name: Hexadecanoic acid
Formula: $C_{16}H_{32}O_2$

CAS-RN: 57-10-3
Group No.: 44-031
Molar Mass: 256.43

Table 44.31.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	355.1	1	nosp	not specified		avg	DSIO	*94BRU
26GAR/MAD	N	349.1	1	nosp	not specified		avg	DSIO	24GAR/RAN
52WAR/SIN		347.0–365.0	3 S	nosp	not specified		*p*	BSAO	44BAI/TOD
67PAC		373.1	1	nosp	not specified		*p*	BDHT	79DU/COM
82SCH/VAN2		340.0–345.0	2 S	nosp	99.56	melpt	sat	BSAO	79SCH/OFF
#00CED/PRI		343.0–428.0	18	1.00	99.3	anal	*p*	BDHT	92BAO/CAC

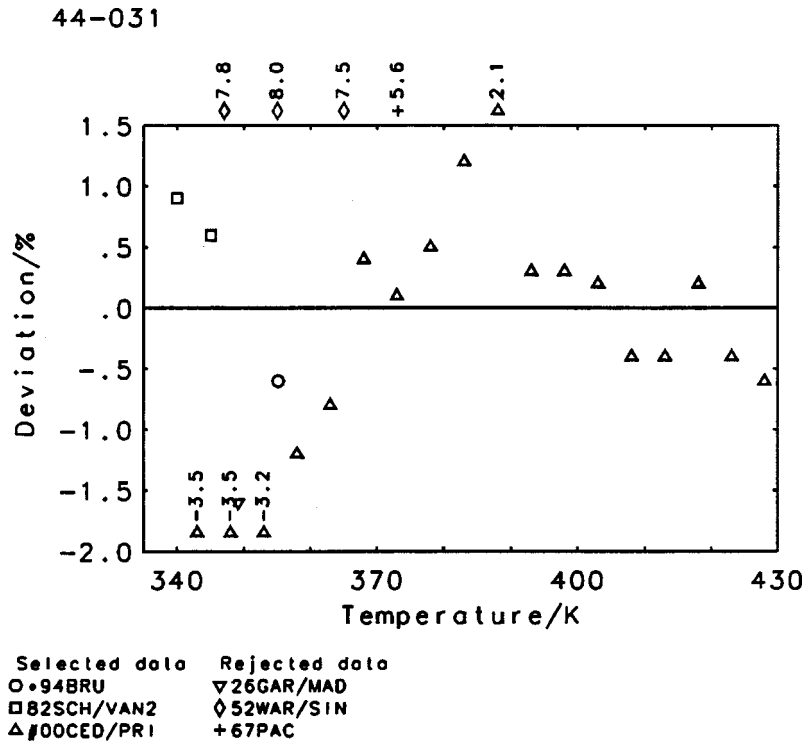
*94BRU average value in temperature range 343–367 K
26GAR/MAD average value in temperature range 336–363 K

Table 44.31.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*94BRU	355.1	1	3.00 #	0.210	4.51–1	0.63	−4.51–1	−1
82SCH/VAN2	340.0–345.0	2	0.40 #	1.883	5.26–1	0.75	5.15–1	2
#00CED/PRI	343.0–428.0	18	1.00	1.565	1.12	1.57	−3.16–1	0
Rejected data								
26GAR/MAD	(1.09,1.57,−1.09,−1)		52WAR/SIN	(6.06,7.74,6.06,3)				
67PAC	(4.55,5.59,4.55,1)							

Table 44.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	26	21	1.687	1.13	1.59	−2.43–1	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
340.0–428.0		2.24196+2	−1.08346+2	1.84461+1			V



Name: (*Z*)-9-Octadecenoic acid
Formula: $C_{18}H_{34}O_2$

CAS-RN: 112-80-1
Group No.: 44-033
Molar Mass: 282.47

Table 44.33.1. Experimental heat capacities

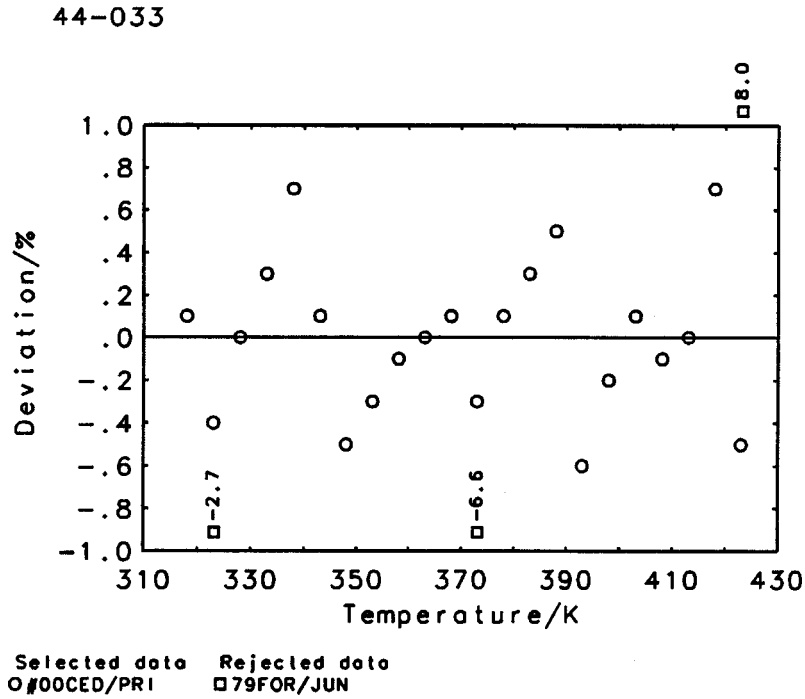
Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
34MEH1	290.1	1	1.50	not specified		*p*	BSIO	49WEI
79FOR/JUN	323.1–423.1	3	nosp	not specified		*p*	not specified	
#00CED/PRI	318.0–423.0	22	1.00	99.9	anal	*p*	BDHT	92BAO/CAC

Table 44.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
#00CED/PRI	318.0–423.0	22	1.00	0.346	2.97–1	0.35	2.06–3	1
Rejected data								
79FOR/JUN	(3.86,5.02,−3.49,−2)							

Table 44.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
total	used						
p	26	22	0.383	3.28–1	0.38	2.06–3	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
318.0–423.0		−2.25054+2	2.35631+2	−6.72962+1	7.04433		V



Name: Octadecanoic acid
Formula: $C_{18}H_{36}O_2$

CAS-RN: 57-11-4
Group No.: 44-034
Molar Mass: 284.48

Table 44.34.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	357.6	1	nosp	not specified		avg	DSIO	*94BRU
50SIN/WAR		350.0	1	nosp	not specified		*p*	BSAO	44BAI/TOD
79FOR/JUN		423.1–523.2	3	nosp	not specified		*p*	not specified	
82SCH/VAN2		350.0–355.0	2 S	nosp	98.87	melpt	sat	BSAO	79SCH/OFF
#00CED/PRI		348.0–418.0	15	1.00	97.	anal	*p*	BDHT	92BAO/CAC

*94BRU average value in temperature range 346–369 K

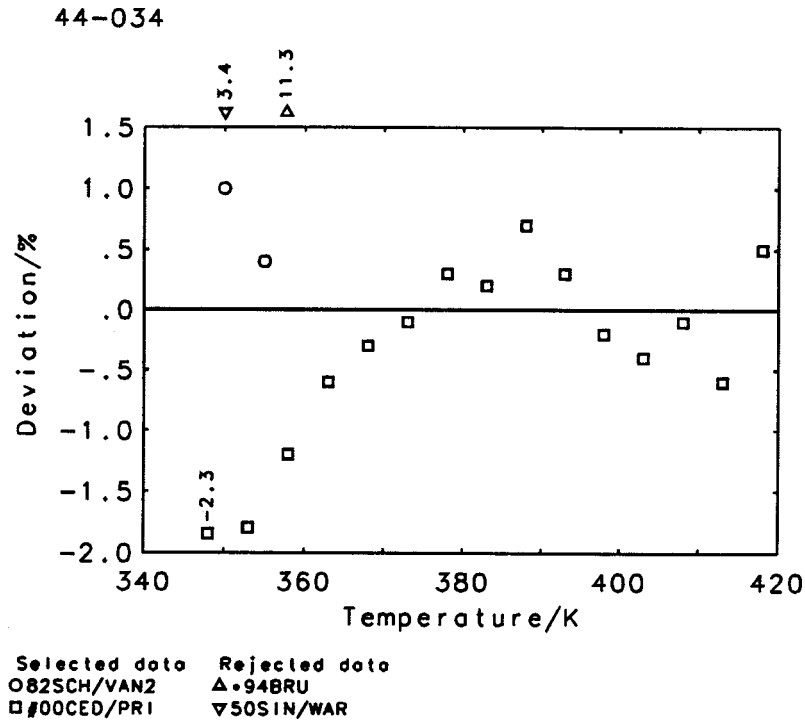
Table 44.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
82SCH/VAN2	350.0–355.0	2	0.50 #	1.560	6.16–1	0.78	5.65–1	2
#00CED/PRI	348.0–418.0	15	1.00	0.893	7.12–1	0.89	−2.83–1	−5
			Rejected data					
*94BRU	(1.02+1,11.31,1.02+1,1)		50SIN/WAR	(2.77,3.43,2.77,1)				

Table 44.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
C	22	17	1.097	7.73–1	0.97	−1.84–1	−3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
348.0–418.0	3.02595+2	−1.49523+2	2.43946+1	V



Name: 2,2-Dimethylpropanoic acid
Formula: $C_5H_{10}O_2$

CAS-RN: 75-98-9
Group No.: 44-037
Molar Mass: 102.13

Table 44.37.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
90SIN/GLI	N	313.0–319.0	eqn	nosp	99.9995	melpt	*p*	BDHT	87PER/COM

90SIN/GLI model of Perkin-Elmer DSC instrument unspecified

Table 44.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	4	4	0.000	2.70−6	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
313.0–319.0	8.14714	5.24350	V

Name: Benzeneacetic acid
Formula: $C_8H_8O_2$

CAS-RN: 103-82-2
Group No.: 44-038
Molar Mass: 136.15

Table 44.38.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	361.65	1.682	nosp	not specified		avg	DSIO	*94BRU

*94BRU average value in temperature range 355–368 K

Name: (±)-2-Ethylhexanoic acid
Formula: $C_8H_{16}O_2$

CAS-RN: 83829-68-9
Group No.: 44-039
Molar Mass: 144.21

Table 44.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI2	310.0–510.1	11	nosp	99.95	chrom	sat	BDHT	89KNI/ARC

Table 44.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	11	11	0.309	1.56–1	0.31	6.71–4	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
310.0–510.1	−3.36413+1	4.32380+1	−9.32460	8.48381–1	IV

Table 44.39.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	11	11	0.378	1.93–1	0.38	9.22–4	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
310.0–510.1	675.00	−1.03011+1	7.34440−1	1.19331+1	3.61202+1	IV

Name: Ethyl formate
Formula: $C_3H_6O_2$

CAS-RN: 109-94-4
Group No.: 45-002
Molar Mass: 74.08

Table 45.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81BER/OGI	N	304.6–306.6	2	nosp	not specified		avg	DSIO	*79BER
34KOL/UDO	N	294.7	1	nosp	not specified		*p*	BSIT	34KOL/UDO
36KUR/VOS		309.0	1	nosp	not specified		avg	DSIO	36KUR/VOS
79FUC		298.1	1	0.50	99.0	chrom	*p*	BSIO	80FUC
97HU/TAM1		298.1	1	nosp	99.97	chrom	*p*	FSIO	85OGA/MUR

*81BER/OGI average values in temperature ranges 287–322 K and 287–326 K
34KOL/UDO same datum in 33KOL/UDO

Table 45.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
				Selected data				
*81BER/OGI	304.6–306.6	2	3.00 #	0.590	3.36–1	1.77	2.87–1	2
36KUR/VOS	309.0	1	3.00 #	0.638	3.64–1	1.91	−3.64–1	−1
79FUC	298.1	1	0.50	0.803	6.97–2	0.40	6.97–2	1
97HU/TAM1	298.1	1	0.30 #	0.512	2.65–2	0.15	−2.65–2	−1

Table 45.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	6	5	0.819	3.49−1	1.84	5.05−2	1

Temp. range K	A_1	A_2	Level of uncertainty
298.1–309.0	−4.06787+1	1.94413+1	V

Name: Methyl acetate
Formula: $C_3H_6O_2$

CAS-RN: 79-20-9
Group No.: 45-003
Molar Mass: 74.08

Table 45.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
26SCH		288.1	1	nosp	not specified		*p*	not specified	
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	*p*	BDHT	71DU/COM
79FUC		298.1	1	0.50	99.0	chrom	*p*	BSIO	80FUC
85COS/PAT8		283.1–313.1	3 S	nosp	99.	estim	*p*	FSIT	71PIC/LED
88PIN/BRA		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
92OKA/OGU		176.7–288.6	56	nosp	99.86	melpt	sat	BSAO	82MOR/MAT
97HOV/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED

71HAL/BAL suspect value

Table 45.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
79FUC	298.1	1	0.50	2.617	2.26−1	1.31	2.26−1	1
85COS/PAT8	283.1–313.1	3	1.00 #	1.937	3.16−1	1.94	−2.09−1	−1
88PIN/BRA	298.1	1	1.00 #	0.479	8.15−2	0.48	−8.15−2	−1
92OKA/OGU	176.7–288.6	56	0.50 #	0.143	1.17−2	0.07	−7.24−4	1
97HOV/ROU	298.1	1	0.50 #	0.088	7.54−3	0.04	7.54−3	1
Rejected data								
26SCH	(5.98−1,3.42,5.98−1,1)		71HAL/BAL	(2.18,14.65,−2.18,−1)				

Table 45.3.3. Parameters of regression polynomial

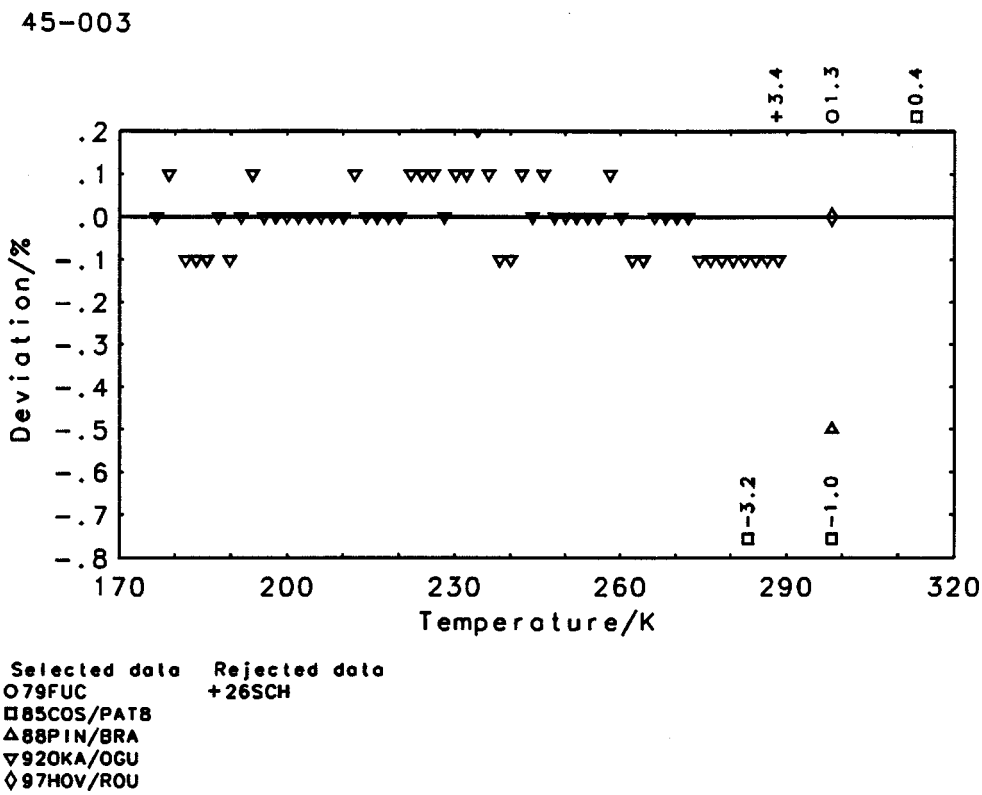
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	64	62	0.575	7.87−2	0.48	−8.29−3	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
176.7–313.1	2.08435+1	−4.78198	1.18059	IV

Table 45.3.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	64	61	0.530	5.00−2	0.30	3.09−3	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
176.7–313.1	506.50	3.01021+1	1.13336+1	4.50685	1.99879+1	IV



Name: Dimethyl carbonate
Formula: $C_3H_6O_3$

CAS-RN: 616-38-6
Group No.: 45-004
Molar Mass: 90.08

Table 45.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*98LOU	N	327.0	1	nosp	not specified		avg	DSIO	*98LOU
97STE/CHI3	N	300.0–540.0	13	1.00	99.95	chrom	sat	BDHT	89KNI/ARC
99PAR/TOV		288.1–308.1	3	nosp	99.	chrom	*p*	BDCT	83ROU/ROU

*98LOU average value in temperature range 293–361 K
97STE/CHI3 same data in 97STE/CHI2

Table 45.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
			Selected data					
97STE/CHI3	300.0–540.0	13	1.00	0.399	9.62–2	0.40	−9.73–3	−1
99PAR/TOV	288.1–308.1	3	0.50 #	0.146	1.44–2	0.07	1.15–2	3
			Rejected data					
*98LOU	(9.90–2,0.48,9.90–2,1)							

Table 45.4.3. Parameters of cubic spline polynomials

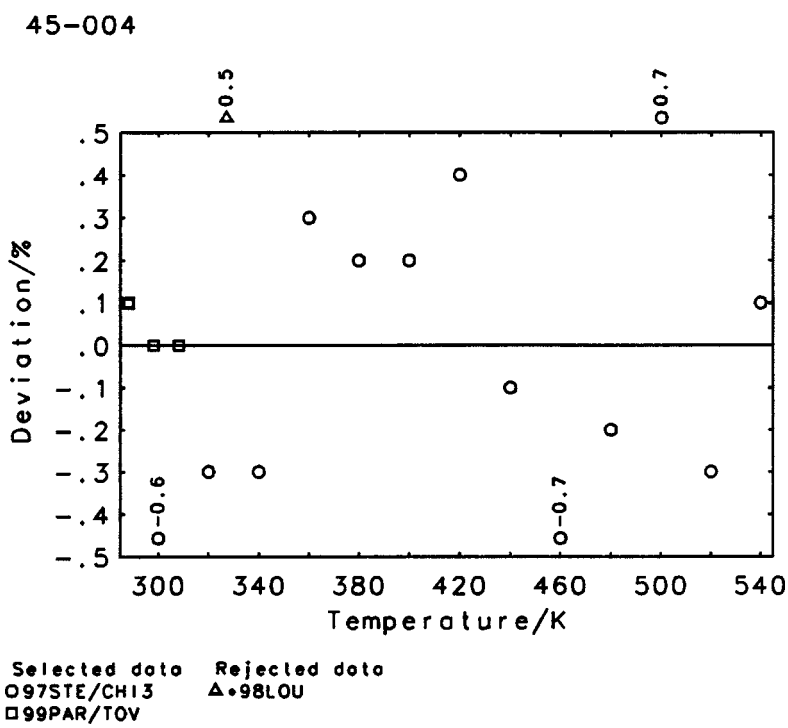
Heat capacity type	No. data points total	used	s_w	s/R	s_r	s_b/R	±
					%		
p	17	16	0.441	1.05–1	0.44	−5.75–3	2
sat	17	16	0.356	8.06–2	0.35	−6.41–3	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
288.1–490.0	1.90928+1	−2.40981−1	−9.90963−2	9.01815−2	IV
490.0–540.0	−7.42507+3	4.55741+3	−9.30231+2	6.33645+1	IV
288.1–490.0	2.60519+1	−6.44355	1.73733	−9.06539−2	IV
490.0–540.0	−4.62830+3	2.84316+3	−5.79814+2	3.94707+1	IV

Table 45.4.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r	s_b/R	±
					%		
p	17	16	0.898	2.05–1	0.88	6.08–2	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
288.1–540.0	557.00	−2.15707	3.12019−1	1.56147+1	3.72809	IV



Name: Ethenyl acetate
Formula: $C_4H_6O_2$

CAS-RN: 108-05-4
Group No.: 45-005
Molar Mass: 86.09

Table 45.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
59BEN/THO	298.1	1	nosp	not specified		avg	BDHT	59BEN/THO
97KUL/LEB1	188.8–330.0	32	0.20	99.75	melpt	*p*	BSAO	76LEB/LIT

Table 45.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
97KUL/LEB1	188.8–330.0	32	0.20	0.798	3.13–2	0.16	9.91–5	1
Rejected data								
59BEN/THO	(2.71–1,1.33,2.71–1,1)							

Table 45.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	33	32	0.854	3.35–2	0.17	9.91–5	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
188.8–330.0		2.95030+1	−1.49299+1	6.05166	−7.05349−1		III

Table 45.5.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	33	32	0.898	3.50–2	0.18	9.78–5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
188.8–330.0	519.10	3.53219+2	3.48596+1	−1.92123+1	3.47562+2	1.47135+1	2.88360+2	III

Name: Ethyl acetate
Formula: $C_4H_8O_2$

CAS-RN: 141-78-6
Group No.: 45-007
Molar Mass: 88.11

Table 45.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH	305.4–309.5	4 S	nosp	not specified		avg	DSIO	*86SCH
26SCH	288.1	1	nosp	not specified		*p*	not specified	
33PAR/HUF	195.7–293.6	8	1.00	not specified		*p*	BSIO	25PAR
36KUR/VOS	309.0–309.0	2	nosp	not specified		avg	DSIO	36KUR/VOS
45ZHD	278.2–319.1	3	nosp	not specified		*p*	BSIT	34KOL/UDO
78ROU/PER1	283.1–313.1	3	0.30	99.8	melpt	*p*	FSIT	71PIC/LED
79FUC	298.1–298.1	2	0.50	99.0	chrom	*p*	BSIO	80FUC
85BAL/BRA	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
85COS/PAT9	283.1–313.1	3	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
86JIM/ROM	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
87ZAB/HYN	293.8–340.3	11	0.50	100.0	anal	sat	BSAO	87ZAB/HYN
88PIN/BRA	298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
91DES/PAT	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
94JIM/ROM	298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
96TAN/TOY1	298.1	1	nosp	100.0	chrom	*p*	FSIT	71PIC/LED
97HU/TAM2	298.1	1	nosp	99.96	chrom	*p*	FSIO	85OGA/MUR
97TOV/CAR3	298.1	1	nosp	99.5	anal	*p*	BDCT	83ROU/ROU
99PIN/BRA	298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED

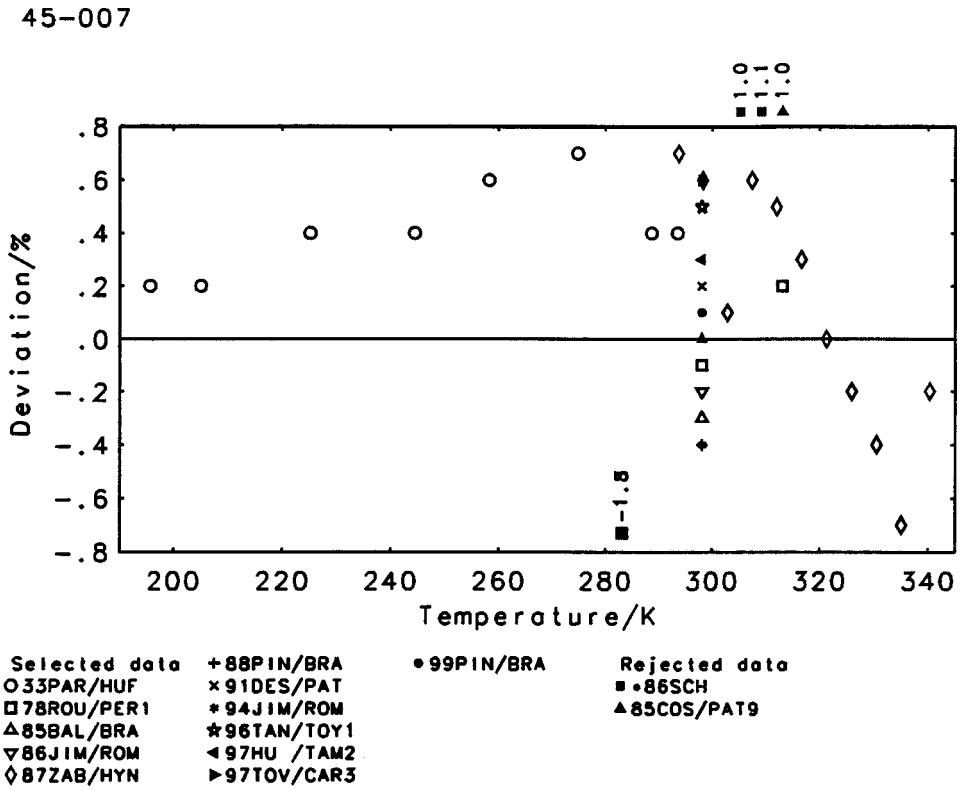
Table 45.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
			Selected data					
33PAR/HUF	195.7–293.6	8	1.00	0.437	8.65–2	0.44	7.97–2	8
78ROU/PER1	283.1–313.1	3	0.30	2.511	1.49–1	0.75	−7.24–2	−1
85BAL/BRA	298.1	1	0.50 #	0.622	6.33–2	0.31	−6.33–2	−1
86JIM/ROM	298.1	1	0.50 #	0.338	3.44–2	0.17	−3.44–2	−1
87ZAB/HYN	293.8–340.3	11	0.50	0.890	9.31–2	0.44	2.54–2	1
88PIN/BRA	298.1	1	0.50 #	0.765	7.77–2	0.38	−7.77–2	−1
91DES/PAT	298.1	1	0.50 #	0.370	3.77–2	0.18	3.77–2	1
94JIM/ROM	298.1	1	0.50 #	0.836	8.49–2	0.42	−8.49–2	−1
96TAN/TOY1	298.1	1	0.50 #	1.095	1.12–1	0.55	1.12–1	1
97HU/TAM2	298.1	1	0.30 #	1.007	6.18–2	0.30	6.18–2	1
97TOV/CAR3	298.1	1	0.50 #	1.165	1.19–1	0.58	1.19–1	1
99PIN/BRA	298.1	1	0.50 #	0.169	1.73–2	0.08	1.73–2	1
			Rejected data					
*86SCH	(2.22–1,1.06,2.22–1,4)		26SCH	(4.34–1,2.11,4.34–1,1)				
36KUR/VOS	(1.29,6.75,−6.23–1,0)		45ZHD	(3.53–1,1.73,−2.29–1,−1)				
79FUC	(2.45–1,1.22,−2.45–1,−2)		85COS/PAT9	(2.34–1,1.17,−4.83–2,0)				

Table 45.7.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
C	46	31	1.361	1.04–1	0.52	−7.02–3	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
195.7–340.3	523.20	1.24186+1	6.62706	1.21932+1	5.81788	IV



Name: Methyl propanoate
Formula: $C_4H_8O_2$

CAS-RN: 554-12-1
Group No.: 45-008
Molar Mass: 88.11

Table 45.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH		305.8–310.3	4 S	nosp	not specified		avg	DSIO	*86SCH
79FUC		298.1–298.1	2	0.50	99.0	chrom	*p*	BSIO	80FUC
84GUS/SHU		205.3–347.9	12	0.50	not specified		*p*	BSAO	54STR/ICK
85BAL/BRA		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
86JIM/ROM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
87ZAB/HYN	N	295.7–341.7	9	0.50	96.5	anal	sat	BSAO	87ZAB/HYN
88PIN/BRA		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
94JIM/ROM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
99PIN/BRA		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

87ZAB/HYN dominant impurity Methanol

Name: Propyl formate
Formula: $C_4H_8O_2$

CAS-RN: 110-74-7
Group No.: 45-009
Molar Mass: 88.11

Table 45.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH	305.1–310.1	4 S	nosp	not specified		avg	DSIO	*86SCH
85BAL/BRA	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
86JIM/ROM	298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
88PIN/BRA	298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
94JIM/ROM	298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED

Name: Butyl formate
Formula: $C_5H_{10}O_2$

CAS-RN: 592-84-7
Group No.: 45-012
Molar Mass: 102.13

Table 45.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86JIM/ROM	298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
94JIM/ROM	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
99PIN/BRA	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

Table 45.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
			Selected data					
86JIM/ROM	298.1	1	0.50 #	0.226	2.72–2	0.11	−2.72–2	−1
94JIM/ROM	298.1	1	0.50 #	0.223	2.69–2	0.11	2.69–2	1
99PIN/BRA	298.1	1	0.50 #	0.004	4.41–4	0.00	4.41–4	0

Table 45.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	3	3	0.225	2.71–2	0.11	4.07–5	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	2.41116+1	IV

Name: Ethyl propanoate
Formula: $C_5H_{10}O_2$

CAS-RN: 105-37-3
Group No.: 45-013
Molar Mass: 102.13

Table 45.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH	309.6–321.7	6 S	nosp	not specified		avg	DSIO	*86SCH
86JIM/ROM	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
87ZAB/HYN	293.9–348.9	13	0.50	****	anal	sat	BSAO	87ZAB/HYN
94JIM/ROM	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
99PIN/BRA	298.1	1	nosp	99.	chrom	*p*	FSIT	71PIC/LED

Name: Propyl acetate
Formula: $C_5H_{10}O_2$

CAS-RN: 109-60-4
Group No.: 45-018
Molar Mass: 102.13

Table 45.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON	324.3–337.7	4 S	nosp	not specified		avg	DSIO	*81VON
*86SCH	307.7–322.7	6 S	nosp	not specified		avg	DSIO	*86SCH
86JIM/ROM	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
94JIM/ROM	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

Name: Diethyl carbonate
Formula: $C_5H_{10}O_3$

CAS-RN: 105-58-8
Group No.: 45-019
Molar Mass: 118.13

Table 45.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		335.6–351.4	3 S	nosp	not specified		avg	DSIO	*81VON
*98LOU	N	344.8	1	nosp	not specified		avg	DSIO	*98LOU
34KOL/UDO	N	294.6	1	nosp	not specified		*p*	BSIT	34KOL/UDO
99PAR/TOV		288.1–308.1	3	nosp	99.	chrom	*p*	BDCT	83ROU/ROU

*98LOU average value in temperature range 293–396 K
34KOL/UDO same datum in 33KOL/UDO

Table 45.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
*81VON	335.6–351.4	3	2.00 #	0.509	2.85–1	1.02	5.34–2	1
*98LOU	344.8	1	5.00 #	0.012	1.71–2	0.06	1.71–2	1
99PAR/TOV	288.1–308.1	3	0.50 #	0.194	2.57–2	0.10	−2.95–3	−1
Rejected data								
34KOL/UDO	(9.82–1,3.87,−9.82–1,−1)							

Table 45.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	8	7	0.422	2.22–1	0.79	2.41–2	1

Temp. range K	A_1	A_2	Level of uncertainty
288.1–351.4	1.54162+1	3.70529	V

Name: 1,2-Ethanediol diacetate
Formula: $C_6H_{10}O_4$

CAS-RN: 111-55-7
Group No.: 45-026
Molar Mass: 146.14

Table 45.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
80CAL/MAR	N	358.0–446.0	eqn	nosp	not specified		*p*	DSIO	71MAR/CIO
86NIL/WAD		298.1	1	nosp	99.9	chrom	*p*	DDCT	71KON/SUU

80CAL/MAR equation calculated from temperature dependence of enthalpy by the authors; suspect values

Name: Butyl acetate
Formula: $C_6H_{12}O_2$

CAS-RN: 123-86-4
Group No.: 45-027
Molar Mass: 116.16

Table 45.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
34KOL/UDO	N	292.5	1	nosp	not specified		*p*	BSIT	34KOL/UDO
79BAL/PET		201.0–364.3	73	nosp	99.62	melpt	*p*	BSAO	77KU/COM
79FUC		298.1	1	nosp	99.0	chrom	*p*	BSIO	80FUC
80VAS/TRE		196.0–280.0	eqn	1.00	99.62	anal	sat	BSAO	80VAS/TRE
80VAS/TRE		280.0–370.0	eqn	1.00	99.62	anal	sat	BSAO	80VAS/TRE
80VAS/TRE		300.0–399.0	eqn	2.00	99.62	anal	sat	BSAO	80VAS/TRE
86JIM/ROM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
87ZAB/HYN	N	293.8–363.8	16	0.50	98.7	anal	sat	BSAO	87ZAB/HYN
94JIM/ROM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
99PIN/BRA		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

34KOL/UDO2 same datum in 33KOL/UDO
87ZAB/HYN dominant impurity Butanol

Name: Propyl propanoate
Formula: $C_6H_{12}O_2$

CAS-RN: 106-36-5
Group No.: 45-035
Molar Mass: 116.16

Table 45.35.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH		307.8–331.8	6 S	nosp	not specified		avg	DSIO	*86SCH
86JIM/ROM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
87ZAB/HYN	N	293.8–367.3	17	0.50	97.9	anal	sat	BSAO	87ZAB/HYN
94JIM/ROM		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
99PIN/BRA		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

87ZAB/HYN dominant impurity Propanol

Name: Butyl 2-propenoate
Formula: $C_7H_{12}O_2$

CAS-RN: 141-32-2
Group No.: 45-036
Molar Mass: 128.17

Table 45.36.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
85KAR/ABD1	N	210.0–333.0	eqn	0.50	not specified		*p*	BSAO	82KAR/IGA
96STE/CHI3		295.0–415.0	6	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

85KAR/ABD1 same data in 85KAR/SAI

Table 45.36.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
96STE/CHI2	295.0–415.0	6	1.00	0.883	2.86–1	0.88	5.12–3	2
Rejected data								
85KAR/ABD1	(1.30,4.22,1.30,3)							

Table 45.36.3. Parameters of regression polynomial

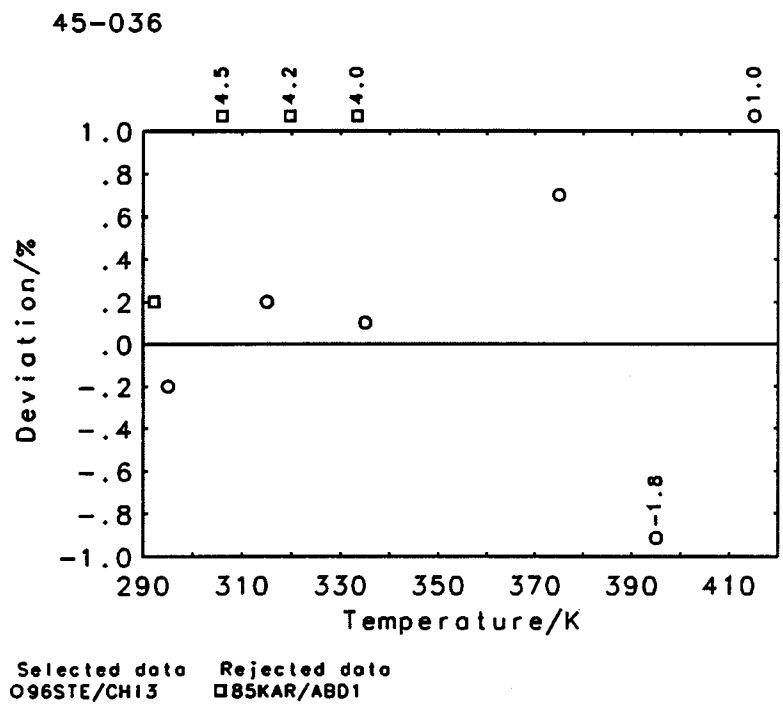
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	16	6	1.082	3.51−1	1.08	5.12−3	2
sat	16	6	1.083	3.51−1	1.08	5.12−3	2

Temp. range K	A_1	A_2	Level of uncertainty
295.0–415.0	1.67318+1	4.03814	IV
295.0–415.0	1.67853+1	4.02128	IV

Table 45.36.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	16	6	1.240	4.00−1	1.24	4.97−3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
295.0–415.0	644.00	−3.40801	1.65773−1	1.82645+1	1.75157+1	V



Name: Diethyl propanedioate
Formula: $C_7H_{12}O_4$

CAS-RN: 105-53-3
Group No.: 45-039
Molar Mass: 160.17

Table 45.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*87SCH	319.4–347.8	6 S	nosp	not specified		*p*	DSIO	*86SCH
33KOL/UDO	294.5	1	nosp	not specified		*p*	BSIT	34KOL/UDO
92VER/BEC	298.1	1	nosp	99.98	chrom	*p*	BDHT	69PER/COM

Table 45.39.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*87SCH	319.4–347.8	6	3.00 #	0.247	2.70–1	0.74	−7.59–2	−2
92VER/BEC	298.1	1	1.00 #	0.148	5.35–2	0.15	5.35–2	1

Table 45.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	8	7	0.278	2.97–1	0.81	−5.74–2	−1

Temp. range K	A_1	A_2	Level of uncertainty
298.1–347.8	2.75460+1	2.85406	V

Name: Ethyl 2,2-dimethylpropanoate
Formula: $C_7H_{14}O_2$

CAS-RN: 3938-95-2
Group No.: 45-040
Molar Mass: 130.19

Table 45.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86NIL/WAD	298.1	1	nosp	99.9	chrom	p	DDCT	71KON/SUU
92VER/BEC	298.1	1	nosp	99.995	chrom	p	BDHT	69PER/COM

Table 45.40.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
86NIL/WAD	298.1	1	0.50 #	0.000	0.00	0.00	0.00	0
Rejected data								
92VER/BEC	(3.19,9.54,3.19,1)							

Table 45.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	3.02243+1	IV

Name: Pentyl acetate
Formula: $C_7H_{14}O_2$

CAS-RN: 628-63-7
Group No.: 45-045
Molar Mass: 130.19

Table 45.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
26SCH	288.1	1	nosp	not specified		*p*	not specified	
39PHI	303.3	1	nosp	not specified		*p*	BSIO	49WEI
96STE/CHI1	300.0–580.0	15 S	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 45.45.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
96STE/CHI1	300.0–580.0	15	1.00	0.213	9.51–2	0.21	5.17–4	1
Rejected data								
39PHI	(3.69,11.11,3.69,1)							

Table 45.45.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	17	15	0.261	1.16–1	0.26	5.17–4	1
sat	17	15	0.177	7.50–2	0.18	2.12–4	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–520.0	−3.25327+1	4.02654+1	−8.71727	7.21408−1	IV
520.0–580.0	−4.48739+3	2.61038+3	−5.02970+2	3.24043+1	IV
300.0–520.0	−2.74214+1	3.59134+1	−7.48833	6.06217−1	IV
520.0–580.0	−2.70019+3	1.57790+3	−3.04024+2	1.96149+1	IV

Table 45.45.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	17	15	0.278	1.08–1	0.28	2.29–4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
300.0–580.0	600.00	−2.17441	3.82317−1	1.68383	7.31481+1	−5.11156+1	1.33319+1	IV

Name: Propyl butanoate
Formula: $C_7H_{14}O_2$

CAS-RN: 105-66-8
Group No.: 45-046
Molar Mass: 130.19

Table 45.46.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH	317.5–346.2	6 S	nosp	not specified		avg	DSIO	*86SCH
94JIM/ROM	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

Table 45.46.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*86SCH	317.5–346.2	6	3.00 #	0.020	1.91–2	0.06	1.55–3	2
94JIM/ROM	298.1	1	0.50 #	0.002	2.56–4	0.00	−2.56–4	0

Table 45.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	7	7	0.024	2.34–2	0.07	1.29–3	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
298.1–346.2	−7.73684	1.82750+1	−1.86796	IV

Name: Methyl benzoate
Formula: $C_8H_8O_2$

CAS-RN: 93-58-3
Group No.: 45-048
Molar Mass: 136.15

Table 45.48.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH		317.8–345.2	6 S	nosp	not specified		avg	DSIO	*86SCH
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	p	BDHT	71DU/COM
79FUC		298.1	1	0.50	99.0	chrom	p	BSIO	80FUC
96ROU/HER		298.1	1	nosp	99.	anal	p	FSIT	71PIC/LED

71HAL/BAL suspect value

Table 45.48.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*86SCH	317.8–345.2	6	3.00 #	0.039	3.32–2	0.12	−7.19–3	−2
79FUC	298.1	1	0.50	1.541	2.05–1	0.77	2.05–1	1
96ROU/HER	298.1	1	0.50 #	1.509	1.98–1	0.75	−1.98–1	−1

Table 45.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	9	8	0.882	1.21–1	0.46	−4.47–3	−2

Temp. range K	A_1	A_2	Level of uncertainty
298.1–345.2	1.28992+1	4.53187	IV

Name: Butyl 2-methyl-2-propenoate
Formula: $C_8H_{14}O_2$

CAS-RN: 97-88-1
Group No.: 45-050
Molar Mass: 142.20

Table 45.50.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
52ERD/JAG		293.1–313.1	3 S	1.00	not specified		*p*	BSIO	49WEI
85KAR/ABD2	N	197.0–350.0	eqn	0.50	not specified		*p*	BSAO	82KAR/IGA
94LEB/KUL	N	199.3–323.8	27	0.20	99.19	melpt	*p*	BSAO	76LEB/LIT

85KAR/ABD2 same data in 85KAR/SAI
94LEB/KUL a graph only in 95LEB/KUL

Table 45.50.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
52ERD/JAG	303.1–313.1	2	1.00	0.472	1.63–1	0.47	9.38–2	0
94LEB/KUL	199.3–323.8	27	0.20	1.273	8.27–2	0.25	1.51–4	−2
Rejected data								
85KAR/ABD2	(8.26–1,2.64,−7.98–1,−11)							

Table 45.50.3. Parameters of regression polynomial

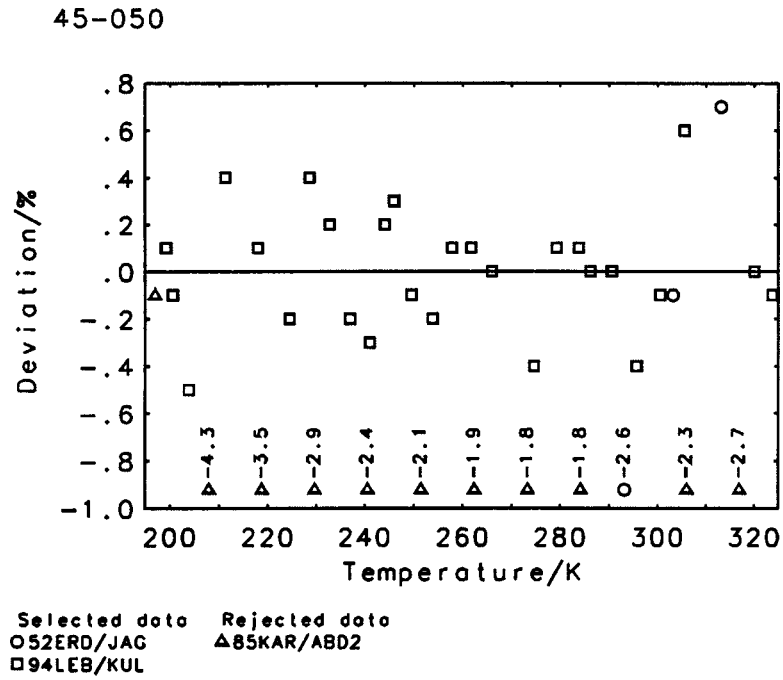
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	45	29	1.304	9.56–2	0.29	6.61–3	−2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
199.3–323.8	3.60401+1	−5.80098	1.67129	III

Table 45.50.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	40	27	1.361	8.88–2	0.27	4.23–4	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
199.3–323.8	619.00	4.43217+1	2.47003+1	5.46405	1.98824+1	III



Name: Hexyl acetate
Formula: $C_8H_{16}O_2$

CAS-RN: 142-92-7
Group No.: 45-057
Molar Mass: 144.21

Table 45.57.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
80BAL/PET	N	220.0–370.0	16 S	1.00	not specified		*p*	not specified	
97SVO/GOT		300.3–318.8	5	0.30	99.7	chrom	*p*	BSAO	91SVO/ZAB1

80BAL/PET error of 0.3–1.0% reported in 84VAS/PET

Table 45.57.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
80BAL/PET	220.0–370.0	16	1.00	0.906	3.04–1	0.91	−1.73–1	−8
97SVO/GOT	300.3–318.8	5	0.60 #	1.014	2.14–1	0.61	2.08–1	5

Table 45.57.3. Parameters of regression polynomial

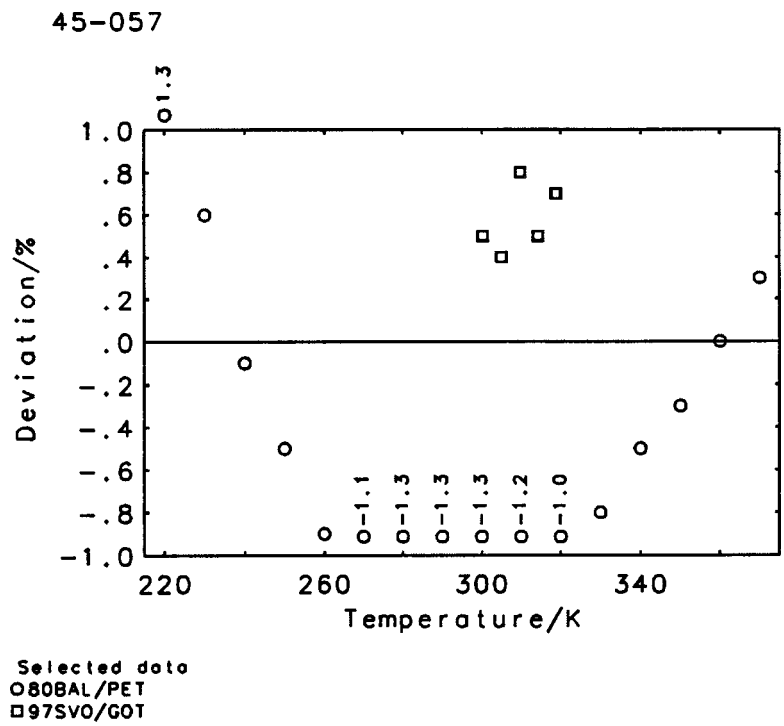
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
total	used						
p	21	21	0.981	3.00–1	0.89	−8.20–2	−3

Temp. range K	A_1	A_2	Level of uncertainty
220.0–370.0	2.22676+1	4.06413	IV

Table 45.57.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	21	21	1.155	2.71−1	0.79	2.43−2	−4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
220.0–370.0	623.50	−6.44657	1.79871	2.37711+1	5.77611	IV



Name: Ethyl benzoate
Formula: $C_9H_{10}O_2$

CAS-RN: 93-89-0
Group No.: 45-064
Molar Mass: 150.18

Table 45.64.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*86SCH		318.4–345.6	5 S	nosp	not specified		avg	DSIO	*86SCH
34KOL/UDO	N	292.7	1	nosp	not specified		*p*	BSIT	34KOL/UDO
36KUR/VOS	N	311.6	1	nosp	not specified		avg	DSIO	36KUR/VOS
79FUC		298.1	1	0.50	99.	chrom	*p*	BSIO	80FUC
96ROU/HER		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

34KOL/UDO2 same datum in 33KOL/UDO
36KUR/VOS average value in temperature range 290–333 K

Table 45.64.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
			Selected data					
*86SCH	318.4–345.6	5	3.00 #	0.008	7.37–3	0.02	1.94–3	1
79FUC	298.1	1	0.50	0.252	3.73–2	0.13	−3.73–2	−1
96ROU/HER	298.1	1	0.50 #	0.251	3.72–2	0.13	3.72–2	1
			Rejected data					
36KUR/VOS	(3.59,10.57,3.59,1)							

Table 45.64.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	9	7	0.159	2.47–2	0.08	1.37–3	1

Temp. range K	A_1	A_2	Level of uncertainty
298.1–345.6	1.21796+1	5.85092	V

Name: Dimethyl 1,2-benzenedicarboxylate
Formula: $C_{10}H_{10}O_4$

CAS-RN: 131-11-3
Group No.: 45-076
Molar Mass: 194.19

Table 45.76.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78MIL		274.0–370.0	eqn	1.00	99.	chrom	p	BDHT	69PER/COM
86RAB/NOV	N	274.2–360.0	11 S	0.50	not specified		p	BDAO	51POP/GAL
98ROH/MUS		308.0–447.2	30	1.00	99.95	chrom	p	BDCT	91BAN/GAR
#00ROH		283.1–323.1	3	0.50	99.95	chrom	p	BDCT	83ROU/ROU

86RAB/NOV some data in 69RAB/MAR and 70MAR/RAB; adiabatic calorimeter 56POP/KOL used below 300 K

Table 45.76.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
			Selected data					
78MIL	284.7–370.3	9	1.00	0.597	2.34–1	0.60	−2.15–1	−9
98MUS/ROH	308.0–447.2	30	1.00	0.205	8.43–2	0.20	2.46–2	10
#00ROH	283.1–323.1	3	0.50	0.609	1.16–1	0.30	1.04–1	3
			Rejected data					
86RAB/NOV	(9.21–1,2.46,−9.20–1,−9)							

Table 45.76.3. Parameters of regression polynomial

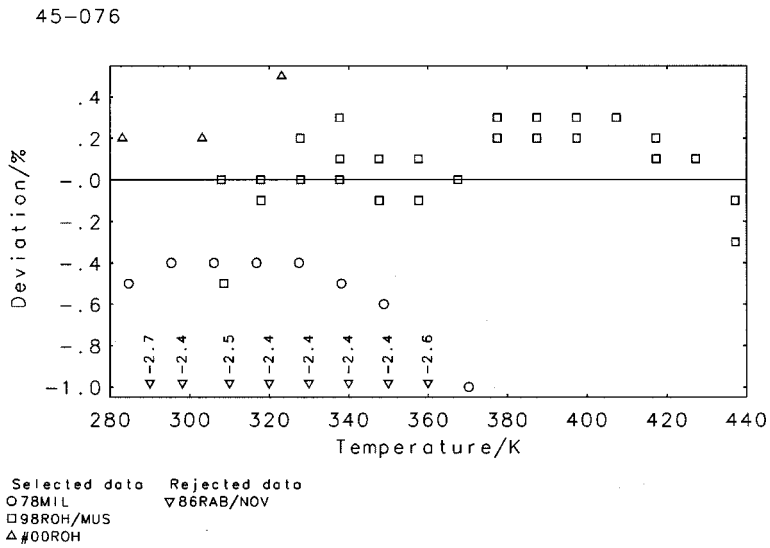
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	56	42	0.378	1.38–1	0.35	−2.12–2	4

Temp. range K	A_1	A_2	A_3	Level of uncertainty
283.1–447.1	3.26009+1	−6.04958−1	7.36242−1	IV

Table 45.76.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	56	42	0.426	1.40−1	0.35	8.84−3	10

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
283.1−447.1	765.00	−9.36281	1.97672	2.50700+1	1.10868+1	IV



Name: Octyl acetate
Formula: $C_{10}H_{20}O_2$

CAS-RN: 112-14-1
Group No.: 45-085
Molar Mass: 172.27

Table 45.85.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91DES/PAT	298.1	1	nosp	98.	anal	p	FSIT	71PIC/LED
97SVO/GOT	300.3−318.8	5	0.30	99.9	chrom	p	BSAO	91SVO/ZAB1

Table 45.85.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
91DES/PAT	298.1	1	0.50 #	0.782	1.62−1	0.39	−1.62−1	−1
97SVO/GOT	300.3−318.8	5	0.30	0.323	4.10−2	0.10	1.18−2	2

Table 45.85.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	6	6	0.532	9.29–2	0.22	−1.71–2	1
Temp. range K		A_1	A_2				Level of uncertainty
298.1–318.8		2.33207+1	6.09863				IV

Name: Diethyl 1,2-benzenedicarboxylate
Formula: $C_{12}H_{14}O_4$

CAS-RN: 84-66-2
Group No.: 45-090
Molar Mass: 222.24

Table 45.90.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
67CHA/HOR	273.2–353.4	25	0.10	99.88	melpt	p	BSAO	65STE/BLA
79FUC	298.1	1	0.50	99.	chrom	p	BSIO	80FUC
#98ROH/SCH	283.1–323.1	3	0.50	99.93	chrom	p	BDCT	83ROU/ROU
#00ROH	305.6–370.1	14	1.00	99.93	chrom	p	BDCT	91BAN/GAR

Table 45.90.2. Correlated heat capacities

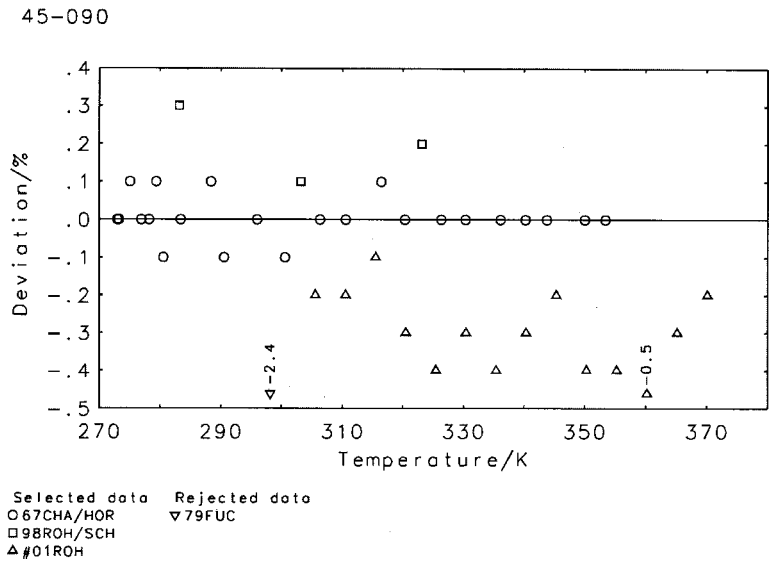
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
67CHA/HOR	273.2–353.4	24	0.10	0.632	2.77–2	0.06	3.57–4	−1
98ROH/SCH	283.1–323.1	3	0.05 #	0.492	1.08–1	0.25	1.02–1	3
#00ROH	305.6–370.1	14	1.00	0.316	1.47–1	0.32	−1.41–1	−14
Rejected data								
79FUC	(1.03,2.40,−1.03,−1)							

Table 45.90.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	71	41	0.555	9.70–2	0.21	−4.05–2	−12
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.2–370.1		3.34046+1	1.40920	7.24886−1			III

Table 45.90.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	71	41	0.718	7.93–2	0.17	−1.78–2	−3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
273.2–370.1	760.20	−1.29396+1	4.61362	2.64527+1	9.07277		IV



Name: Decyl acetate
Formula: $C_{12}H_{24}O_2$

CAS-RN: 112-17-4
Group No.: 45-098
Molar Mass: 200.32

Table 45.98.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97SVO/GOT	300.3–318.8	5	0.30	99.4	chrom	*p*	BSAO	91SVO/ZAB1

Table 45.98.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	5	5	0.511	7.57−2	0.15	1.36−4	1
Temp. range K		A_1	A_2				Level of uncertainty
300.3–318.8		3.35480+1	5.10275				IV

Name: Dibutyl 1,2-benzenedicarboxylate
Formula: $C_{16}H_{22}O_4$

CAS-RN: 84-74-2
Group No.: 45-104
Molar Mass: 278.35

Table 45.104.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
48BER/MEL		353.1–423.1	2	nosp	not specified		*p*	BSIO	34LON/REY
70MAR/RAB	N	173.5–360.0	5 S	0.30	not specified		*p*	BSAO	56POP/KOL
85RAB/NOV		173.9–300.1	40	nosp	99.7	chrom	*p*	BSAO	66NIK/LEB
#00ROH		312.8–447.3	30	1.00	99.97	chrom	*p*	BDCT	91BAN/GAR

70MAR/RAB same data in 69RAB/MAR at 300 K and 360 K

Table 45.104.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
70MAR/RAB	200.0–360.0	4	0.30	1.699	3.13–1	0.51	−1.55–1	−2
85RAB/NOV	179.2–300.1	36	0.50 #	0.276	7.24–2	0.14	−3.92–3	−5
#00ROH	312.8–447.3	30	1.00	0.480	3.03–1	0.48	2.57–1	26
Rejected data								
48BER/MEL	(2.45,3.44,1.99,2)							

Table 45.104.3. Parameters of cubic spline polynomials

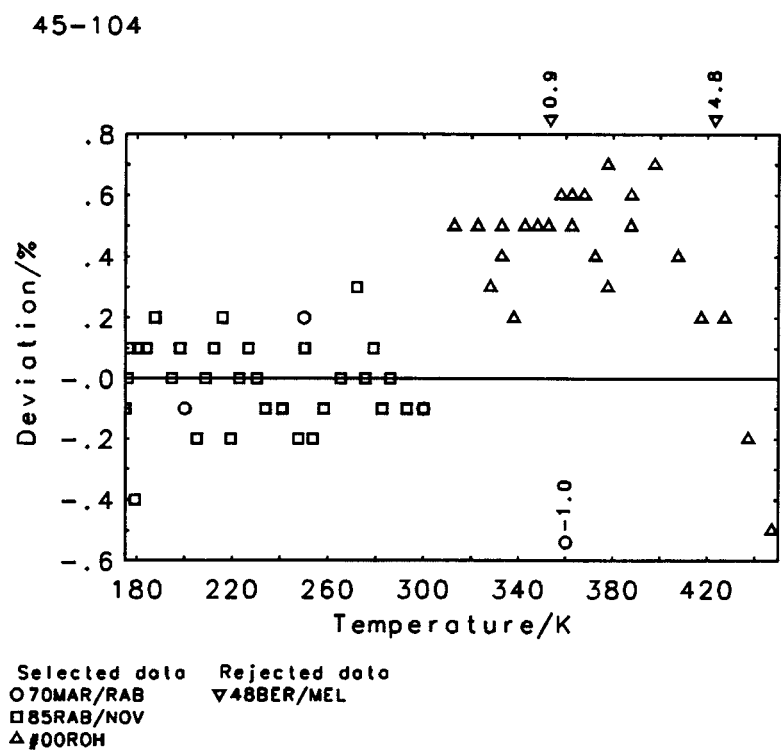
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	77	70	0.571	2.27–1	0.36	9.94–2	19

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
179.2–290.0	1.09651+2	−7.17062+1	2.76630+1	−3.18754	III
290.0–447.3	2.43773+1	1.65077+1	−2.75563	3.08848−1	IV

Table 45.104.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	77	63	1.116	4.89–1	0.78	5.61–2	11

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
200.0–447.3	790.00	−1.02711+1	1.56931+1	2.64437+1	1.68061	IV



Name: Bis(2-ethylhexyl) hexanedioate
Formula: $C_{22}H_{42}O_4$

CAS-RN: 103-23-1
Group No.: 45-107
Molar Mass: 370.57

Table 45.107.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
85OVC/MOS	180.0–300.0	7 S	0.20	99.	chrom	*p*	BSAO	76LEB/LIT
93CON/GIR2	297.0–426.0	eqn	nosp	not specified		sat	BDHT	93CON/GIR1

Name: Bis(2-ethylhexyl)-1,2-benzenedicarboxylate
Formula: $C_{24}H_{38}O_4$

CAS-RN: 117-81-7
Group No.: 45-110
Molar Mass: 390.56

Table 45.110.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
70MAR/RAB	N	182.5–360.0	5 S	0.30	not specified		*p*	BSAO	56POP/KOL
85RAB/NOV		184.4–300.2	38	nosp	99.7	chrom	*p*	BSAO	66NIK/LEB
#00ROH		313.0–461.9	35	1.00	99.64	chrom	*p*	BDCT	91BAN/GAR

70MAR/RAB same data in 69RAB/MAR at 300 K and 360 K

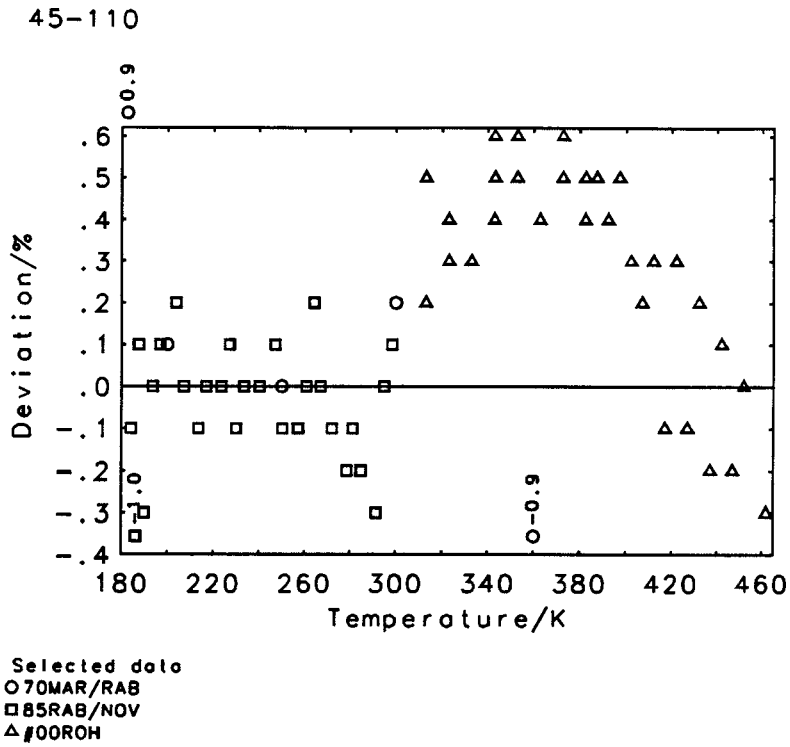
Table 45.110.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
70MAR/RAB	200.0–360.0	4	0.30	1.475	4.07–1	0.44	−1.60–1	0
85RAB/NOV	190.0–300.2	35	0.50 #	0.234	9.36–2	0.12	−1.51–2	−4
#00ROH	313.0–461.9	35	1.00	0.373	3.51–1	0.37	2.72–1	25

Table 45.110.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	78	74	0.474	2.76–1	0.30	1.13–1	21

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
190.0–300.0	1.27061+2	−6.16255+1	2.27638+1	−2.30250	III
300.0–461.9	8.52931+1	−1.98572+1	8.84107	−7.55525−1	IV



Name: 1,2,3-Propanetriyl ester dodecanoic acid
Formula: $C_{39}H_{74}O_6$

CAS-RN: 538-24-9
Group No.: 45-120
Molar Mass: 639.01

Table 45.120.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
47CHA/SIN		330.9–370.2	6	nosp	98.	estim	*p*	BSAO	44BAI/TOD
76PHI/MAT	N	323.0–398.0	4	nosp	not specified		*p*	BDHT	73PER/COM
95MOR/IDR1		328.0–443.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1
95MOR/IDR2		328.0–443.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1
95MOR/IDR2		443.0–523.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1

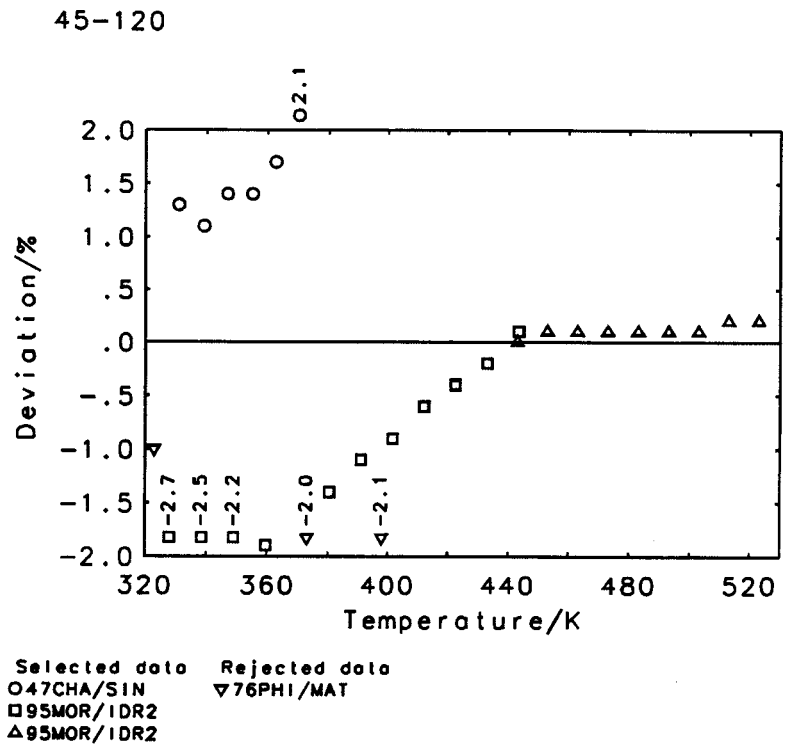
76PHI/MAT reproducibility given as 5%

Table 45.120.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
47CHA/SIN	330.9–370.2	6	1.50 #	1.007	2.53	1.51	2.46	6
95MOR/IDR2	328.0–438.0	12	2.00 #	0.795	2.55	1.59	−2.19	−12
95MOR/IDR2	443.0–523.0	9	2.00 #	0.059	2.20–1	0.12	2.03–1	9
Rejected data								
76PHI/MAT	(5.38,3.41,−4.90,−3)		95MOR/IDR1	(2.56,1.60,−2.20,−12)				

Table 45.120.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	43	27	0.740	2.16	1.33	−3.59−1	3
Temp. range K		A_1	A_2				Level of uncertainty
328.0–523.0		1.11431+2	1.49714+1				V



Name: 1,2,3-Propanetriyl ester tetradecanoic acid
Formula: $C_{45}H_{86}O_6$

CAS-RN: 555-45-3
Group No.: 45-124
Molar Mass: 723.17

Table 45.124.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
47CHA/SIN		331.5–365.0	6	nosp	98.	estim	*p*	BSAO	44BAI/TOD
76PHI/MAT	N	333.0–433.0	5	nosp	not specified		*p*	BDHT	73PER/COM
95MOR/IDR2		338.0–454.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1
95MOR/IDR2		454.0–523.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1

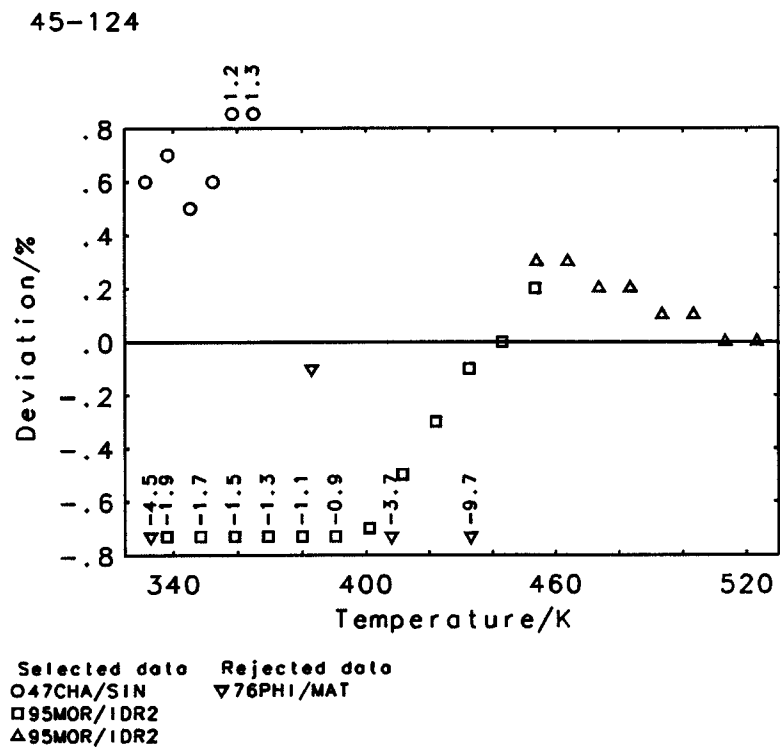
76PHI/MAT reproducibility given as 5%

Table 45.124.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
47CHA/SIN	331.5–365.0	6	1.50 #	0.574	1.65	0.86	1.53	6
95MOR/IDR2	338.0–453.5	12	2.00 #	0.513	1.93	1.03	−1.51	−8
95MOR/IDR2	454.0–523.3	8	2.00 #	0.090	3.80−1	0.18	3.24−1	7
			Rejected data					
76PHI/MAT	(9.86,5.33,−8.05,−5)							

Table 45.124.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	31	26	0.466	1.61	0.85	−2.44−1	5
Temp. range K		A_1	A_2				Level of uncertainty
331.5–523.3		1.28043+2	1.74669+1				V



Name: 1,2,3-Propanetriyl ester hexadecanoic acid
Formula: $C_{51}H_{98}O_6$

CAS-RN: 555-44-2
Group No.: 45-127
Molar Mass: 807.34

Table 45.127.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
47CHA/SIN		338.8–369.1	6	nosp	98.	estim	*p*	BSAO	44BAI/TOD
76PHI/MAT	N	343.0–418.0	4	nosp	not specified		*p*	BDHT	73PER/COM
82OLL/PER		340.0	1	nosp	not specified		*p*	BDHT	73PER/COM
93KAP/BAL		345.0–365.0	2	nosp	99.	anal	*p*	BDCT	86MER/BEN
95MOR/IDR2		348.0–457.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1
95MOR/IDR2		457.0–523.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1
99VAN/TEN		341.2–354.9	7	0.20	96.9	melpt	*p*	BSAO	98VAN/VAN

76PHI/MAT reproducibility given as 5%

Table 45.127.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
82OLL/PER	340.0	1	1.00 #	0.662	1.37	0.66	−1.37	−1
95MOR/IDR2	348.0–457.2	15	1.00 #	0.055	1.22–1	0.06	4.43–2	7
95MOR/IDR2	457.0–522.8	8	1.50 #	0.044	1.66–1	0.07	−6.27–2	−1
99VAN/TEN	341.2–354.9	7	0.20	0.189	7.94–2	0.04	5.50–3	−1
			Rejected data					
47CHA/SIN	(3.47,1.60,3.46,5)		76PHI/MAT	(5.96,2.91,−3.13,0)				
93KAP/BAL	(1.92+1,8.31,1.91+1,2)							

Table 45.127.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	43	31	0.164	2.91–1	0.14	−3.77–2	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
340.0–522.8		1.38924+2	1.80896+1	7.03888−1			IV

Name: 1,2,3-Propanetriyl ester octadecanoic acid
Formula: $C_{57}H_{110}O_6$

CAS-RN: 555-43-1
Group No.: 45-130
Molar Mass: 891.50

Table 45.130.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
47CHA/SIN		346.5–371.6	6	nosp	98.	estim	*p*	BSAO	44BAI/TOD
76PHI/MAT	N	353.0–453.0	5	nosp	not specified		*p*	BDHT	73PER/COM
95MOR/IDR2		353.0–460.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1
95MOR/IDR2		460.0–523.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1

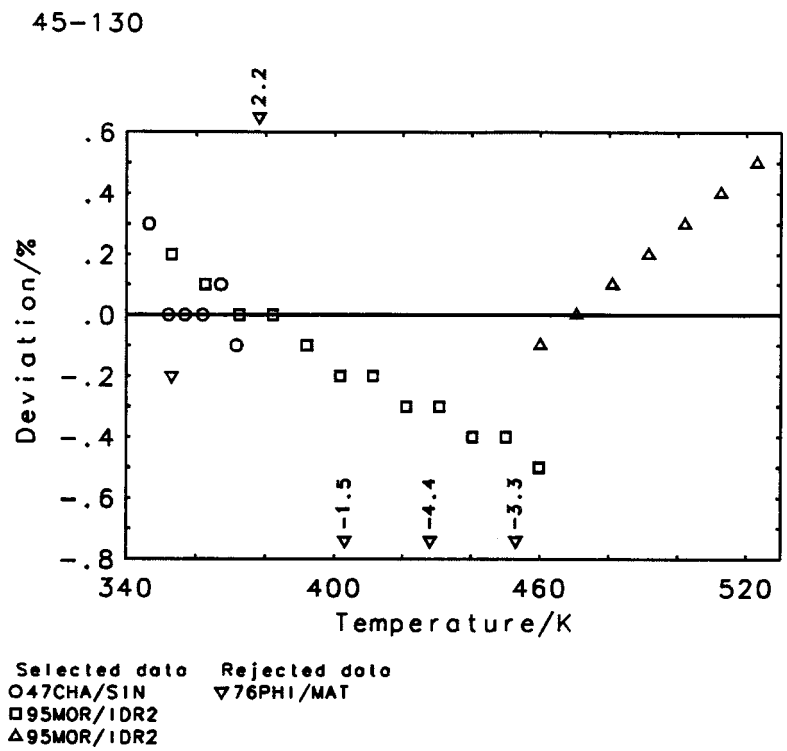
76PHI/MAT reproducibility given as 5%

Table 45.130.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
47CHA/SIN	346.5–371.6	6	1.50 #	0.098	3.49–1	0.15	1.71–1	2
95MOR/IDR2	353.0–459.7	12	2.00 #	0.136	7.11–1	0.27	−4.66–1	−6
95MOR/IDR2	460.0–523.0	7	2.00 #	0.135	7.70–1	0.27	5.56–1	4
Rejected data								
76PHI/MAT	(6.86,2.73,−3.62,−3)							

Table 45.130.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	30	25	0.133	6.90–1	0.26	−2.67–2	0
Temp. range K		A_1	A_2				Level of uncertainty
346.5–523.0		1.36516+2	2.87329+1				V



Name: Dimethyl ester ethanedioic acid
Formula: $C_4H_6O_4$

CAS-RN: 553-90-2
Group No.: 45-131
Molar Mass: 118.09

Table 45.131.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	339.15	2.151	nosp	not specified		avg	DSIO	*94BRU
*94BRU	average value in temperature range 329–349 K								

Name: Dimethyl ester propanedioic acid
Formula: $C_5H_8O_4$

CAS-RN: 108-59-8
Group No.: 45-132
Molar Mass: 132.12

Table 45.132.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92VER/BEC	298.15	1.590	nosp	99.995	chrom	*p*	BDHT	69PER/COM

Name: Dimethyl ester methylpropanedioic acid
Formula: $C_6H_{10}O_4$

CAS-RN: 609-02-9
Group No.: 45-133
Molar Mass: 146.14

Table 45.133.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92VER/BEC	298.15	1.791	nosp	99.995	chrom	*p*	BDHT	69PER/COM

Name: Dimethyl ester dimethylpropanedioic acid
Formula: $C_7H_{12}O_4$

CAS-RN: 6065-54-9
Group No.: 45-134
Molar Mass: 160.17

Table 45.134.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92VER/BEC	298.15	1.619	nosp	99.995	chrom	*p*	BDHT	69PER/COM

Name: Ethyl ester 2-methylbutanoic acid
Formula: $C_7H_{14}O_2$

CAS-RN: 7452-79-1
Group No.: 45-135
Molar Mass: 130.19

Table 45.135.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92VER/BEC	298.15	2.515	nosp	99.995	chrom	*p*	BDHT	69PER/COM

Name: Butyl-d_9 ester 2-(methyl-d_3)-2-propenoic-3,3-d_2 acid
Formula: $C_8D_{14}O_2$

CAS-RN: 158612-79-4
Group No.: 45-136
Molar Mass: 156.28

Table 45.136.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94LEB/KUL	N	208.3–329.4	32	0.20	99.64	melpt	*p*	BSAO	76LEB/LIT
94LEB/KUL	degree of deuteration was 99%; a graph only in 95LEB/KUL								

Table 45.136.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	32	32	1.201	8.72–2	0.24	3.82–4	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
208.3–329.4	2.62719+1	1.80271	6.40006–1	III

Name: Heptyl acetate
Formula: $C_9H_{18}O_2$

CAS-RN: 112-06-1
Group No.: 45-137
Molar Mass: 158.24

Table 45.137.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97SVO/GOT	300.3–318.8	5	0.30	100.0	chrom	*p*	BSAO	91SVO/ZAB1

Table 45.137.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	5	5	0.518	6.00–2	0.16	1.11–4	0

Temp. range K	A_1	A_2	Level of uncertainty
300.3–318.8	2.48991+1	4.36749	IV

Name: Dimethyl ester 1,3-benzenedicarboxylic acid
Formula: $C_{10}H_{10}O_4$

CAS-RN: 1459-93-4
Group No.: 45-138
Molar Mass: 194.19

Table 45.138.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI3	360.0–740.0	20	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 45.138.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	20	20	0.209	1.22–1	0.21	4.76–4	−1
sat	20	20	0.142	7.99–2	0.14	2.06–4	−2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
360.0–670.0	−9.61110	2.38821+1	−3.70702	2.44568−1	IV
670.0–740.0	−7.72297+3	3.47762+3	−5.19191+2	2.58905+1	IV
360.0–670.0	−4.37496	2.03677+1	−2.92911	1.87734−1	IV
670.0–740.0	−5.19945+3	2.34652+3	−3.50116+2	1.74607+1	IV

Table 45.138.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	20	20	0.088	4.57–2	0.09	1.35–4	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
360.0–740.0	766.00	−2.33736	4.65526−1	5.49457	9.67417+1	−7.04743+1	1.91624+1	IV

Name: Methyl ester pentacyclo[4.3.0.0^{2,5}.0^{3,8}.0^{4,7}]nonane-4-carboxylic acid
Formula: $C_{11}H_{12}O_2$

CAS-RN: 40317-63-3
Group No.: 45-139
Molar Mass: 176.22

Table 45.139.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
84BEC/RUE	298.15	1.636	nosp	99.95	chrom	*p*	BDHT	69PER/COM

Name: Butyl benzoate
Formula: $C_{11}H_{14}O_2$

CAS-RN: 136-60-7
Group No.: 45-140
Molar Mass: 178.23

Table 45.140.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96ROU/HER	298.15	1.706	nosp	99.	anal	*p*	FSIT	71PIC/LED

Name: Nonyl acetate
Formula: $C_{11}H_{22}O_2$

CAS-RN: 143-13-5
Group No.: 45-141
Molar Mass: 186.29

Table 45.141.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97SVO/GOT	300.3–318.8	5	0.30	100.0	chrom	*p*	BSAO	91SVO/ZAB1

Table 45.141.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	5	5	0.457	6.27−2	0.14	1.07−4	1

Temp. range K	A_1	A_2	Level of uncertainty
300.3–318.8	2.88879+1	5.41999	IV

Name: Monobutyl ester 1,2-benzenedicarboxylic acid
Formula: $C_{12}H_{14}O_4$

CAS-RN: 131-70-4
Group No.: 45-142
Molar Mass: 222.24

Table 45.142.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
48BER/MEL	353.1–423.1	2	nosp	not specified		*p*	BSIO	34LON/REY

Table 45.142.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	−3.82−6	0

Temp. range K	A_1	A_2	Level of uncertainty
353.1–423.1	−2.59139+1	2.02901+1	VI

Name: Undecyl acetate
Formula: $C_{13}H_{26}O_2$

CAS-RN: 1731-81-3
Group No.: 45-143
Molar Mass: 214.35

Table 45.143.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97SVO/GOT	300.3–318.8	5	0.30	99.8	chrom	*p*	BSAO	91SVO/ZAB1

Table 45.143.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	5	5	0.326	5.24−2	0.10	6.26−5	0
Temp. range K		A_1	A_2				Level of uncertainty
300.3–318.8		3.62670+1	5.59038				IV

Name: Dimethyl ester 2,6-naphthalenedicarboxylic acid
Formula: $C_{14}H_{12}O_4$

CAS-RN: 840-65-3
Group No.: 45-144
Molar Mass: 244.25

Table 45.144.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91STE/CHI2	480.0–660.0	10	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 45.144.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	10	10	0.267	1.65−1	0.27	5.71−4	−2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
480.0–660.0		2.04783+2	−8.73066+1	1.62903+1	−9.38663−1		IV

Name: Dibutyl ester hexanedioic acid
Formula: $C_{14}H_{26}O_4$

CAS-RN: 105-99-7
Group No.: 45-145
Molar Mass: 258.36

Table 45.145.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93CON/GIR2	299.0–435.0	eqn	nosp	not specified		sat	BDHT	93CON/GIR1

Table 45.145.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	14	14	0.000	3.64−6	0.00	1.63−6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
299.0–435.5		5.28236	2.27611+1	−2.05208			VI

Name: Dodecyl acetate
Formula: $C_{14}H_{28}O_2$

CAS-RN: 112-66-3
Group No.: 45-146
Molar Mass: 228.38

Table 45.146.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91DES/PAT	N	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
97SVO/GOT		300.3–318.8	5	0.30	99.5	chrom	*p*	BSAO	91SVO/ZAB1

91DES/PAT the compound was not Decyl acetate as given in the original paper (corrected after correspondence with author)

Table 45.146.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
97SVO/GOT	300.3–318.8	5	0.30	0.256	4.42–2	0.08	6.41–5	−2

Table 45.146.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	6	5	0.331	5.70–2	0.10	6.41–5	−2

Temp. range K	A_1	A_2	Level of uncertainty
300.3–318.8	3.30848+1	7.88680	IV

Name: Tetradecyl acetate
Formula: $C_{16}H_{32}O_2$

CAS-RN: 638-59-5
Group No.: 45-147
Molar Mass: 256.43

Table 45.147.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97SVO/GOT	300.3–318.8	5	0.30	98.6	chrom	*p*	BSAO	91SVO/ZAB1

Table 45.147.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	5	5	0.275	5.40–2	0.08	5.65–5	0

Temp. range K	A_1	A_2	Level of uncertainty
300.3–318.8	3.98921+1	8.09271	IV

Name: 1-Methylethyl ester tetradecanoic acid
Formula: $C_{17}H_{34}O_2$

CAS-RN: 110-27-0
Group No.: 45-148
Molar Mass: 270.46

Table 45.148.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93CON/GIR2	298.0–426.0	eqn	nosp	not specified		sat	BDHT	93CON/GIR1

Table 45.148.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	13	13	0.000	4.18−6	0.00	5.87−7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.0−426.4		4.66453+1	4.85325	4.36846−1			VI

Name: Butyl phenylmethyl ester 1,2-benzenedicarboxylic acid
Formula: $C_{19}H_{20}O_4$

CAS-RN: 85-68-7
Group No.: 45-149
Molar Mass: 312.37

Table 45.149.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00ROH	313.1−382.7	20	1.00	99.82	chrom	p	BDCT	91BAN/GAR

Table 45.149.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	20	0.133	8.62−2	0.13	1.93−4	0
Temp. range K		A_1	A_2				Level of uncertainty
313.1−382.7		3.20501+1	9.39194				IV

Name: 1-Methylethyl ester hexadecanoic acid
Formula: $C_{19}H_{38}O_2$

CAS-RN: 142-91-6
Group No.: 45-150
Molar Mass: 298.51

Table 45.150.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93CON/GIR2	334.0−471.0	eqn	nosp	not specified		sat	BDHT	93CON/GIR1

Table 45.150.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	15	15	0.000	9.85−6	0.00	8.14−6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
334.0−471.2		−2.80756+1	3.30336+1	−3.05959			VI

Name: 1-Methyl-1,2-ethanediyl ester nonanoic acid
Formula: $C_{21}H_{40}O_4$

CAS-RN: 41395-83-9
Group No.: 45-151
Molar Mass: 356.55

Table 45.151.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93CON/GIR2	298.0−428.0	eqn	nosp	not specified		sat	BDHT	93CON/GIR1

Table 45.151.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
sat	13	13	0.000	5.91−6	0.00	−1.17−6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.0–427.6		−5.36025	3.24577+1	−2.71488			VI

Name: Decyl ester (*Z*)-9-octadecenoic acid
Formula: $C_{28}H_{54}O_2$

CAS-RN: 3687-46-5
Group No.: 45-152
Molar Mass: 422.74

Table 45.152.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93CON/GIR2	297.0–426.0	eqn	nosp	not specified		sat	BDHT	93CON/GIR1

Table 45.152.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
sat	13	13	0.000	7.24−6	0.00	2.93−6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
297.0–426.6		7.37224+1	1.38450	2.03830			VI

Name: Bis(2,4-diethyloctyl) ester 1,2-benzenedicarboxylic acid
Formula: $C_{32}H_{54}O_4$

CAS-RN: 40989-56-8
Group No.: 45-153
Molar Mass: 502.78

Table 45.153.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
84OVC/MOS	195.0–302.4	29	0.20	not specified		*p*	BSAO	76LEB/LIT

Table 45.153.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	29	29	0.853	1.70−1	0.17	5.08−4	7
Temp. range K		A_1	A_2	A_3			Level of uncertainty
195.0–302.4		1.01881+2	−1.18477+1	4.82618			IV

Name: (*Z*)-9-Octadecenyl ester (*Z*)-9-octadecenoic acid
Formula: $C_{36}H_{68}O_2$

CAS-RN: 3687-45-4
Group No.: 45-154
Molar Mass: 532.93

Table 45.154.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93CON/GIR2	298.0–438.0	eqn	nosp	not specified		sat	BDHT	93CON/GIR1

Table 45.154.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	14	14	0.000	3.45−5	0.00	−2.23−5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.0−438.4		−3.24202+2	2.32992+2	−2.97923+1			VI

Name: 2,3-Bis[(1-oxotetradecyl)oxy]propyl ester hexadecanoic acid
Formula: $C_{47}H_{90}O_6$

CAS-RN: 60138-13-8
Group No.: 45-155
Molar Mass: 751.23

Table 45.155.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95MOR/IDR2	333.0−454.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1
95MOR/IDR2	454.0−523.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1

Table 45.155.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
			Selected data					
95MOR/IDR2	333.0−454.0	12	2.00 #	0.039	1.56−1	0.08	1.72−2	3
95MOR/IDR2	454.0−523.3	8	2.00 #	0.037	1.57−1	0.07	−2.51−2	1

Table 45.155.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	20	0.041	1.70−1	0.08	2.62−4	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
333.0−523.3		1.44283+2	9.26419	1.21300			V

Name: 2,3-Bis[(1-oxotetradecyl)oxy]propyl ester (*Z*)-9-octadecenoic acid
Formula: $C_{49}H_{92}O_6$

CAS-RN: 74160-01-3
Group No.: 45-156
Molar Mass: 777.27

Table 45.156.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95MOR/IDR2	308.0−443.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1
95MOR/IDR2	443.0−523.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1

Table 45.156.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
			Selected data					
95MOR/IDR2	308.0−443.2	14	2.00 #	0.014	5.74−2	0.03	4.29−3	3
95MOR/IDR2	443.0−522.8	8	2.00 #	0.014	5.96−2	0.03	−7.40−3	1

Table 45.156.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	22	22	0.015	6.27−2	0.03	3.68−5	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
308.0–522.8		1.20496+2	1.96340+1	3.63136−1			V

Name: 2,3-Bis[(1-oxohexadecyl)oxy]propyl ester (*Z*)-9-octadecenoic acid
Formula: $C_{53}H_{100}O_6$

CAS-RN: 1867-91-0
Group No.: 45-157
Molar Mass: 833.37

Table 45.157.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95MOR/IDR2	323.0–453.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1
95MOR/IDR2	453.0–523.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1

Table 45.157.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
95MOR/IDR2	323.0–452.6	13	2.00 #	0.047	2.18−1	0.09	−1.15−1	−3
95MOR/IDR2	453.0–523.2	10	2.00 #	0.066	3.21−1	0.13	1.51−1	3

Table 45.157.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	23	23	0.060	2.87−1	0.12	5.85−4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
323.0–523.2		1.32789+2	2.04905+1	5.47847−1			V

Name: 1-[[(1-Oxohexadecyl)oxy]methyl]-1,2-ethanediyl ester (*Z*)-9-octadecenoic acid
Formula: $C_{55}H_{102}O_6$

CAS-RN: 2190-30-9
Group No.: 45-158
Molar Mass: 859.41

Table 45.158.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95MOR/IDR2	308.0–435.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1
95MOR/IDR2	435.0–523.0	eqn	nosp	99.0	anal	*p*	BDHT	95MOR/IDR1

Table 45.158.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
95MOR/IDR2	308.0–435.4	14	2.00 #	0.024	1.09−1	0.05	−7.42−3	−2
95MOR/IDR2	435.0–523.0	9	2.00 #	0.020	9.92−2	0.04	1.18−2	−2

Table 45.158.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	23	23	0.024	1.13−1	0.05	1.03−4	−4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
308.0–523.0		1.04850+2	3.51001+1	−7.75735−1			V

Name: (*all-Z*)-1,2,3-Propanetriyl ester 9,12,15-octadecatrienoic acid
Formula: $C_{57}H_{92}O_6$

CAS-RN: 14465-68-0
Group No.: 45-159
Molar Mass: 873.35

Table 45.159.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93KAP/BAL	300.0–363.0	2	nosp	99.	anal	*p*	BDCT	86MER/BEN

Table 45.159.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
300.0–363.0		3.57135+2					VI

Name: 2,3,6,7,10,11-Triphenylenehexayl ester octanoic acid
Formula: $C_{66}H_{96}O_{12}$

CAS-RN: 70351-94-9
Group No.: 45-160
Molar Mass: 1081.48

Table 45.160.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86VAN/KAJ	403.3–422.5	10	nosp	not specified		*p*	BSAO	83YOS/SOR1

Table 45.160.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	10	10	0.197	2.73−1	0.10	4.21−4	4
Temp. range K		A_1	A_2				Level of uncertainty
403.3–422.5		7.50248+1	4.90152+1				IV

Name: 1,3-Dioxolane
Formula: $C_3H_6O_2$

CAS-RN: 646-06-0
Group No.: 46-004
Molar Mass: 74.08

Table 46.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
69CLE/MEL4	175.9–300.0	16 S	nosp	99.93	melpt	sat	BSAO	68CLE/MEL
76CON/GIA	298.1	1	nosp	not specified		*p*	BDCT	76CON/GIA
88ING	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
99BRO/CAL	298.1	1	nosp	99.8	anal	*p*	FSIT	71PIC/LED

Name: Ethyloxirane
Formula: C_4H_8O

CAS-RN: 106-88-7
Group No.: 46-008
Molar Mass: 72.11

Table 46.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
73GOO/FIN	136.8–322.5	24	0.20	99.93	melpt	sat	BSAO	47HUF
97RIG/COM	288.1–313.1	3	1.00	99.8	chrom	*p*	BDHT	95DIO/MAN

Name: Tetrahydrofuran
Formula: C_4H_8O

CAS-RN: 109-99-9
Group No.: 46-009
Molar Mass: 72.11

Table 46.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
76BON/CER		298.1	1	nosp	not specified		*p*	BSIO	76BON/CER
76CON/GIA		298.1	1	nosp	not specified		*p*	BDCT	76CON/GIA
78LEB/RAB2	N	161.6–322.6	50	0.20	99.8	melpt	*p*	BSAO	76LEB/LIT
79KIY/DAR		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
85COS/PAT9		283.1–313.1	3	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
88ING		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
94CON/GIA1		298.1	1	nosp	not specified		*p*	FSIT	88CON/GIA
94CON/GIA2		298.1	1	nosp	99.5	anal	*p*	FSIT	88CON/GIA
97CON/GIA		298.1	1	nosp	not specified		*p*	FSIT	88CON/GIA
99BRO/CAL		298.1	1	nosp	99.9	anal	*p*	FSIT	71PIC/LED

78LEB/RAB2 same data in 79LEB/LIT and smoothed data in 77LEB/LIT1

Name: 1,4-Dioxane
Formula: $C_4H_8O_2$

CAS-RN: 123-91-1
Group No.: 46-011
Molar Mass: 88.11

Table 46.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
29HER/LOR	296.1	1	nosp	not specified		*p*	DSIO	22HER/SCH
33ROT/MEY1	291.1	1	nosp	not specified		*p*	DSIO	33ROT/MEY2
34JAC/PAR	288.7–298.2	3	nosp	not specified		*p*	BSIO	25PAR
52STA/AMI	313.1	1	nosp	not specified		*p*	BSIO	52STA/AMI
61ROU	296.9–313.7	14	nosp	not specified		*p*	BSAO	61ROU
71DES/BHA	298.1–318.1	3 S	nosp	not specified		*p*	BSIO	58MUR/VAN
71KHA/SUB	298.1–313.1	2	nosp	not specified		*p*	BSIO	64MOE/THO
76BON/CER	298.1	1	nosp	not specified		*p*	BSIO	76BON/CER
76CON/GIA	298.1	1	nosp	not specified		*p*	BDCT	76CON/GIA
79MUR/SUB	298.1	1	nosp	not specified		*p*	BSIO	64MOE/THO
84GRO/ING	298.1	1	0.30	99.5	melpt	*p*	FSIT	71PIC/LED
84ING/GRO	298.1	1	0.30	99.5	chrom	*p*	FSIT	71PIC/LED
88ING	298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
89BAR/KOO2	298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
91GRO/ROU	298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
91TRE/COS	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
93GRO/ROU	298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
94GRO/ROU	298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED
99BRO/CAL	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

Name: Tetrahydropyran
Formula: $C_5H_{10}O$

CAS-RN: 142-68-7
Group No.: 46-014
Molar Mass: 86.13

Table 46.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
64MOE/THO	297.6–327.5	4 S	0.50	not specified		*p*	BSIO	64MOE/THO
76CON/GIA	298.1	1	nosp	not specified		*p*	BDCT	76CON/GIA
84ING/GRO	298.1	1	0.30	99.	chrom	*p*	FSIT	71PIC/LED
88ING	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
99BRO/CAL	298.1	1	nosp	99.	chrom	*p*	FSIT	71PIC/LED

Name: Dibenzofuran
Formula: $C_{12}H_8O$

CAS-RN: 132-64-9
Group No.: 46-026
Molar Mass: 168.19

Table 46.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
90CHI/GAM	362.0–520.3	17	0.10	99.955	melpt	sat	BSAO	47HUF
90CHI/GAM	400.0–720.0	17	1.00	99.955	melpt	sat	BDHT	89KNI/ARC
95FUJ/FUJ	361.1–375.7	5	0.30	99.93	melpt	sat	BSAO	93FUJ/OGU1

Name: Tetrahydro-d_4-furan-d_4
Formula: C_4D_8O

CAS-RN: 1693-74-9
Group No.: 46-027
Molar Mass: 80.16

Table 46.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95KUL/LEB	171.9–320.4	43	0.20	99.52	melpt	*p*	BSAO	76LEB/LIT

Table 46.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	43	43	3.671	1.13−1	0.73	1.53−3	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
171.9–320.4		2.46267	1.26294+1	−5.07995	8.48634−1		IV

Name: 2,5-Dimethylfuran
Formula: C_6H_8O

CAS-RN: 625-86-5
Group No.: 46-028
Molar Mass: 96.13

Table 46.28.1. Experimental heat capacities

Reference	Temp. range K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98VER/WEL	298.15	1.550	nosp	100.0	chrom	p	BDHT	69PER/COM

Name: 2,5-Dihydrobenzo-3,4-furan
Formula: C_8H_8O

CAS-RN: 496-14-0
Group No.: 46-029
Molar Mass: 120.15

Table 46.29.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93STE/CHI2	N	300.0–620.0	17	1.00	99.95	chrom	sat	BDHT	89KNI/ARC
93STE/CHI2	same data in 96STE/CHI2								

Table 46.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	17	17	0.212	6.95–2	0.21	2.37–4	−1
sat	17	17	0.152	4.69–2	0.15	1.16–4	−1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
300.0–620.0		6.64717	7.09333	−7.71325−1	6.74175−2		IV
300.0–620.0		1.08190+1	3.88489	3.92652−2	6.74175−2		IV

Table 46.29.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	17	17	0.180	5.85–2	0.18	7.38–5	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–620.0	700.00	−1.32136	1.66608−2	1.08467+1	2.61990+1	IV

Name: 2-(1,1-Dimethylethyl)furan
Formula: $C_8H_{12}O$

CAS-RN: 7040-43-9
Group No.: 46-030
Molar Mass: 124.18

Table 46.30.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98VER/WEL	298.15	2.220	nosp	99.91	chrom	*p*	BDHT	69PER/COM

Name: 2,5-Bis(1,1-dimethylethyl)furan
Formula: $C_{12}H_{20}O$

CAS-RN: 4789-40-6
Group No.: 46-031
Molar Mass: 180.29

Table 46.31.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98VER/WEL	298.15	2.210	nosp	99.91	chrom	*p*	BDHT	69PER/COM

Name: 2(3*H*)-Dihydrofuranone
Formula: $C_4H_6O_2$

CAS-RN: 96-48-0
Group No.: 47-006
Molar Mass: 86.09

Table 47.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
79FUC		298.1	1	0.50	99.	chrom	*p*	BSIO	80FUC
83LEB/EVS	N	232.5–328.6	28	0.30	99.83	melpt	*p*	BSAO	76LEB/LIT
88ISM/GAB		290.0–410.0	14 S	2.00	not specified		*p*	BDCT	86MER/BEN
89STE/CHI3		298.1	1	1.00	99.98	chrom	*p*	BDHT	89KNI/ARC

83LEB/EVS same data in 79EVS/LEB1 and smoothed data in 80EVS/LEB

Table 47.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
79FUC	298.1	1	0.50	0.038	3.26–3	0.02	3.26–3	1
83LEB/EVS	232.5–328.6	28	0.30	0.455	2.29–2	0.14	7.80–4	−2
88ISM/GAB	290.0–410.0	14	2.00	0.212	7.67–2	0.42	−6.70–2	−12
Rejected data								
89STE/CHI3	(1.68+1,49.69,1.68+1,1)							

Table 47.6.3. Parameters of regression polynomial

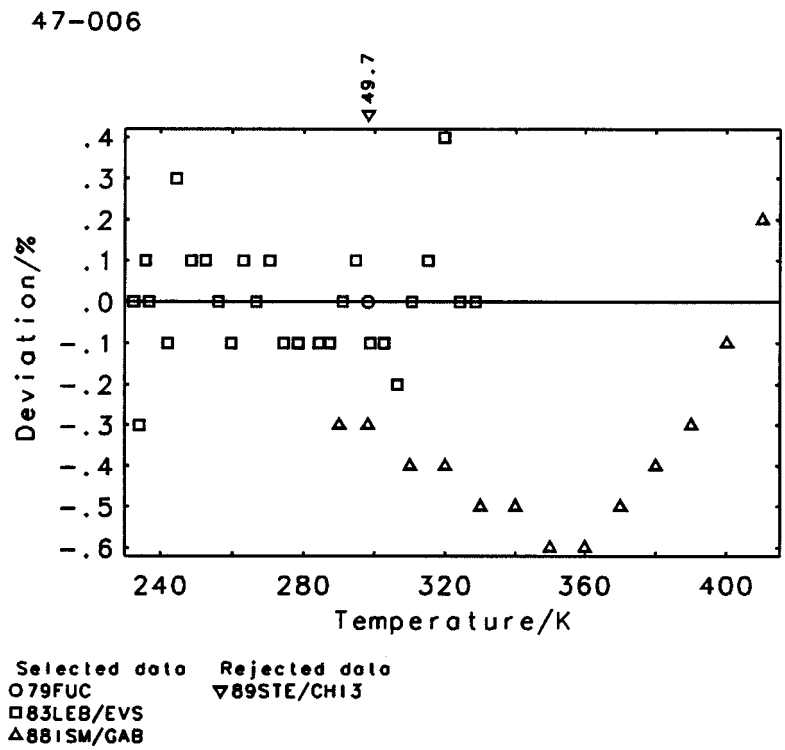
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	44	43	0.406	4.98–2	0.28	−2.12–2	−13

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
232.5–410.0	2.26588+1	−9.01216	3.34748	−3.22327−1	II

Table 47.6.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
total	used						
p	44	43	0.751	5.69−2	0.31	−8.93−4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
232.5–410.0	730.00	−3.14046	3.32605	9.39934	7.41304−1	III



Name: 4-Methyl-1,3-dioxolan-2-one
Formula: $C_4H_6O_3$

CAS-RN: 108-32-7
Group No.: 47-007
Molar Mass: 102.09

Table 47.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
58PEP		323.1	1	nosp	not specified		p	not specified	
76MAS/PET	N	235.5–325.8	13	5.00	not specified		p	BDHT	66PER/COM
76VAS/KOR	N	226.7–416.3	93	nosp	99.32	melpt	p	BSAO	77KU/COM
91WIL/JIM		298.1	1	nosp	99.	anal	p	FSIT	71PIC/LED
93ANG/BOE	N	229.0	1	nosp	99.	anal	p	BDHT	69PER/COM
94FUJ/OGU		222.1–300.9	37	0.30	99.974	melpt	sat	BSAO	93FUJ/OGU1
97RIG/COM		288.1–313.1	3	1.00	99.7	chrom	p	BDHT	95DIO/MAN

76MAS/PET data from a graph only
76VAS/KOR smoothed data in 74VAS/KOR
93ANG/BOE data from a graph only

Table 47.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
76VAS/KOR	226.7–416.3	93	1.00 #	0.597	1.26–1	0.60	4.42–2	42
94FUJ/OGU	222.1–300.9	37	0.30	0.306	1.82–2	0.09	−9.63–3	−17
			Rejected data					
58PEP	(1.46,6.58,1.46,1)		76MAS/PET	(2.42,10.48,2.26,13)				
91WIL/JIM	(5.32–1,2.73,−5.32–1,−1)		93ANG/BOE	(3.76–1,2.03,−3.76–1,−1)				
97RIG/COM	(1.67–1,0.83,1.65–-1,3)							

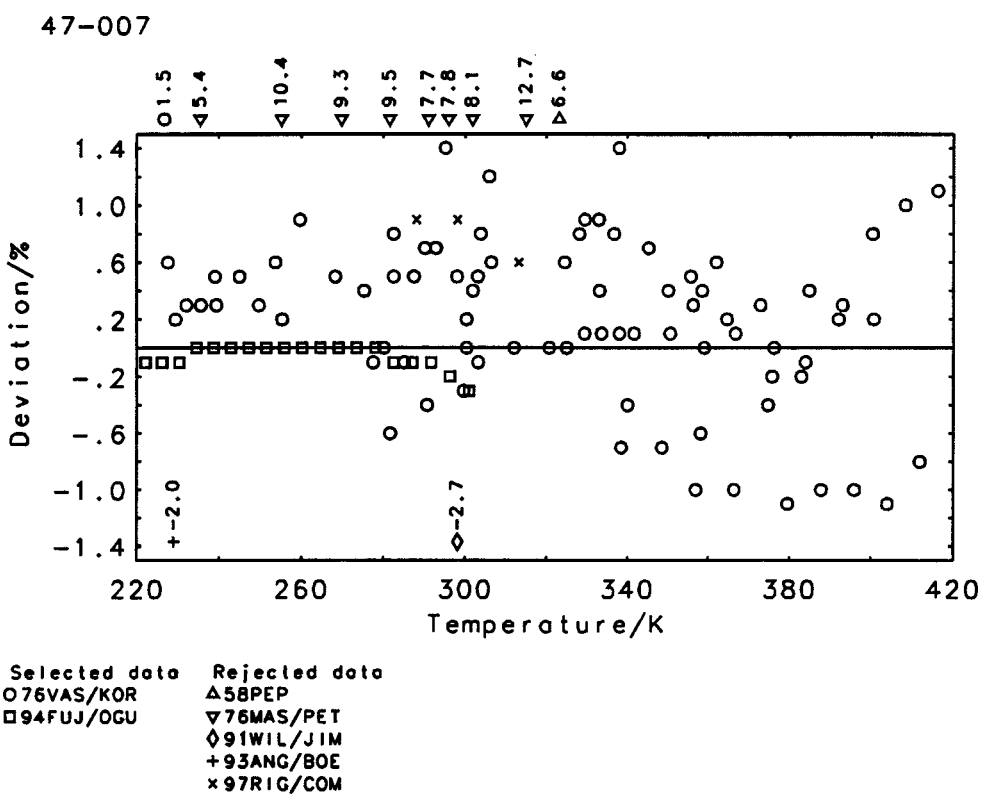
Table 47.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	149	130	0.539	1.09–1	0.52	2.89–2	25
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
222.1–416.3		2.86994+1	−1.11544+1	3.77458	−3.37408−1		III

Table 47.7.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
C	149	130	0.876	1.09–1	0.52	−6.05–3	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
222.1–416.3	779.00	2.13236+2	1.99823+1	−2.05453	1.93867+2	7.43416+1	1.35532+2	IV



Name: 2-Ethoxyethanol
Formula: $C_4H_{10}O_2$

CAS-RN: 110-80-5
Group No.: 47-008
Molar Mass: 90.12

Table 47.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		*p*	not specified	
73KUS/SUU		298.1	1	0.10	not specified		*p*	DDCT	71KON/SUU
78ROU/PER2		283.1–313.1	3	nosp	99.	chrom	*p*	FSIT	71PIC/LED
89COB/GAR		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
91SVO/ZAB2		300.6–328.3	7	0.50	99.95	chrom	*p*	BSAO	91SVO/ZAB1
98TAM/TAB		298.1–303.1	2	nosp	99.98	chrom	*p*	FSIO	85OGA/MUR

52CUR/JOH technical product, purity in question

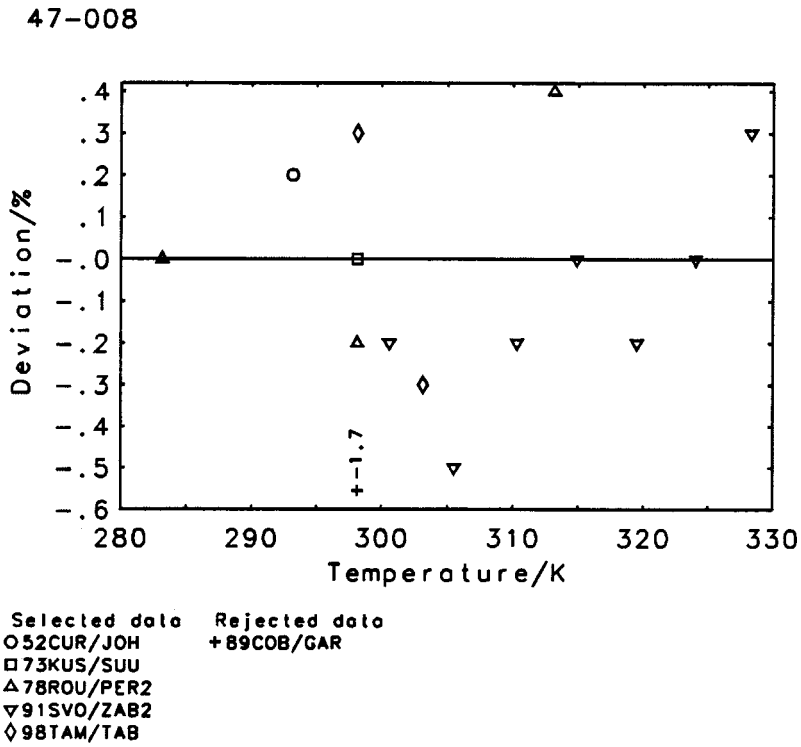
Table 47.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
Selected data								
52CUR/JOH	293.1	1	1.00 #	0.190	4.77–2	0.19	4.77–2	1
73KUS/SUU	298.1	1	0.10	0.206	5.23–3	0.02	5.23–3	1
78ROU/PER2	283.1–313.1	3	0.50 #	0.499	6.47–2	0.25	1.73–2	1
91SVO/ZAB2	300.6–328.3	7	0.50	0.503	6.51–2	0.25	−2.64–2	−1
98TAM/TAB	298.1–303.1	2	0.30 #	0.975	7.45–2	0.29	−6.91–4	0
Rejected data								
89COB/GAR	(4.26–1,1.71,−4.26–1,−1)							

Table 47.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	15	14	0.612	6.81–2	0.26	−5.81–3	2

Temp. range K	A_1	A_2	Level of uncertainty
283.1–328.3	1.18757+1	4.51866	III



Name: 2,2′-Oxybisethanol
Formula: $C_4H_{10}O_3$

CAS-RN: 111-46-6
Group No.: 47-009
Molar Mass: 106.12

Table 47.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		*p*	not specified	
59DEA/EVA	N	303.1–473.1	3 S	nosp	not specified		*p*	not specified	
79STE/TAM		273.1–513.2	14 S	nosp	99.9	chrom	sat	BDHT	69PER/COM
82ZAR		298.0–363.0	3	0.60	99.5	chrom	*p*	BDCT	82ZAR
88MUK/ZAR		300.5–422.3	6	nosp	not specified		*p*	BDCT	82ZAR

52CUR/JOH technical product, purity in question
59DEA/EVA data of firm Shell Development Company Emeryville, Calif.

Table 47.9.2. Correlated heat capacities

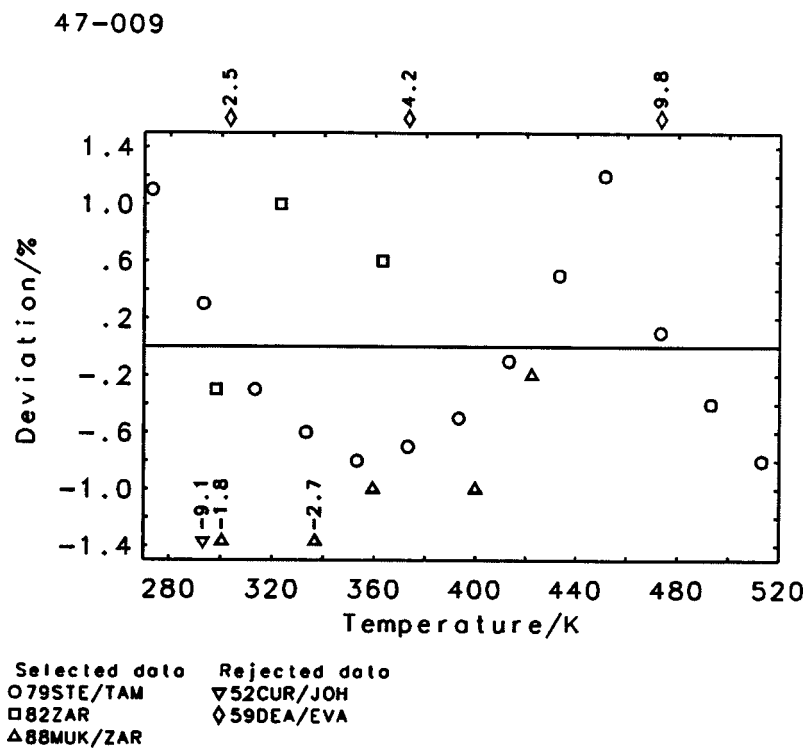
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
79STE/TAM	273.1–513.2	14	1.00 #	0.706	2.42–1	0.71	1.04–3	−2
82ZAR	298.0–363.0	3	0.60	1.198	2.27–1	0.72	1.53–1	1
88MUK/ZAR	300.5–422.3	6	1.50 #	1.083	4.94–1	1.63	−4.36–1	−6
Rejected data								
52CUR/JOH	(2.42,9.08,−2.42,−1)		59DEA/EVA	(2.52,6.33,2.09,3)				

Table 47.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	27	23	0.957	3.49–1	1.10	−9.33–2	−7
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.1–513.2		5.48991	1.03054+1	−7.64956−1			IV

Table 47.9.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	27	23	1.056	3.22–1	0.99	6.80–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
273.1–513.2	760.00	2.27848+1	1.76410	8.89494	7.35714+1		IV



Name: 2-Furancarboxaldehyde
Formula: $C_5H_4O_2$

CAS-RN: 98-01-1
Group No.: 47-010
Molar Mass: 96.09

Table 47.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		317.5–370.7	3 S	nosp	not specified		avg	DSIO	*81VON
34MIL	N	256.0–267.9	2	nosp	not specified		avg	BSIO	20GIB/LAT
47BUE/BOA	N	288.7–422.0	7	nosp	not specified		*p*	not specified	
62OME2		288.6–422.0	6	nosp	not specified		*p*	not specified	
67RAS/GAN		293.1–373.1	5 S	0.50	not specified		*p*	BSAO	67RAS/GAN

34MIL average values in temperature ranges 240–272 K and 262–274 K
47BUE/BOA data from Quaker Oats Co., Tech. Div., ‘‘Furfural as a Selective Solvent’’ (1940)

Table 47.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*81VON	317.5–370.7	3	2.00 #	0.550	2.29–1	1.10	1.68–1	1
47BUE/BOA	288.7–422.0	7	2.00 #	0.744	3.23–1	1.49	2.77–1	5
67RAS/GAN	293.1–373.1	5	0.50	1.192	1.22–1	0.60	−2.79-2	−1
Rejected data								
62OME2	(6.80–1,2.90,5.07–1,5)							

Table 47.10.3. Parameters of regression polynomial

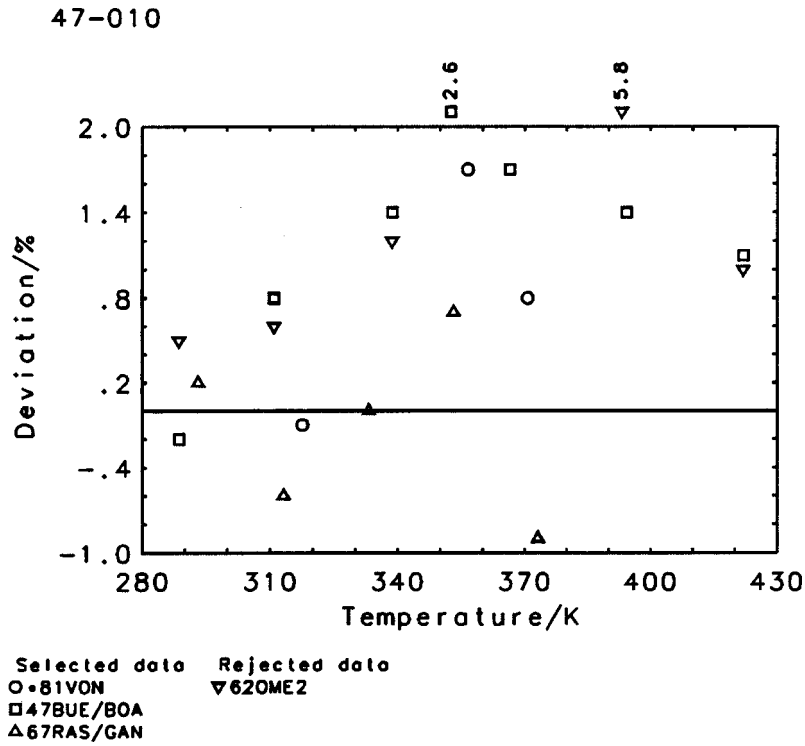
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	23	15	1.040	2.96–1	1.38	1.54–1	5

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
288.7–422.0	−2.81207+2	2.70728+2	−8.14232+1	8.19410	V

Table 47.10.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	23	15	1.419	2.89–1	1.42	7.94-2	5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
288.7–422.0	670.00	6.39332+3	9.29674+2	−9.63048+2	5.89198+3	9.30916+2	3.01129+3	V



Name: 2-Methoxyethanol acetate
Formula: $C_5H_{10}O_3$

CAS-RN: 110-49-6
Group No.: 47-014
Molar Mass: 118.13

Table 47.14.1. Experimental heat capacities

Reference		Temp range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
52CUR/JOH		303.1	1	nosp	not specified		*p*	not specified	
80CAL/MAR	N	359.0–409.0	eqn	nosp	not specified		*p*	DSIO	71MAR/CIO
97HOV/ROU		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

80CAL/MAR equation calculated from temperature dependence of enthalpy by the authors

Table 47.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
97HOV/ROU	298.1	1	0.50 #	0.000	0.00	0.00	0.00	0

Table 47.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	7	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	2.81376+1	IV

Name: 2-(1-Methylethoxy)ethanol
Formula: $C_5H_{12}O_2$

CAS-RN: 109-59-1
Group No.: 47-015
Molar Mass: 104.15

Table 47.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
73KUS/SUU	298.1	1	0.10	not specified		*p*	DDCT	71KON/SUU
99TAM/OSA	298.1	1	nosp	99.95	chrom	*p*	FSIO	85OGA/MUR

Table 47.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
73KUS/SUU	298.1	1	0.10	0.316	9.09–3	0.03	−9.09–3	−1
99TAM/OSA	298.1	1	0.30 #	0.952	8.23–2	0.29	8.23-2	1

Table 47.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	2	2	1.004	8.28–2	0.29	3.66–2	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	2.87300+1	III

Name: 2-Propoxyethanol
Formula: $C_5H_{12}O_2$

CAS-RN: 2807-30-9
Group No.: 47-016
Molar Mass: 104.15

Table 47.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
73KUS/SUU	298.1	1	0.10	not specified		*p*	DDCT	71KON/SUU
78ROU/PER2	298.1	1	nosp	99.	chrom	*p*	FSIT	71PIC/LED
91SVO/ZAB2	300.6–328.3	7	0.50	99.95	chrom	*p*	BSAO	91SVO/ZAB1
99TAM/OSA	298.1	1	nosp	99.95	chrom	*p*	FSIO	85OGA/MUR

Name: Ethyl ester 3-oxobutanoic acid
Formula: $C_6H_{10}O_3$

CAS-RN: 141-97-9
Group No.: 47-020
Molar Mass: 130.14

Table 47.20.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON		315.7–376.2	5 S	nosp	not specified		avg	DSIO	*81VON
34KOL/UDO	N	297.5	1	nosp	not specified		*p*	BSIT	34KOL/UDO
97HOV/ROU		298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED

34KOL/UDO same datum in 33KOL/UDO

Table 47.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*81VON	315.7–376.2	5	3.00 #	0.443	3.99–1	1.33	−1.28–1	−1
97HOV/ROU	298.1	1	0.50 #	0.128	1.94–2	0.06	1.94–2	1

Table 47.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	7	6	0.500	4.46–1	1.49	−1.04–1	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–376.2	2.27999+1	2.48405	V

Name: 2-Ethoxyethanol acetate
Formula: $C_6H_{12}O_3$

CAS-RN: 111-15-9
Group No.: 47-022
Molar Mass: 132.16

Table 47.22.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
52CUR/JOH		293.1	1	nosp	not specified		p	not specified	
80CAL/MAR	N	354.0–418.0	eqn	nosp	not specified		p	DSIO	71MAR/CIO
96STE/CHI1		300.0–600.0	16 S	1.00	99.95	chrom	sat	BDHT	89KNI/ARC
97HOV/ROU		298.1	1	nosp	99.	anal	p	FSIT	71PIC/LED

80CAL/MAR equation calculated from temperature dependence of enthalpy by the authors

Table 47.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
96STE/CHI1	300.0–600.0	16	1.00	0.676	2.75–1	0.68	−3.38–2	−2
97HOV/ROU	298.1	1	1.00 #	1.984	6.43–1	1.98	6.43–1	1
Rejected data								
80CAL/MAR	(3.52–1,1.06,−2.66–1,−3)							

Table 47.22.3. Parameters of cubic spline polynomials

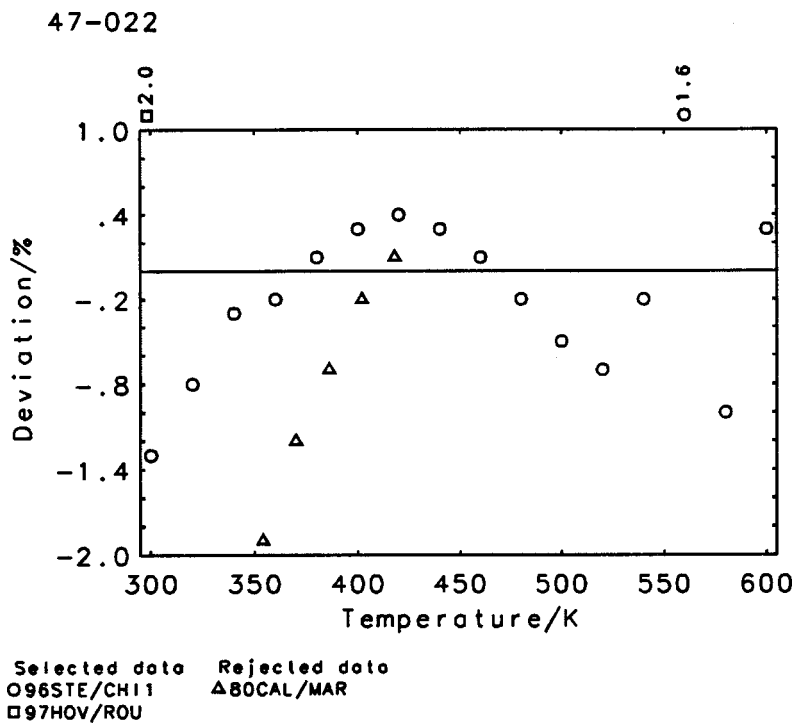
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	23	17	0.968	3.68–1	0.97	6.00–3	−1
sat	23	17	0.837	2.92–1	0.84	3.61–3	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
298.1–550.0	2.00707+1	6.05745	−1.14721	1.44555−1	IV
550.0–600.0	−2.91992+4	1.59439+4	−2.89893+3	1.75768+2	V
298.1–550.0	2.68077+1	4.30666−1	4.05552−1	2.84452−3	IV
550.0–600.0	−1.85087+4	1.01107+4	−1.83782+3	1.11411+2	V

Table 47.22.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	23	17	0.857	2.88−1	0.86	−1.11−2	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
298.1–600.0	611.00	−1.24875	4.93364−1	1.54174+1	4.21175+1	−2.97869+1	8.43815	IV



Name: 2-Butoxyethanol
Formula: $C_6H_{14}O_2$

CAS-RN: 111-76-2
Group No.: 47-023
Molar Mass: 118.18

Table 47.23.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		p	not specified	
59ONK		298.1–373.1	16 S	nosp	not specified		p	BSAO	59ONK
73KUS/SUU		298.1	1	0.10	not specified		p	DDCT	71KON/SUU
78ROU/PER2		277.1–328.1	5	nosp	99.	chrom	p	FSIT	71PIC/LED
89COB/GAR		298.1	1	nosp	98.	anal	p	FSIT	71PIC/LED
99TAM/OSA		298.1	1	nosp	99.88	chrom	p	FSIO	85OGA/MUR

52CUR/JOH technical product, purity in question

Name: 2-(2-Ethoxyethoxy)ethanol
Formula: $C_6H_{14}O_3$

CAS-RN: 111-90-0
Group No.: 47-024
Molar Mass: 134.18

Table 47.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		*p*	not specified	
87COB		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED
89COB/GAR		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED

52CUR/JOH technical product, purity in question

Table 47.24.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
87COB	298.1	1	0.50 #	0.289	5.19−2	0.14	5.19−2	1
89COB/GAR	298.1	1	0.50 #	0.289	5.16−2	0.14	−5.16−2	−1

Table 47.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	2	0.409	7.31−2	0.20	1.51−4	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	3.58011+1	IV

Name: 2,2′-[1,2-Ethanediylbis(oxy)]bisethanol
Formula: $C_6H_{14}O_4$

CAS-RN: 112-27-6
Group No.: 47-025
Molar Mass: 150.17

Table 47.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		*p*	not specified	
79STE/TAM		273.1–533.2	15 S	nosp	99.9	chrom	sat	BDHT	69PER/COM
82ZAR		298.0–363.0	3	0.60	98.5	chrom	*p*	BDCT	82ZAR

52CUR/JOH technical product, purity in question

Name: 2-(2-Butoxyethoxy)ethanol
Formula: $C_8H_{18}O_3$

CAS-RN: 112-34-5
Group No.: 47-033
Molar Mass: 162.23

Table 47.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		*p*	not specified	
87COB	N	298.1	1	nosp	99.	anal	*p*	FSIT	71PIC/LED
87COB/CAS		298.1	1	nosp	98.	anal	*p*	FSIT	71PIC/LED

52CUR/JOH technical product, purity in question
87COB misprint in the name of substance; instead of 2-(2-Ethoxybutoxy). should be 2-(2-Butoxyethoxy)ethanol

Table 47.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
87COB/CAS	298.1	1	0.50 #	0.979	2.09–1	0.49	−2.09–1	−1
87COB	298.1	1	0.50 #	0.989	2.13–1	0.49	2.13–1	1

Table 47.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	3	2	1.392	2.99–1	0.70	2.08–3	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	4.28922+1	IV

Name: 2,2′-[Oxybis(2,1-ethanediyloxy)]bisethanol
Formula: $C_8H_{18}O_5$

CAS-RN: 112-60-7
Group No.: 47-034
Molar Mass: 194.23

Table 47.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
79STE/TAM	273.1–533.2	14 S	nosp	99.9	chrom	sat	BDHT	69PER/COM
82ZAR	298.0–363.0	3	0.60	99.9	chrom	p	BDCT	82ZAR

Name: (Phenoxymethyl)oxirane
Formula: $C_9H_{10}O_2$

CAS-RN: 122-60-1
Group No.: 47-036
Molar Mass: 150.18

Table 47.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
87LES/LIC	240.0–390.0	eqn	2.00	99.	estim	p	BDHT	69PER/COM
88LEB/BYK	276.8–330.0	4 S	0.30	99.3	melpt	p	BSAO	76LEB/LIT
97STE/CHI1	290.0–520.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 47.36.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
88LEB/BYK	276.8–330.0	4	0.30	0.756	758–2	0.23	5.38–3	0
97STE/CHI1	290.0–520.0	24	1.00	0.117	3.97–2	0.12	−9.23–3	2
Rejected data								
87LES/LIC	(4.80–1,1.38,−1.14–1,−2)							

Table 47.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	44	28	0.324	4.93−2	0.15	−7.15−3	2
sat	44	28	0.325	5.06−2	0.15	−6.89−3	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
276.8–520.0	2.58169+1	1.44429	3.39970−1	IV
276.8–520.0	2.57231+1	1.50020	3.31793−1	IV

Table 47.36.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	44	28	0.361	5.98−2	0.17	−1.97−2	−5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
276.8–520.0	720.00	−4.52410	2.87529−1	2.28641+1	1.77961+1	IV

Name: Methyl ester hydroxyacetic acid
Formula: $C_3H_6O_3$

CAS-RN: 96-35-5
Group No.: 47-052
Molar Mass: 90.08

Table 47.52.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96STE/CHI3	315.0–375.0	4	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 47.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	4	4	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
315.0–375.0	1.75996+1	1.99996	IV

Name: 1,2-Ethanediol monoacetate
Formula: $C_4H_8O_3$

CAS-RN: 542-59-6
Group No.: 47-053
Molar Mass: 104.11

Table 47.53.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
80CAL/MAR	N	359.0–415.0	eqn	nosp	not specified		*p*	DSIO	71MAR/CIO

80CAL/MAR equation calculated from temperature dependence of enthalpy by the authors; suspect values

Name: Methyl ester methoxyacetic acid
Formula: $C_4H_8O_3$

CAS-RN: 6290-49-9
Group No.: 47-054
Molar Mass: 104.11

Table 47.54.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97HOV/ROU	298.15	1.962	nosp	99.	chrom	*p*	FSIT	71PIC/LED

Name: Methyl ester 3-oxobutanoic acid
Formula: $C_5H_8O_3$

CAS-RN: 105-45-3
Group No.: 47-055
Molar Mass: 116.12

Table 47.55.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97HOV/ROU	298.15	1.921	nosp	99.	chrom	*p*	FSIT	71PIC/LED

Name: (3*S*,6*S*)-3,6-Dimethyl-1,4-dioxane-2,5-dione
Formula: $C_6H_8O_4$

CAS-RN: 4511-42-6
Group No.: 47-056
Molar Mass: 144.13

Table 47.56.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99LEB/KUL1	N	368.3–438.9	22	1.50	not specified		*p*	BDHT	69YAG

99LEB/KUL1 data below 391 K rejected from correlation; sharp maximum

Table 47.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	22	14	1.385	1.02	2.08	3.92–2	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
394.9–438.9		7.73774+4	−5.45080+4	1.28031+4	−1.00223+3		V

Name: 2-(2-Methylpropoxy)ethanol
Formula: $C_6H_{14}O_2$

CAS-RN: 4439-24-1
Group No.: 47-057
Molar Mass: 118.18

Table 47.57.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93PER/QUI	N	283.7–298.4	4	nosp	not specified		*p*	FSIT	71PIC/LED
93PER/QUI	N	288.6–298.4	3	nosp	not specified		*p*	FSIT	71PIC/LED
99TAM/OSA		298.1	1	nosp	99.95	chrom	*p*	FSIO	85OGA/MUR

93PER/QUI measured on 10 mW scale
93PER/QUI measured on 30 mW scale

Table 47.57.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93PER/QUI	283.7–298.4	4	0.50 #	1.143	1.96–1	0.57	−7.74–2	0
93PER/QUI	288.6–298.4	3	0.50 #	0.702	1.23–1	0.35	1.07–1	3
Rejected data								
99TAM/OSA	(1.74,5.20,−1.74,−1)							

Table 47.57.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	8	7	1.158	1.99–1	0.58	1.66–3	3

Temp. range K	A_1	A_2	Level of uncertainty
283.7–298.4	1.29369+1	7.48574	V

Name: 2-(2-Hydroxypropoxy)-1-propanol
Formula: $C_6H_{14}O_3$

CAS-RN: 106-62-7
Group No.: 47-058
Molar Mass: 134.18

Table 47.58.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
82ZAR	298.0–363.0	3	0.60	99.32	chrom	p	BDCT	82ZAR

Table 47.58.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	3	3	0.256	6.24–2	0.15	1.27–4	1

Temp. range K	A_1	A_2	Level of uncertainty
298.0–363.0	1.54605+1	7.80443	V

Name: 2-Hydroxyethyl ester 2,2-dimethylpropanoic acid
Formula: $C_7H_{14}O_3$

CAS-RN: 20267-19-0
Group No.: 47-059
Molar Mass: 146.19

Table 47.59.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
82BIR/SIK	270.0–370.0	eqn	1.00	99.	chrom	p	BDHT	69PER/COM

Table 47.59.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	10	10	0.000	4.99−6	0.00	−3.05−6	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
270.0–369.9	1.89917	1.60803+1	−1.43964	V

Name: 2-(2-Propoxyethoxy)ethanol
Formula: $C_7H_{16}O_3$

CAS-RN: 6881-94-3
Group No.: 47-060
Molar Mass: 148.20

Table 47.60.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96STE/CHI1	300.0–540.0	13 S	1.00	99.9	chrom	sat	BDHT	89KNI/ARC

Table 47.60.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	13	13	0.083	3.82−2	0.08	3.70−5	1
sat	13	13	0.087	4.01−2	0.09	4.20−5	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–540.0	−2.41737	2.20581+1	−3.40807	2.16376−1	IV
300.0–540.0	−8.38939−1	2.07506+1	−3.05009	1.83967−1	IV

Table 47.60.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	13	13	0.096	4.40−2	0.10	4.99−5	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
300.0–540.0	680.00	2.46071−2	4.61056−1	1.65552	1.24040+2	−1.09976+2	3.67219+1	IV

Name: α-Oxobenzeneacetic acid
Formula: $C_8H_6O_3$

CAS-RN: 611-73-4
Group No.: 47-061
Molar Mass: 150.13

Table 47.61.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91STE/CHI2	355.0–415.0	4	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 47.61.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	4	4	0.159	5.37−2	0.16	1.06−4	0
Temp. range K		A_1	A_2				Level of uncertainty
355.0−415.0		1.78265+1	4.06757				IV

Name: Bis(1,1-dimethylethyl) peroxide
Formula: $C_8H_{18}O_2$

CAS-RN: 110-05-4
Group No.: 47-062
Molar Mass: 146.23

Table 47.62.1. Experimental heat capacities

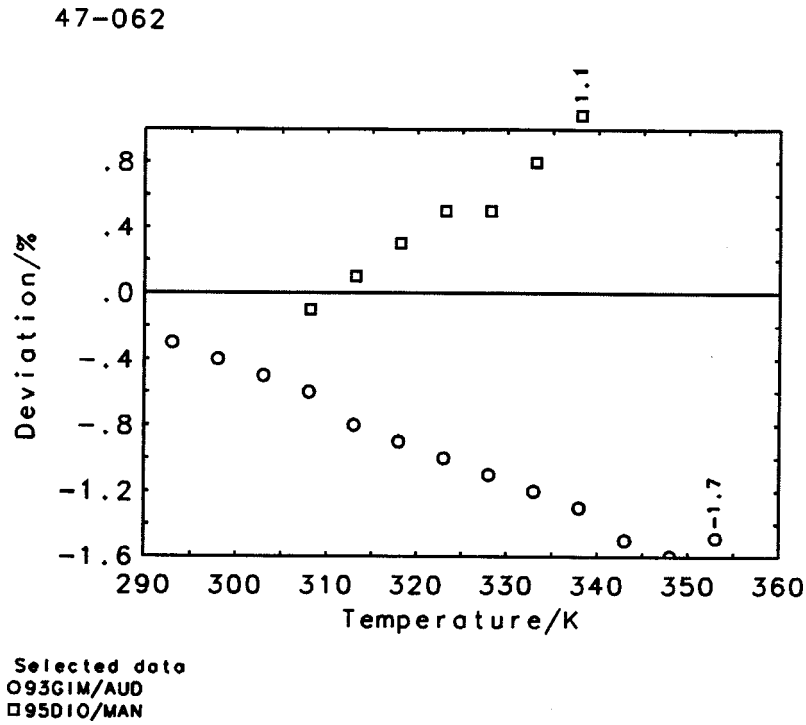
Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93GIM/AUD	293.0−353.0	eqn	nosp	98.	anal	*p*	BDHT	93GIM/AUD
95DIO/MAN	308.1−338.1	7	nosp	99.54	chrom	*p*	BDHT	95DIO/MAN

Table 47.62.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93GIM/AUD	293.0−353.0	13	2.00 #	0.539	4.04−1	1.08	−3.67−1	−13
95DIO/MAN	308.1−338.1	7	1.00 #	0.597	2.28−1	0.60	1.77−1	5

Table 47.62.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	20	20	0.590	3.72−1	0.99	−1.76−1	−8
Temp. range K		A_1	A_2				Level of uncertainty
293.0−353.0		1.85233+1	5.78440				V



Name: 2-(2′-Hydroxyethoxy)ethyl ester 2,2-dimethylpropanoic acid
Formula: $C_9H_{18}O_4$

CAS-RN: 20267-21-4
Group No.: 47-063
Molar Mass: 190.24

Table 47.63.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
82BIR/SIK	N	270.0–370.0	eqn	1.00	99.	chrom	*p*	BDHT	69PER/COM

82BIR/SIK an error in correlating equation that gives negative C_p over entire temperature range

Name: 1,1′-[(1-Methyl-1,2-ethanediyl)bis(oxy)]bis-2-propanol
Formula: $C_9H_{20}O_4$

CAS-RN: 1638-16-0
Group No.: 47-064
Molar Mass: 192.26

Table 47.64.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
82ZAR	298.0–363.0	3	0.60	99.72	chrom	*p*	BDCT	82ZAR

Table 47.64.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	3	3	0.004	1.44−3	0.00	1.27−6	0

Temp. range K	A_1	A_2	Level of uncertainty
298.0–363.0	3.00982+1	7.68416	V

Name: 1,1-Dimethylethyl ester benzenecarboperoxoic acid
Formula: $C_{11}H_{14}O_3$

CAS-RN: 614-45-9
Group No.: 47-065
Molar Mass: 194.23

Table 47.65.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93GIM/AUD	293.0–353.0	eqn	nosp	98.	anal	*p*	BDHT	93GIM/AUD

Table 47.65.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	6	6	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
293.0–353.0	2.40612+1	4.97577	V

Name: 2-[2-[2-(2-Hydroxypropoxy)propoxy]propoxy]-1-propanol
Formula: $C_{12}H_{26}O_5$

CAS-RN: 24800-25-7
Group No.: 47-066
Molar Mass: 250.34

Table 47.66.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
82ZAR	298.0–363.0	3	0.60	98.8	chrom	*p*	BDCT	82ZAR

Table 47.66.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	3	0.601	2.52−1	0.36	7.78−4	1

Temp. range K	A_1	A_2	Level of uncertainty
298.0–363.0	3.39818+1	1.11589+1	V

Name: 3,6,9,12,15-Pentaoxaheptadecane-1,17-diol
Formula: $C_{12}H_{26}O_7$

CAS-RN: 2615-15-8
Group No.: 47-067
Molar Mass: 282.33

Table 47.67.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
82ZAR	298.0–363.0	3	0.60	98.7	chrom	*p*	BDCT	82ZAR

Table 47.67.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	3	1.087	4.95−1	0.65	2.29−3	1

Temp. range K	A_1	A_2	Level of uncertainty
298.0–363.0	5.17517+1	7.57702	V

Name: 2,5,8,11-Tetramethyl-3,6,9,12-tetraoxapentadecane-1,14-diol
Formula: $C_{15}H_{32}O_6$

CAS-RN: 21482-12-2
Group No.: 47-068
Molar Mass: 308.42

Table 47.68.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
82ZAR	298.0–363.0	3	0.60	98.20	chrom	*p*	BDCT	82ZAR

Table 47.68.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	3	1.281	6.55−1	0.77	3.81−3	1

Temp. range K	A_1	A_2	Level of uncertainty
298.0–363.0	4.16885+1	1.35787+1	V

Name: 2,5,8,11,14-Pentamethyl-3,6,9,12,15-pentaoxaoctadecane
Formula: $C_{18}H_{38}O_7$

CAS-RN: 74388-92-4
Group No.: 47-069
Molar Mass: 366.50

Table 47.69.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
82ZAR	298.0–363.0	3	0.60	98.73	chrom	*p*	BDCT	82ZAR

Table 47.69.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	3	1.616	9.76−1	0.97	7.18−3	1

Temp. range K	A_1	A_2	Level of uncertainty
298.0–363.0	4.24512+1	1.81884+1	V

Name: 3,6,9,12,15-Pentaoxapentacosan-1-ol
Formula: $C_{20}H_{42}O_6$

CAS-RN: 23244-49-7
Group No.: 47-070
Molar Mass: 378.55

Table 47.70.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94JHA/AHL	298.15	2.171	nosp	99.	chrom	*p*	BDCT	89BRE/LIC

Name: 3,6,9,12,15-Pentaoxaheptacosan-1-ol
Formula: $C_{22}H_{46}O_6$

CAS-RN: 3055-95-6
Group No.: 47-071
Molar Mass: 406.60

Table 47.71.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
83OLO	298.1	1	nosp	98.	chrom	*p*	DDCT	74SUU/WAD
94JHA/AHL	298.1	1	nosp	99.	chrom	*p*	BDCT	89BRE/LIC

Table 47.71.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	±
			Selected data					
83OLO	298.1	1	0.70 #	0.162	1.20–1	0.11	−1.20–1	−1
94JHA/AHL	298.1	1	0.70 #	0.162	1.20–1	0.11	1.20–1	1

Table 47.71.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.229	1.70–1	0.16	2.75–4	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	1.06079+2	IV

Name: 3,6,9,12,15,18-Hexaoxaoctacosan-1-ol
Formula: $C_{22}H_{46}O_7$

CAS-RN: 5168-89-8
Group No.: 47-072
Molar Mass: 422.60

Table 47.72.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94JHA/AHL	298.15	2.172	nosp	99.	chrom	p	BDCT	89BRE/LIC

Name: 3,6,9,12,15,18-Hexaoxatriacontan-1-ol
Formula: $C_{24}H_{50}O_7$

CAS-RN: 3055-96-7
Group No.: 47-073
Molar Mass: 450.66

Table 47.73.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94JHA/AHL	298.15	2.179	nosp	99.	chrom	p	BDCT	89BRE/LIC

Name: 4-(Octadecyloxy)benzoic acid
Formula: $C_{25}H_{42}O_3$

CAS-RN: 15872-50-1
Group No.: 47-074
Molar Mass: 390.61

Table 47.74.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
77IKE/HAT	408.0–420.0	7	4.00	not specified		p	BDHT	69PER/COM

Table 47.74.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	7	7	0.113	1.30–1	0.45	−2.39–2	−3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
408.0–420.0	3.88204+5	−2.79651+5	6.71547+4	−5.37536+3	VI

Name: 3,6,9,12,15,18,21,24-Octaoxatetratriacontan-1-ol
Formula: $C_{26}H_{54}O_9$

CAS-RN: 24233-81-6
Group No.: 47-075
Molar Mass: 510.71

Table 47.75.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94JHA/AHL	298.15	2.170	nosp	99.	chrom	*p*	BDCT	89BRE/LIC

Name: 1,1′-Thiobisbenzene
Formula: $C_{12}H_{10}S$

CAS-RN: 139-66-2
Group No.: 51-023
Molar Mass: 186.28

Table 51.23.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
31SMI/AND2		259.8–298.5	4	nosp	97.5	estim	*p*	DSIO	26AND/LYN
95STE/CHI1		239.1–439.5	22	0.10	99.94	melpt	sat	BSAO	88STE/ARC
95STE/CHI1	N	300.0–700.0	21 S	1.00	99.94	melpt	sat	BDHT	89KNI/ARC

95STE/CHI1 in the temperature range 620–700 K values C_{sat} were extrapolated by the authors because of sample decomposition

Table 51.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
95STE/CHI1	239.1–299.9	11	0.10	0.167	5.33–3	0.02	2.06–4	−1
95STE/CHI1	300.0–700.0	21	1.00	0.105	4.53–2	0.10	−1.07–2	−1
			Rejected data					
31SMI/AND2	(2.70–1,0.84,−2.53–1,−4)							

Table 51.23.3. Parameters of cubic spline polynomials

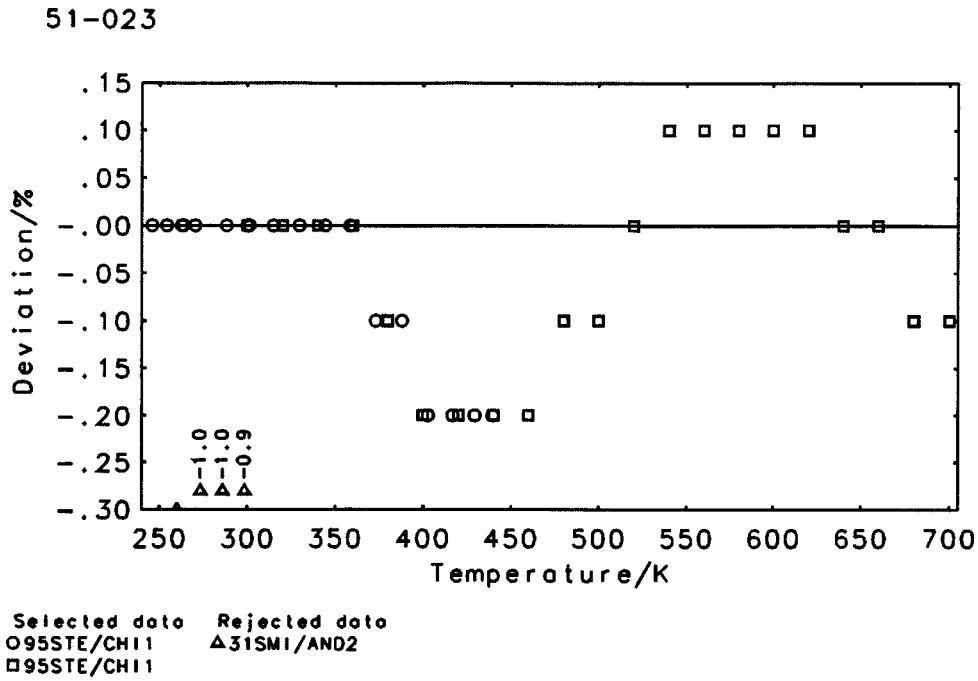
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	47	32	0.141	4.01–2	0.09	−6.93–3	−2
sat	47	32	0.160	4.89–2	0.11	−7.30–3	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
239.1–400.0	3.05649+1	−5.98837	3.09179	−2.75775−1	II
400.0–700.0	6.84680	1.18002+1	−1.35534	9.48198−2	IV
239.1–400.0	3.02139+1	−5.63837	2.97787	−2.63740−1	II
400.0–700.0	9.14835	1.01608+1	−9.71917−1	6.54092−2	IV

Table 51.23.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	47	32	0.645	1.87–1	0.42	3.44–2	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
239.1–700.0	795.00	6.09100	1.10753−1	2.09831+1	3.04703+1	2.04381+1	4.99161	IV



Name: 1,1′-Thiobisoctane
Formula: $C_{16}H_{34}S$

CAS-RN: 2690-08-6
Group No.: 51-026
Molar Mass: 258.51

Table 51.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
82TUT/GAB	273.0–373.0	eqn	0.40	99.7	chrom	*p*	BSAO	62KOL/SER
97STE/CHI4	290.0–550.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 51.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
97STE/CHI4	290.0–550.0	27	1.00	0.004	2.20−3	0.00	1.84−6	1
Rejected data								
82TUT/GAB	(2.18+1,31.42,2.18+1,8)							

Table 51.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	37	27	0.004	2.33−3	0.00	1.84−6	1
sat	37	27	0.000	1.74−6	0.00	−4.24−7	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
290.0–550.0	4.66375+1	−2.83779	9.36382−1	IV
290.0–550.0	4.65500+1	−2.78999	9.29999−1	IV

Table 51.26.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	37	27	0.175	9.11−2	0.17	2.65−4	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
290.0–550.0	780.00	−8.06216	3.12026	3.54628+1	5.20777	IV

Name: 1-Ethylthiooctane
Formula: $C_{10}H_{22}S$

CAS-RN: 3698-94-0
Group No.: 51-029
Molar Mass: 174.35

Table 51.29.1. Experimental heat capacities

Reference	Temp range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96STE/CHI1	300.0–600.0	16 S	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 51.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	16	16	0.064	3.59−2	0.06	4.39−5	0
sat	16	16	0.000	2.50−6	0.00	−1.43−6	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
300.0–600.0	2.10585+1	6.43977	7.23019−2	IV
300.0–600.0	1.99996+1	6.99985	7.23019−2	IV

Table 51.29.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	16	16	0.034	1.85−2	0.03	−4.10−5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–600.0	700.00	−8.06736−1	3.45290−3	2.03654+1	4.71215+1	IV

Name: 1,1′-Thiobiscyclohexane
Formula: $C_{12}H_{22}S$

CAS-RN: 7133-46-2
Group No.: 51-030
Molar Mass: 198.37

Table 51.30.1. Experimental heat capacities

Reference		Temp range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI4	N	290.0–520.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

97STE/CHI4 the original equation gives negative heat capacities; the sign of the 2nd parameter was changed to positive

Table 51.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	24	24	0.004	1.95−3	0.00	9.54−7	0
sat	24	24	0.000	2.20−6	0.00	−1.59−7	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
290.0–520.0	1.38007+1	7.83471	1.89840−1	IV
290.0–520.0	1.37200+1	7.88000	1.83600−1	IV

Table 51.30.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	24	24	0.018	8.74−3	0.02	1.49−5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
290.0–520.0	770.00	−4.53067	8.27716−2	1.24785+1	6.19989+1	IV

Name: 1,1′-[(1-Methylethylidene)bis(thio)]bisbenzene
Formula: $C_{15}H_{16}S_2$

CAS-RN: 14252-46-1
Group No.: 51-031
Molar Mass: 260.42

Table 51.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI1	329.0–420.0	eqn	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 51.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	10	10	0.000	1.91−6	0.00	7.63−7	0

Temp. range K	A_1	A_2	Level of uncertainty
329.0–419.9	2.63600+1	7.20000	IV

Name: 1-Hexanethiol
Formula: $C_6H_{14}S$

CAS-RN: 111-31-9
Group No.: 52-016
Molar Mass: 118.24

Table 52.16.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
66GOO/DEP	N	298.1	1	nosp	99.97	melpt	p	not specified	
70FIN/MCC		200.3–371.9	20	0.20	99.978	melpt	sat	BSAO	47HUF

66GOO/DEP from unpublished measurement of Bureau of Mines, Bartlesville (USA)

Name: 1-Heptanethiol
Formula: $C_7H_{16}S$

CAS-RN: 1639-09-4
Group No.: 52-017
Molar Mass: 132.27

Table 52.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
66GOO/DEP	N	298.1	1	nosp	99.97	melpt	*p*	not specified	
70FIN/MCC		232.1–359.4	16	0.20	99.97	melpt	sat	BSAO	47HUF

66GOO/DEP from unpublished measurement of Bureau of Mines, Bartlesville (USA)

Name: 1-Decanethiol
Formula: $C_{10}H_{22}S$

CAS-RN: 143-10-2
Group No.: 52-018
Molar Mass: 174.35

Table 52.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
66GOO/DEP	N	298.1	1	nosp	99.88	melpt	*p*	not specified	
70FIN/MCC		255.1–375.2	30	0.20	99.88	melpt	sat	BSAO	47HUF

66GOO/DEP from unpublished measurement of Bureau of Mines, Bartlesville (USA)

Name: Dibenzothiophene
Formula: $C_{12}H_8S$

CAS-RN: 132-65-0
Group No.: 53-013
Molar Mass: 184.26

Table 53.13.1. Experimental heat capacities

Reference		Temp range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
83ORO/MRA		380.0–550.0	24 S	1.50	99.9	chrom	*p*	BDHT	69PER/COM
91CHI/KNI1		377.2–515.7	16	0.10	99.986	melpt	sat	BSAO	47HUF
91CHI/KNI1		380.0–860.0	25	1.00	99.986	melpt	sat	BDHT	89KNI/ARC
95STE/CHI1	N	500.0–800.0	16 S	1.00	99.986	melpt	sat	BDHT	89KNI/ARC

95STE/CHI1 revised values based on the new measurement densities along the saturation line

Table 53.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
91CHI/KNI1	377.2–515.8	16	0.10	0.169	6.71–3	0.02	−1.02–4	−1
95STE/CHI1	500.0–800.0	16	1.00	0.042	1.91–2	0.04	1.04–2	6
Rejected data								
83ORO/MRA	(4.24–1,1.21,−2.55–1,−12)		91CHI/KNI1	(2.29–1,0.45,1.41–1,10)				

Table 53.13.3. Parameters of cubic spline polynomials

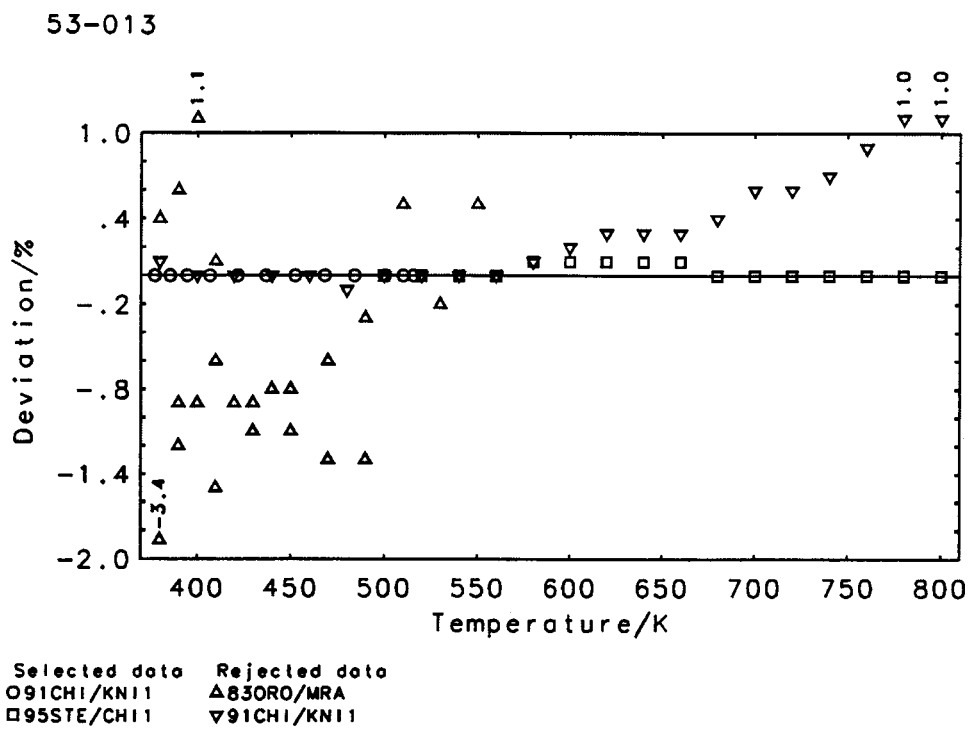
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%	w	
p	81	32	0.137	1.59−2	0.04	5.17−3	5
sat	81	32	0.136	1.38−2	0.03	4.47−3	6

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
377.2–520.0	9.54676	8.15897	−4.96261−1	1.95933−2	II
520.0–740.0	1.42058+1	5.47103	2.06494−2	−1.35420−2	IV
740.0–800.0	−6.97902+2	2.94164+2	−3.89919+1	1.74378	IV
377.2–520.0	9.47419	8.20789	−5.07171−1	2.03981−2	II
520.0–740.0	1.81594+1	3.19718	4.56428−1	−4.13711−2	IV
740.0–800.0	−3.13966+2	1.37843+2	−1.77389+1	7.78239−1	IV

Table 53.13.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	81	32	0.154	4.29−2	0.09	4.22−3	3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
377.2–800.0	897.00	−3.71128−1	1.34134−3	1.08236+1	6.49215+1	−2.39479+1	2.95451	IV



Name: Thianthrene
Formula: $C_{12}H_8S_2$

CAS-RN: 92-85-3
Group No.: 53-014
Molar Mass: 216.33

Table 53.14.1. Experimental heat capacities

Reference	Temp range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93STE/CHI1	435.7–518.4	12	0.10	99.997	melpt	sat	BSAO	88STE/ARC
93STE/CHI1	440.0–700.0	14 S	1.00	99.997	melpt	sat	BDHT	89KNI/ARC

Table 53.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93STE/CHI1	435.7–518.4	12	0.10	0.088	3.84–3	0.01	1.21–4	1
93STE/CHI1	440.0–700.0	14	1.00	0.063	3.03–2	0.06	−1.03–2	−5

Table 53.14.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	26	26	0.084	2.49–2	0.05	−5.49–3	−4
sat	26	26	0.084	2.44–2	0.05	−5.52–3	−4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
435.7–520.0	2.71286+1	−1.14920	1.57355	−1.30609−1	II
520.0–700.0	−1.79927+1	2.48823+1	−3.43250	1.90291−1	IV
435.7–520.0	2.75711+1	−1.42934	1.63254	−1.34742−1	II
520.0–700.0	−1.64752+1	2.39820+1	−3.25426	1.78514−1	IV

Table 53.14.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	26	26	0.176	4.45–2	0.09	−1.08–2	−2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
435.7–700.0	920.00	−2.74010	2.88568−1	9.36362	8.60828+1	−5.65524+1	1.34505+1	IV

Name: 2,2,2-Trifluoroethanol
Formula: $C_2H_3F_3O$

CAS-RN: 75-89-8
Group No.: 61-008
Molar Mass: 100.04

Table 61.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
89JAD/FRA	315.0–355.0	5	nosp	99.	anal	p	BDCT	86MER/BEN
92MIY/TAMI	298.1	1	nosp	99.95	chrom	p	FSIO	85OGA/MUR
97NIS/TAM	308.1	1	nosp	99.97	chrom	p	FSIO	85OGA/MUR

Table 61.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
92MIY/TAM1	298.1	1	0.30 #	0.000	0.00	0.00	0.00	0
97NIS/TAM	308.1	1	0.30 #	0.000	0.00	0.00	0.00	0

Table 61.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	7	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–308.1	4.42059	5.68885	III

Name: Pentafluorophenol
Formula: C_6HF_5O

CAS-RN: 771-61-9
Group No.: 61-034
Molar Mass: 184.07

Table 61.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
68AND/COU1	315.6–376.9	16	nosp	99.97	melpt	p	BSAO	63AND/COU1
69PAU/LAV2	318.0–328.5	4	nosp	98.76	melpt	p	BSAO	69PAU/LAV2
97STE/CHI3	320.0–580.0	14	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 61.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
68AND/COU1	315.6–376.9	16	0.20 #	0.307	2.06–2	0.06	8.42–5	0
97STE/CHI3	320.0–580.0	14	1.00	0.294	1.14–1	0.29	−8.41–4	−2
Rejected data								
69PAU/LAV2	(5.89–1,1.73,5.89–1,4)							

Table 61.34.3. Parameters of cubic spline polynomials

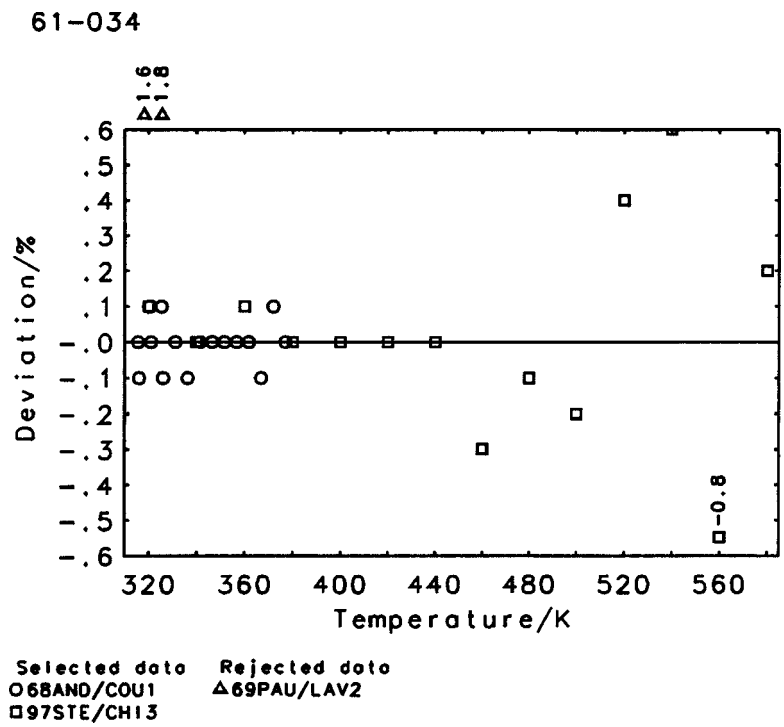
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	34	30	0.337	8.90–2	0.23	−3.47–4	−2
sat	34	30	0.312	7.14–2	0.19	−7.51–4	−3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
315.7–400.0	4.38341+1	−3.51873	−4.74950−1	1.78930−1	II
400.0–520.0	8.26306+1	−3.26160+1	6.79938	−4.27264−1	IV
520.0–580.0	−4.49205+3	2.60662+3	−5.00747+2	3.21078+1	IV
315.7–400.0	4.42762+1	−3.98006	−3.17982−1	1.61437−1	II
400.0–520.0	9.25689+1	−4.01996+1	8.73690	−5.93137−1	IV
520.0–580.0	−3.11543+3	1.81057+3	−3.47181+2	2.22221+1	IV

Table 61.34.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	34	13	0.507	1.81−1	0.47	−1.57−3	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
371.8–580.0	605.00	−1.19863	4.36410−1	3.06003+1	8.23029−1	IV



Name: 2-Chlorophenol
Formula: C_6H_5ClO

CAS-RN: 95-57-8
Group No.: 61-037
Molar Mass: 128.56

Table 61.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
16BRA	283.1–323.1	2	nosp	not specified		avg	DSTO	16BRA
37ELL	298.1–351.1	3 S	nosp	not specified		p	BSIO	37ELL
#00ROH	293.1–353.1	7	0.50	99.97	chrom	p	BDCT	91BAN/GAR

Table 61.37.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
#00ROH	293.1–353.1	7	0.50	0.142	1.87–2	0.07	2.59–5	0
Rejected data								
16BRA	(6.72–1,2.62,−6.72–1,−1)		37ELL	(5.89–1,2.31,−4.27–1,−1)				

Table 61.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	12	7	0.187	2.48−2	0.09	2.59−5	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
293.1−353.1	4.16416+1	−1.04980+1	1.77851	IV

Name: (Difluoromethoxy)trifluoromethane
Formula: C_2HF_5O

CAS-RN: 3822-68-2
Group No.: 61-047
Molar Mass: 136.02

Table 61.47.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92HWA/DES	313.15	1.327	3.00	not specified		*p*	BDHT	92HWA/DES

Name: 4,5-Dichloro-1,3-dioxolan-2-one
Formula: $C_3H_2Cl_2O_3$

CAS-RN: 3967-55-3
Group No.: 61-048
Molar Mass: 156.95

Table 61.48.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
76MAS/PET	N	274.8−335.2	11	5.00	not specified		*p*	BDHT	66PER/COM
76MAS/PET	data from a graph only								

Table 61.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	11	11	0.204	2.37−1	1.02	4.31−3	5

Temp. range K	A_1	A_2	Level of uncertainty
274.8−335.2	3.20668	6.87970	VI

Name: 4-Chloro-1,3-dioxolan-2-one
Formula: $C_3H_3ClO_3$

CAS-RN: 3967-54-2
Group No.: 61-049
Molar Mass: 122.51

Table 61.49.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
76MAS/PET	N	241.8−310.5	11	5.00	not specified		*p*	BDHT	66PER/COM
76MAS/PET	data from a graph only								

Table 61.49.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	11	11	0.106	1.44−1	0.53	9.46−4	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
241.8–310.5	−1.83134+2	2.61701+2	−1.08544+2	1.49441+1	VI

Name: 4-(Chloromethyl)-1,3-dioxolan-2-one
Formula: $C_4H_5ClO_3$

CAS-RN: 2463-45-8
Group No.: 61-050
Molar Mass: 136.53

Table 61.50.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
76MAS/PET	N	274.2–304.8	7	5.00	not specified		*p*	BDHT	66PER/COM
76MAS/PET	data from a graph only								

Table 61.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	7	7	0.181	2.69−1	0.90	3.60−3	1

Temp. range K	A_1	A_2	Level of uncertainty
274.2–304.8	−1.18927+1	1.40300+1	VI

Name: 3-Chlorophenol
Formula: C_6H_5ClO

CAS-RN: 108-43-0
Group No.: 61-051
Molar Mass: 128.56

Table 61.51.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00ROH	313.1–353.1	5	0.50	99.97	chrom	*p*	BDCT	83ROU/ROU

Table 61.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
total	used						
p	5	5	0.250	3.47−2	0.13	3.36−5	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
313.1–353.1	−2.62580+1	3.04931+1	−4.26736	IV

Name: 4-Chlorophenol
Formula: C_6H_5ClO

CAS-RN: 106-48-9
Group No.: 61-052
Molar Mass: 128.56

Table 61.52.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00ROH	323.1–353.1	4	0.50	99.81	chrom	*p*	BDCT	83ROU/ROU

Table 61.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	4	4	0.090	1.26−2	0.04	6.20−6	0

Temp. range K	A_1	A_2	Level of uncertainty
323.1–353.1	2.25112+1	1.65996	IV

Name: 2-Fluorophenol
Formula: C_6H_5FO

CAS-RN: 367-12-4
Group No.: 61-053
Molar Mass: 112.10

Table 61.53.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91LIC	289.25	1.902	2.00	99.	anal	*p*	BDCT	89BRE/LIC

Name: 3-Fluorophenol
Formula: C_6H_5FO

CAS-RN: 372-20-3
Group No.: 61-054
Molar Mass: 112.10

Table 61.54.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91LIC	286.85	1.897	2.00	99.	anal	*p*	BDCT	89BRE/LIC

Name: 1-[1-[Difluoro(pentafluoroethoxy)methyl]-1,2,2,2-tetrafluoroethoxy]-1,1,2,2,3,3,3-heptafluoropropane
Formula: $C_8F_{18}O_2$

CAS-RN: 66804-94-2
Group No.: 61-055
Molar Mass: 470.06

Table 61.55.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98MUS/NAZ	293.1–373.1	5	1.50	99.	anal	*p*	BDIO	96MUS

Table 61.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	5	5	0.034	3.17−2	0.05	1.30−5	−1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
293.1–373.1	4.23552+1	1.79370	1.29623	V

Name: Formamide
Formula: CH_3NO

CAS-RN: 75-12-7
Group No.: 62-001
Molar Mass: 45.04

Table 62.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
65SOM/COO	N	298.1	1	0.20	not specified		*p*	BSAO	56COO/BAL
66EGA/LUF		298.1	1	nosp	not specified		*p*	BSIO	61EGA/LUF
67RAS/GAN		293.1–373.1	5 S	0.50	not specified		*p*	BSAO	67RAS/GAN
74DEV/SOM	N	298.1	1	0.50	not specified		*p*	BSIO	70LKB/COM
76BON/CER		298.1	1	nosp	not specified		*p*	BSIO	76BON/CER
76SKO/SUU		298.1	1	0.10	not specified		*p*	DDCT	71KON/SUU
77VOR/PRI		297.4	1	0.80	not specified		sat	BSAO	77VOR/PRI
78DEV/HEU		298.1	1	1.00	99.8	chrom	*p*	BSIO	70LKB/COM
83DEW/DEK		276.8–293.7	8	nosp	99.57	melpt	*p*	BSAO	79SCH/OFF
85KOL/KUL	N	293.1–313.1	3	nosp	not specified		*p*	BSAO	75VYU/ZVE
89PET/PES2	N	278.1–318.1	3	0.10	not specified		*p*	BSAO	83KUK/KOR
92KOL/KUL1	N	283.1–328.1	4	0.05	not specified		*p*	BSAO	75VYU/ZVE
93BAS/VOL	N	298.1	1	nosp	99.0	chrom	*p*	DDCT	71KON/SUU

65SOM/COO high purity of substance with water content below 0.02%
74DEV/SOM C_p values for Formamide and *N*,*N*-Dimethylformamide were interchanged
85KOL/KUL water content below 0.03%
89PET/PES2 water content below 0.01%
92KOL/KUL1 content of water 0.01%–0.02% by Karl Fischer method
93BAS/VOL content of water less than 0.05 mol. % by Karl Fischer method

Table 62.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
65SOM/COO	298.1	1	0.20	0.989	2.56–2	0.20	−2.56–2	−1
66EGA/LUF	298.1	1	0.50 #	0.136	8.81–3	0.07	8.81–3	1
74DEV/SOM	298.1	1	0.50	0.531	3.45–2	0.27	3.45–2	1
76SKO/SUU	298.1	1	0.10	1.791	2.32–2	0.18	−2.32–2	−1
77VOR/PRI	297.5	1	0.80	0.237	2.46–2	0.19	2.46–2	1
78DEV/HEU	298.1	1	1.00	0.081	1.05–2	0.08	1.05–2	1
83DEW/DEK	276.8–293.7	8	0.50 #	0.920	5.90–2	0.46	−5.55–2	−8
85KOL/KUL	293.1–313.1	3	0.50 #	0.104	6.75–3	0.05	4.63–3	1
89PET/PES2	278.1–318.1	3	0.10	2.178	2.85–2	0.22	−7.64–3	−1
92KOL/KUL1	283.1–328.1	4	0.05	0.873	5.70–3	0.04	4.27–3	3
Rejected data								
67RAS/GAN	(2.97–1,2.33,−2.96–1,−2)		76BON/CER	(9.78–2,0.76,−9.78–2,−1)				
93BAS/VOL	(3.88–2,0.30,−3.88–2,−1)							

Table 62.1.3. Parameters of regression polynomial

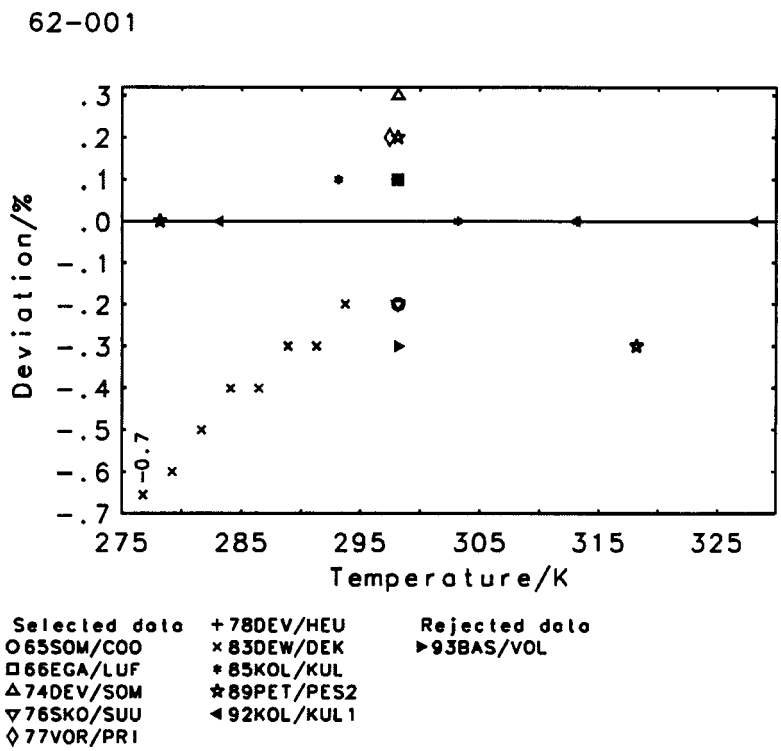
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	31	24	1.168	4.01–2	0.31	−1.69–2	−3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
276.8–328.1	2.10920+1	−6.09729	1.13100	III

Table 62.1.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	31	24	2.111	2.88−2	0.22	5.38−3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
276.8–328.1	775.00	1.10520+2	4.38420+1	−3.14205+1	6.96517+1	IV



Name: Nitromethane
Formula: CH_3NO_2

CAS-RN: 75-52-5
Group No.: 62-002
Molar Mass: 61.04

Table 62.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
07WAL		290.1	1	nosp	not specified		avg	DSIO	07WAL
25WIL	N	303.0–343.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
25WIL	N	288.0–343.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
47JON/GIA		249.8–297.1	11	nosp	99.7	melpt	*p*	BSIO	37GIA/EGA
50HOU/MAS2		313.1–363.1	6 S	0.40	99.8	estim	*p*	BSAO	50SAG/HOU
65ZIE	N	316.0–333.9	2	nosp	not specified		avg	DSIO	58SWI/ZIEI
69BER/WES		308.1–473.1	18 S	0.10	99.99	melpt	sat	BSAO	68WES/WES
99CER/TOV		288.1–308.1	4	nosp	99.	chrom	*p*	BDCT	83ROU/ROU

25WIL sample was dried P_2O_5
25WIL sample was dried $CaCl_2$
65ZIE average values in temperature ranges 294–374 K and 294–338 K

Table 62.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
47JON/GIA	249.8–297.1	11	0.40 #	0.405	2.06–2	0.16	−6.01–3	0
69BER/WES	308.1–473.1	18	0.10	0.134	1.87–3	0.01	−7.14–5	−2
99CER/TOV	288.1–308.1	4	0.50 #	0.538	3.45–2	0.27	3.45–2	4
			Rejected data					
07WAL	(7.19–2,0.57,−7.19–2,−1)		25WIL	(6.70–1,5.43,−6.67–1,−4)				
25WIL	(7.18–1,5.88,−6.28–1,−5)		50HOU/MAS2	(1.32–1,0.99,1.31–1,6)				
65ZIE	(2.80–1,2.20,−2.75–1,−2)							

Table 62.2.3. Parameters of cubic spline polynomials

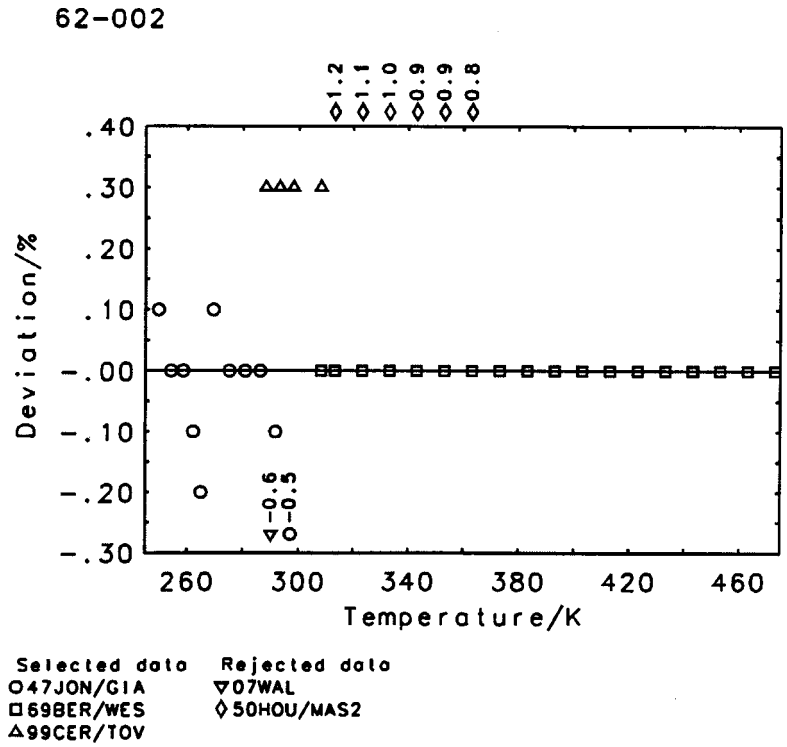
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	51	33	0.343	1.84–2	0.14	2.13–3	2
sat	51	33	0.345	1.82–2	0.14	1.83–3	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
249.8–360.0	2.09372+1	−7.96430	2.31812	−1.89026−1	III
360.0–473.2	−1.00995	1.03251+1	−2.76226	2.81379−1	III
249.8–360.0	2.05129+1	−7.60099	2.21965	−1.80790−1	III
360.0–473.2	3.26255	6.77427	−1.77348	1.88944−1	III

Table 62.2.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	51	33	2.418	6.45–2	0.49	1.30–2	8

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
249.8–473.1	588.00	−1.20159	6.02375−1	1.04261+1	5.99223−1	IV



Name: *N*-Methylformamide
Formula: C_2H_5NO

CAS-RN: 123-39-7
Group No.: 62-006
Molar Mass: 59.07

Table 62.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
74DEV/SOM		298.1	1	0.50	not specified		*p*	BSIO	70LKB/COM
76BON/CER		298.1	1	nosp	not specified		*p*	BSIO	76BON/CER
76SKO/SUU		298.1	1	0.10	not specified		*p*	DDCT	71KON/SUU
79DEV/SOM		298.1	1	1.00	99.8	chrom	*p*	BSIO	70LKB/COM
85KOL/KUL	N	293.1–303.1	2	nosp	not specified		*p*	BSAO	75VYU/ZVE
89KUL/KRE		308.0	1	nosp	not specified		*p*	BSAO	83KUK/KOR
92KOL/KUL1	N	283.1–328.1	4	0.05	not specified		*p*	BSAO	75VYU/ZVE

85KOL/KUL water content below 0.03%
92KOL/KUL1 content of water 0.01%–0.02% by Karl Fischer method

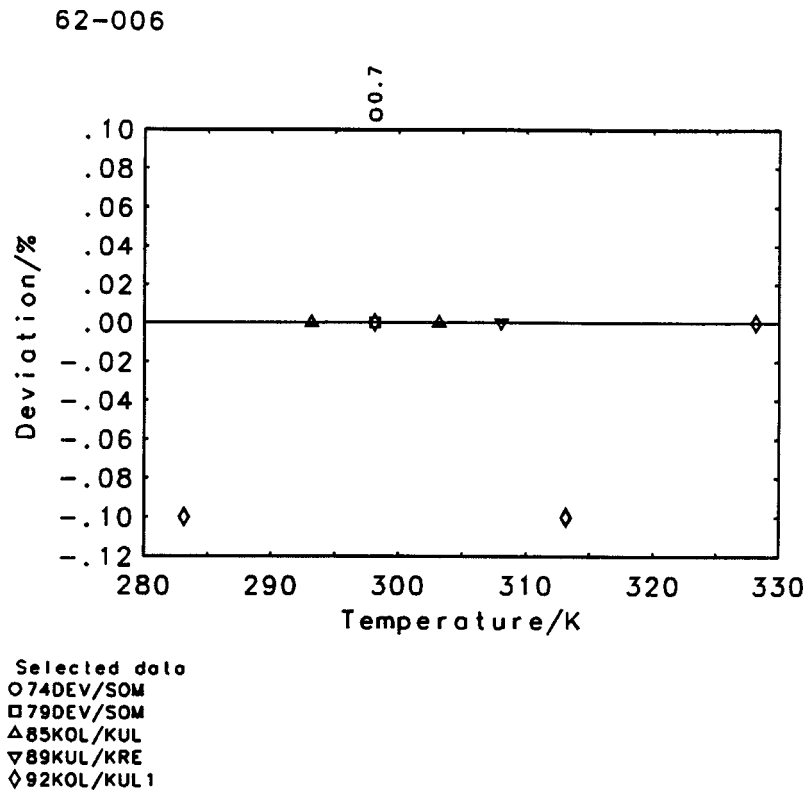
Table 62.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
74DEV/SOM	298.1	1	0.50	1.485	1.13–1	0.74	1.13–1	1
79DEV/SOM	298.1	1	1.00	0.029	4.37–3	0.03	4.37–3	1
85KOL/KUL	293.1–303.1	2	0.30 #	0.055	2.49–3	0.02	−2.36–3	−2
89KUL/KRE	308.0	1	0.50 #	0.049	3.69–3	0.02	−3.69–3	−1
92KOL/KUL1	283.1–328.1	4	0.30 #	0.241	1.08–2	0.07	−8.56–3	−3
Rejected data								
76BON/CER	(3.80–1,2.59,−3.80–1,−1)		76SKO/SUU	(1.64–1,1.10,−1.64–1,−1)				

Table 62.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	11	9	0.591	4.34−2	0.29	8.26−3	−4

Temp. range K	A_1	A_2	Level of uncertainty
283.1–328.1	9.60363	1.82794	III



Name: Isoxazole
Formula: C_3H_3NO

CAS-RN: 288-14-2
Group No.: 62-010
Molar Mass: 69.06

Table 62.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78MCC/HAM		298.1	1	nosp	not specified		p	BDHT	73PER/COM
93STE/CHI2	N	300.0–480.0	10	1.00	99.95	chrom	sat	BDHT	89KNI/ARC
93STE/CHI2	same data in 96STE/CHI2								

Table 62.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93STE/CHI2	300.0–480.0	10	1.00	0.419	6.10−2	0.42	8.35−4	−3

Table 62.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	11	10	0.468	6.82−2	0.47	8.35−4	−3
sat	11	10	0.454	7.04−2	0.45	5.59−4	0

Temp. range K	A_1	A_2	Level of uncertainty
300.0–480.0	4.98573	2.63620	IV
300.0–480.0	5.32295	2.53491	IV

Table 62.10.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	11	10	0.447	6.89−2	0.45	4.95−4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–480.0	590.00	−6.53318−1	7.91038−3	5.58899	1.34894+1	IV

Name: *N*,*N*-Dimethylformamide
Formula: C_3H_7NO

CAS-RN: 68-12-2
Group No.: 62-016
Molar Mass: 73.09

Table 62.16.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
61GEL		273.0–323.0	5 S	nosp	not specified		*p*	not specified	
70ANO		293.2–423.2	8 S	nosp	not specified		sat	not specified	
73MOS/NIK		212.6–298.1	4 S	nosp	99.5	melpt	*p*	BSAO	66NIK/LEB
74DEV/SOM	N	298.1	1	0.50	not specified		*p*	BSIO	70LKB/COM
76BON/CER		298.1	1	nosp	not specified		*p*	BSIO	76BON/CER
77BON/BED	N	298.1	1	0.10	not specified		*p*	BSIO	76BON/CER
77DEV/PER2		298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
77DEV/PER3		298.1	1	0.50	not specified		*p*	FSIT	71PIC/LED
77VYU		298.0	1	nosp	not specified		*p*	not specified	
78MAR/CIO1	N	298.1–429.1	2	nosp	not specified		*p*	DSIO	71MAR/CIO
79DEV/SOM		298.1	1	1.00	99.8	chrom	*p*	BSIO	70LKB/COM
82VOR/YAK		298.1	1	nosp	not specified		*p*	BSAO	77VOR/PRI
84ZEG/SOM2		298.1	1	0.30	99.5	chrom	*p*	FSIT	71PIC/LED
86KOR/KUK		278.0–298.0	2	0.20	not specified		*p*	BSAO	83KUK/KOR
87PIE		298.1	1	nosp	99.5	chrom	*p*	FSIT	71PIC/LED
89KUL/KRE		308.0	1	nosp	not specified		*p*	BSAO	83KUK/KOR
89PET/PES1		258.1–318.1	4	nosp	not specified		*p*	BSAO	83KUK/KOR
91GRO/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
92KOL/KUL2	N	283.1–323.1	6	0.05	not specified		*p*	BSAO	75VYU/ZVE
92MIY/TAM2		298.1	1	nosp	99.9	chrom	*p*	FSIO	85OGA/MUR
93NAK/CHU		298.1	1	0.50	99.96	chrom	*p*	FSIO	85OGA/MUR
94CON/GIA1		298.1	1	nosp	not specified		*p*	FSIT	88CON/GIA
94PRA/RAJ		293.1–323.1	4	nosp	not specified		*p*	BDHT	89PRA/RAJ

74DEV/SOM	C_p values for *N*,*N*-Dimethylformamide and Formamide were interchanged
77BON/BED	infrared spectrum indicated that sample was water-free
78MAR/CIO1	constant value calculated from temperature dependence of enthalpy by the authors
92KOL/KUL2	content of water 0.01%–0.02% by Karl Fischer method

Table 62.16.2. Correlated heat capacities

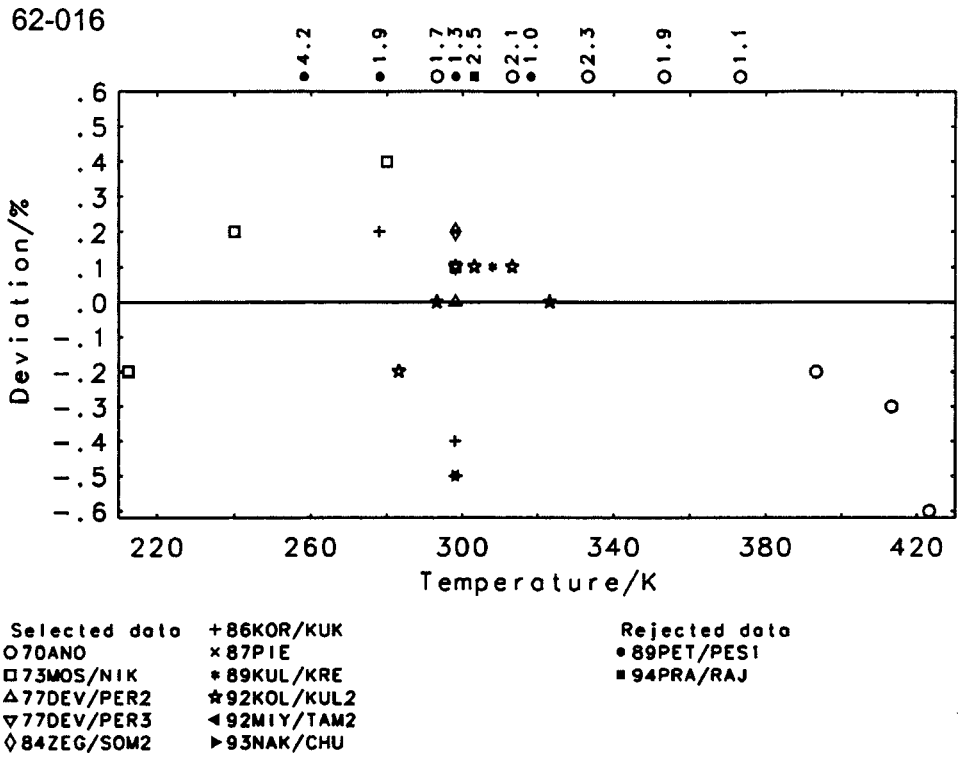
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
			Selected data					
70ANO	293.2–423.2	8	1.50 #	1.003	2.82–1	1.50	1.85–1	2
73MOS/NIK	212.6–298.1	4	0.50 #	0.502	4.38–2	0.25	2.05–2	2
77DEV/PER2	298.1	1	0.30	0.019	1.00–3	0.01	−1.00–3	0
77DEV/PER3	298.1	1	0.50	0.259	2.31–2	0.13	2.31–2	1
84ZEG/SOM2	298.1	1	0.30	0.790	4.23–2	0.24	4.23–2	1
86KOR/KUK	278.0–298.0	2	0.20	1.663	5.89–2	0.33	−1.42–2	0
87PIE	298.1	1	0.50 #	0.475	4.23–2	0.24	4.23–2	1
89KUL/KRE	308.0	1	0.50 #	0.245	2.20–2	0.12	2.20–2	1
92KOL/KUL2	283.1–323.1	6	0.30 #	0.331	1.77–2	0.10	6.37–3	4
92MIY/TAM2	298.1	1	0.30 #	1.785	9.48–2	0.54	−9.48–2	−1
93NAK/CHU	298.1	1	0.50	1.085	9.60–2	0.54	−9.60–2	−1
			Rejected data					
61GEL	(1.44,7.38,1.30,5)		74DEV/SOM	(4.80–1,2.63,4.80–1,1)				
76BON/CER	(2.42–1,1.38,−2.42–1,−1)		77BON/BED	(3.10–1,1.77,−3.10–1,−1)				
77VYU	(4.52–1,2.48,4.52–1,1)		78MAR/CIO1	(3.31,22.83,−3.31,−1)				
79DEV/SOM	(3.36–1,1.85,3.36–1,1)		82VOR/YAK	(3.00–1,1.66,3.00–1,1)				
89PET/PES1	(4.48–1,2.47,3.85–1,4)		91GRO/ROU	(2.35–1,1.34,−2.35–1,−1)				
94CON/GIA1	(1.91–1,1.09,−1.91–1,−1)		94PRA/RAJ	(4.40–1,2.39,4.37–1,4)				

Table 62.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	50	27	0.946	1.71–1	0.92	5.58–2	10
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
212.6–423.2		1.30506+1	4.51158	−1.84340	2.89996−1		IV

Table 62.16.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	50	27	2.943	2.46–1	1.41	8.28–2	8
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
212.6–423.2	660.00	−3.63232	8.64272−1	1.23295+1	3.81644		V



Name: 2-Amino-2-methyl-1-propanol
Formula: $C_4H_{11}NO$

CAS-RN: 124-68-5
Group No.: 62-028
Molar Mass: 89.14

Table 62.28.1. Experimental heat capacities

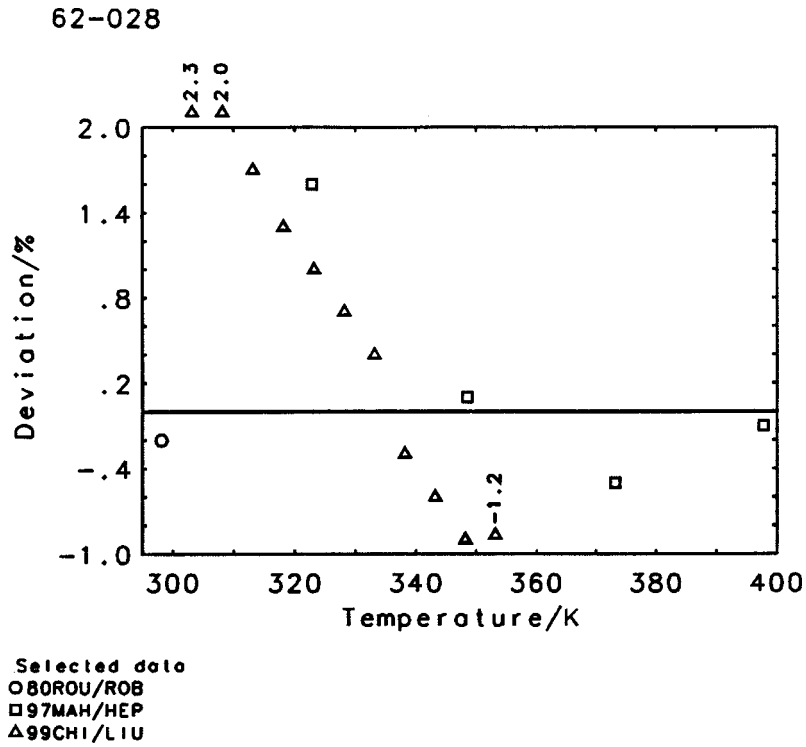
Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
80ROU/ROB	298.1	1	0.30	not specified		*p*	FSIT	71PIC/LED
97MAH/HEP	322.8–397.8	4	nosp	99.0	chrom	*p*	BDCT	91BAN/GAR
99CHI/LIU	303.1–353.1	11	3.00	95.	anal	*p*	BDHT	99CHI/LIU

Table 62.28.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
80ROU/ROB	298.1	1	0.30	0.507	4.20–2	0.15	−4.20–2	−1
97MAH/HEP	322.8–397.8	4	1.00 #	0.828	2.53–1	0.83	7.21–2	0
99CHI/LIU	303.1–353.1	11	3.00	0.427	3.78–1	1.28	1.65–1	3

Table 62.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	16	16	0.598	3.62–1	1.22	1.29–1	2
Temp. range K		A_1	A_2				Level of uncertainty
298.1–397.8		2.88532	8.30421				V



Name: Nitrobenzene
Formula: $C_6H_5NO_2$

CAS-RN: 98-95-3
Group No.: 62-045
Molar Mass: 123.11

Table 62.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*81VON	323.4–392.1	4 S	nosp	not specified		avg	DSIO	*81VON
12SCH2	283.1–393.1	12	nosp	not specified		*p*	BSIO	12SCH1
24WIL/DAN	303.0–358.0	eqn	nosp	not specified		*p*	BSAO	24WIL/DAN
34PAR/TOD	280.6–297.4	5	0.60	not specified		*p*	BSIO	25PAR
36PAR/TOD1	280.0–300.0	3 S	0.70	not specified		*p*	BSIO	25PAR
39MAZ1	278.5–293.4	50	nosp	not specified		*p*	BSIO	39MAZ3
39MAZ3	279.0–293.4	10	nosp	not specified		*p*	BSIO	39MAZ3
58LUT/PAN	335.6–414.6	15	0.70	not specified		*p*	BDHO	58LUT/PAN
67PAC	303.1	1	nosp	not specified		*p*	BDHT	79DU/COM
67RAS/GAN	293.1–373.1	5 S	0.50	not specified		*p*	BSAO	67RAS/GAN
85LAI/ROD	298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
94GRO/ROU	298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED

Name: 2-Nitrophenol
Formula: $C_6H_5NO_3$

CAS-RN: 88-75-5
Group No.: 62-046
Molar Mass: 139.11

Table 62.46.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	337.1	1	nosp	not specified		avg	DSIO	*94BRU
16KUR	N	430.6	1	nosp	not specified		avg	not specified	
59LUT/PAN		335.0–409.0	eqn	nosp	not specified		*p*	BDHO	58LUT/PAN

*94BRU average value in temperature range 325–349 K
16KUR average value in temperature range 413–448 K

Name: 2,2′,2″-Nitrilotrisethanol
Formula: $C_6H_{15}NO_3$

CAS-RN: 102-71-6
Group No.: 62-059
Molar Mass: 149.19

Table 62.59.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
34MEH1		290.1	1	1.50	not specified		*p*	BSIO	49WEI
82MIN/SAB	N	298.1	1	nosp	99.	anal	*p*	not specified	
94LEE		303.1–353.1	11 S	nosp	not specified		*p*	not specified	
97MAH/HEP		299.1–397.8	5	nosp	99.8	anal	*p*	BDCT	91BAN/GAR
99CHI/LIU		303.1–353.1	11	1.00	99.	anal	*p*	BDHT	99CHI/LIU

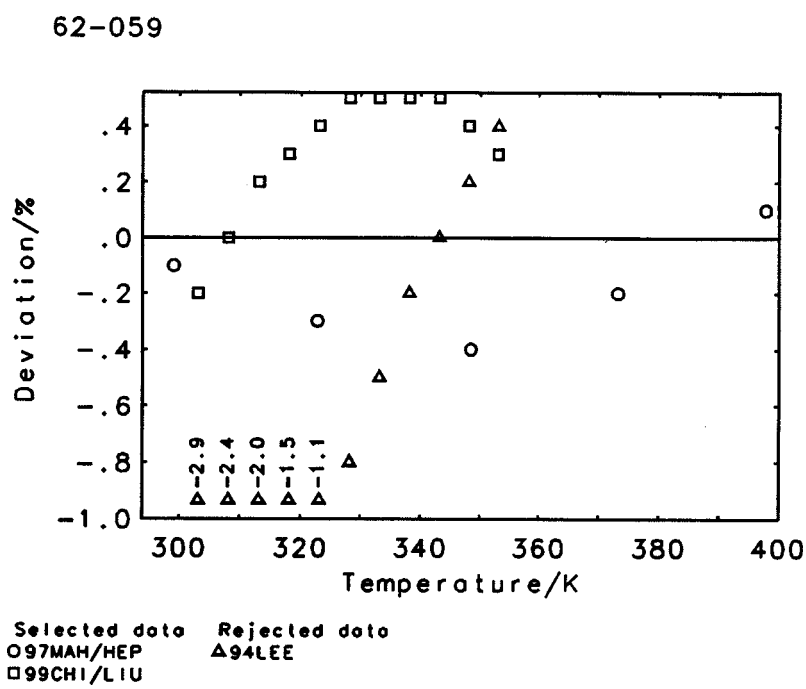
82MIN/SAB thermopile conduction calorimeter (Tian-Calvet) used, but not specified

Table 62.59.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
97MAH/HEP	299.1–397.8	5	0.50 #	0.497	1.12–1	0.25	−7.59–2	−3
99CHI/LIU	303.1–353.1	11	1.00	0.377	1.69–1	0.38	1.40–1	9
Rejected data								
94LEE	(6.22–1,1.45,−4.27–1,−6)							

Table 62.59.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	29	16	0.464	1.70–1	0.38	7.28–2	6
Temp. range K		A_1	A_2	A_3			Level of uncertainty
299.1–397.8		6.47378+1	−1.56172+1	2.86003			IV



Name: 1,1′-Methylenebis[4-isocyanatobenzene]
Formula: $C_{15}H_{10}N_2O_2$

CAS-RN: 101-68-8
Group No.: 62-099
Molar Mass: 250.26

Table 62.99.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
66ZAL/STR	N	335.1	1	nosp	not specified		avg	not specified	
77LEB/EVS3		321.3–331.5	9	0.30	99.81	melpt	*p*	BSAO	66NIK/LEB
77LEB/RAB1	N	313.6–330.0	3 S	0.30	not specified		*p*	BSAO	76LEB/LIT

66ZAL/STR average value in temperature range 319–351 K
77LEB/RAB1 only a graph given in the paper; smoothed values provided by the authors

Table 62.99.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
77LEB/EVS3	321.3–331.5	9	0.30	0.160	2.28–2	0.05	−1.28–3	1
77LEB/RAB1	313.6–330.0	3	0.30	0.033	4.70–3	0.01	3.91–3	1

Table 62.99.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	13	12	0.153	2.18–2	0.05	1.46–5	2

Temp. range K	A_1	A_2	Level of uncertainty
313.6–331.5	3.27509+1	4.50946	III

Name: 2-Aminoethanol
Formula: C_2H_7NO

CAS-RN: 141-43-5
Group No.: 62-128
Molar Mass: 61.08

Table 62.128.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93PAG/HUO2	283.1–313.1	3	nosp	99.7	anal	*p*	FSIT	71PIC/LED
94LEE	303.1–353.1	11 S	nosp	not specified		*p*	not specified	
97MAH/HEP	299.1–397.8	5	nosp	99.0	anal	*p*	BDCT	91BAN/GAR
99CHI/LIU	303.1–353.1	11	1.00	99.	anal	*p*	BDHT	99CHI/LIU

Table 62.128.2. Correlated heat capacities

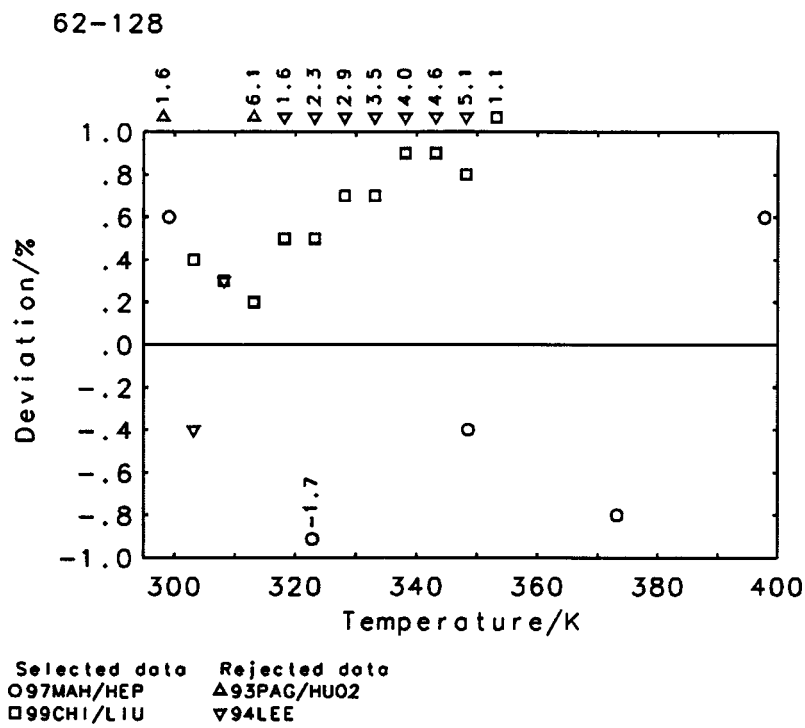
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
97MAH/HEP	299.1–397.8	5	0.50 #	1.883	1.97–1	0.94	−6.92–2	−1
99CHI/LIU	303.1–353.1	11	1.00	0.689	1.47–1	0.69	1.35–1	11
Rejected data								
93PAG/HUO2	(1.34,6.15,1.34,1)		94LEE	(7.53–1,3.37,6.14–1,9)				

Table 62.128.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	30	16	1.281	1.76−1	0.83	7.11−2	10
Temp. range K		A_1	A_2				Level of uncertainty
299.1–397.8		1.03390+1	3.20506				IV

Table 62.128.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	30	16	1.429	1.65−1	0.78	−2.76−3	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
299.1–397.8	641.73	−6.20579−1	5.01843−3	1.06637+1	1.91852+1		IV



Name: Methoxyacetonitrile
Formula: C_3H_5NO

CAS-RN: 1738-36-9
Group No.: 62-129
Molar Mass: 71.08

Table 62.129.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95VER/BEC	298.00	2.110	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 1-Nitropropane
Formula: $C_3H_7NO_2$

CAS-RN: 108-03-2
Group No.: 62-130
Molar Mass: 89.09

Table 62.130.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96TAN/TOY1	298.15	1.801	nosp	99.9	chrom	*p*	FSIT	71PIC/LED

Name: 2-(Methylamino)ethanol
Formula: C_3H_9NO

CAS-RN: 109-83-1
Group No.: 62-131
Molar Mass: 75.11

Table 62.131.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97MAH/HEP	299.1–397.8	5	nosp	99.0	anal	*p*	BDCT	91BAN/GAR
97STE/CHI2	300.0–620.0	17	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 62.131.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
97MAH/HEP	299.1–397.8	5	1.00 #	1.026	2.59–1	1.03	−2.38–1	−5
97STE/CHI2	300.0–620.0	17	1.00	0.816	2.89–1	0.82	7.82–2	6

Table 62.131.3. Parameters of cubic spline polynomials

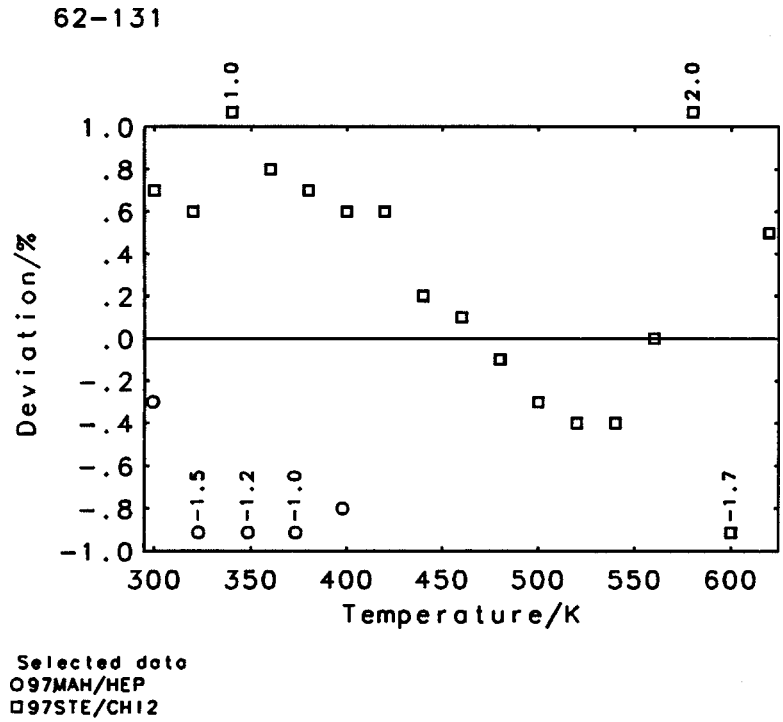
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	22	22	0.988	3.21–1	0.99	6.36–3	1
sat	22	22	0.828	2.37–1	0.83	3.33–3	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
299.1–570.0	3.42554+1	−1.56382+1	5.29539	−4.39149−1	IV
570.0–620.0	−3.44752+4	1.81472+4	−3.18117+3	1.85904+2	IV
299.1–570.0	4.04063+1	−2.06783+1	6.65786	−5.60728−1	IV
570.0–620.0	−2.17024+4	1.14229+4	−2.00099+3	1.16846+2	IV

Table 62.131.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	22	22	1.750	5.46–1	1.75	2.83–2	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
299.1–620.0	630.00	3.95675−1	4.21461−1	−1.64733+1	1.27628+2	−1.16651+2	3.99963+1	V



Name: Methyl ester cyanoacetic acid
Formula: $C_4H_5NO_2$

CAS-RN: 105-34-0
Group No.: 62-132
Molar Mass: 99.09

Table 62.132.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95VER/BEC	298.00	2.190	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: Ethoxyacetonitrile
Formula: C_4H_7NO

CAS-RN: 62957-60-2
Group No.: 62-133
Molar Mass: 85.11

Table 62.133.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95VER/BEC	298.00	2.090	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: Tetrahydro-2*H*-1,3-oxazin-2-one
Formula: $C_4H_7NO_2$

CAS-RN: 5259-97-2
Group No.: 62-134
Molar Mass: 101.11

Table 62.134.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97LEB/SMI	N	400.3–446.2	22	2.50	not specified		*p*	BDHT	69YAG

97LEB/SMI anomaly of Cp=f(T) relationship in the range 350–400 K associated with melting of crystals (n.m.t. 354 K)

Table 62.134.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	22	22	0.157	1.07−1	0.39	7.50−4	−1
Temp. range K		A_1	A_2				Level of uncertainty
400.3–446.2		4.06571	5.54567				V

Name: 2-(Dimethylamino)ethanol
Formula: $C_4H_{11}NO$

CAS-RN: 108-01-0
Group No.: 62-135
Molar Mass: 89.14

Table 62.135.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97MAH/HEP	299.1–397.8	5	nosp	99.0	anal	p	BDCT	91BAN/GAR

Table 62.135.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	5	5	0.546	1.55−1	0.55	8.55−4	−1
Temp. range K		A_1	A_2				Level of uncertainty
299.1–397.8		6.94478	5.94073				IV

Name: 2-(Ethylamino)ethanol
Formula: $C_4H_{11}NO$

CAS-RN: 110-73-6
Group No.: 62-136
Molar Mass: 89.14

Table 62.136.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97MAH/HEP	299.1–397.8	5	nosp	99.0	anal	p	BDCT	91BAN/GAR

Table 62.136.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	5	5	0.622	1.84−1	0.62	9.26−4	−1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
299.1–397.8		5.90834+1	−2.33923+1	4.28873			IV

Name: 2-(2-Aminoethoxy)ethanol
Formula: $C_4H_{11}NO_2$

CAS-RN: 929-06-6
Group No.: 62-137
Molar Mass: 105.14

Table 62.137.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99CHI/LIU	303.1–353.1	11	1.00	98.	anal	p	BDHT	99CHI/LIU

Table 62.137.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	11	11	0.113	3.68−2	0.11	6.61−5	−1
Temp. range K		A_1	A_2				Level of uncertainty
303.1–353.1		1.78663+1	4.46222				V

Name: 2,2′-Iminobisethanol
Formula: $C_4H_{11}NO_2$

CAS-RN: 111-42-2
Group No.: 62-138
Molar Mass: 105.14

Table 62.138.1. Experimental heat capacities

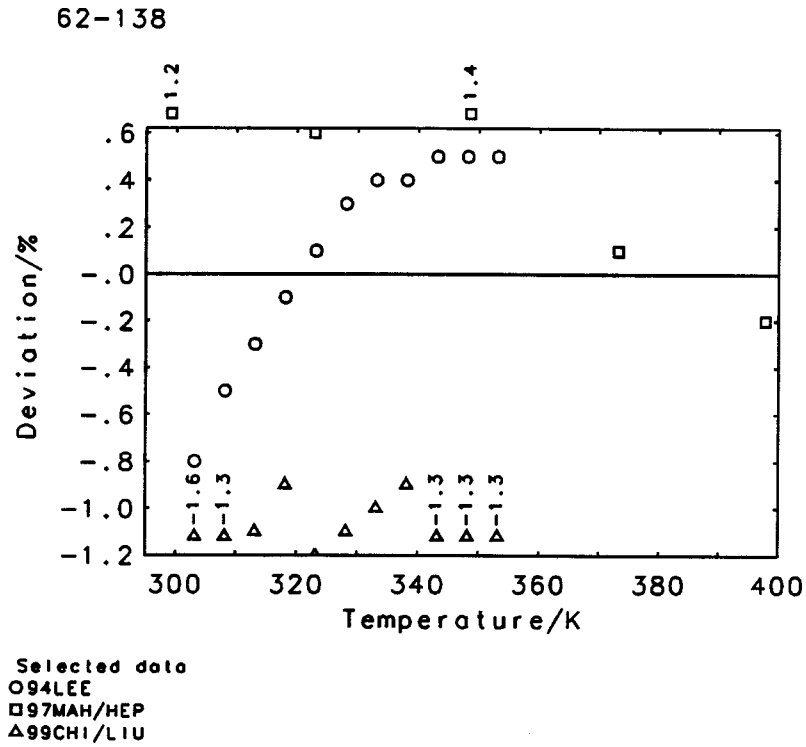
Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94LEE	303.1–353.1	11 S	nosp	not specified		*p*	not specified	
97MAH/HEP	299.1–397.8	5	nosp	99.0	anal	*p*	BDCT	91BAN/GAR
99CHI/LIU	303.1–353.1	11	1.00	99.	anal	*p*	BDHT	99CHI/LIU

Table 62.138.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94LEE	303.1–353.1	11	1.00 #	0.451	1.47−1	0.45	3.44−2	3
97MAH/HEP	299.1–397.8	5	0.50 #	1.749	2.91−1	0.87	2.00−1	3
99CHI/LIU	303.1–353.1	11	1.00	1.188	3.84−1	1.19	−3.80−1	−11

Table 62.138.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	27	27	1.173	3.08−1	0.95	−1.04−1	−5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
299.1–397.8		2.96248+1	−5.13210	1.85100			IV



Name: Methyl ester 2-cyanopropanoic acid
Formula: $C_5H_7NO_2$

CAS-RN: 14618-77-0
Group No.: 62-139
Molar Mass: 113.12

Table 62.139.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86KUL/DZH	255.6–304.6	18	nosp	not specified		*p*	BSAO	54STR/ICK

Table 62.139.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	18	18	0.234	3.06–2	0.12	6.47–5	0
Temp. range K		A_1	A_2				Level of uncertainty
255.6–304.6		2.14563+1	1.71248				IV

Name: 2-Methoxy-2-methylpropanenitrile
Formula: C_5H_9NO

CAS-RN: 76474-09-4
Group No.: 62-140
Molar Mass: 99.13

Table 62.140.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95VER/BEC	298.00	1.760	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 4-Methyl-3-morpholinone
Formula: $C_5H_9NO_2$

CAS-RN: 20721-78-2
Group No.: 62-141
Molar Mass: 115.13

Table 62.141.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92KOL/POT	N	293.1–333.1	5 S	nosp	not specified		*p*	not specified	
92KOL/POT	the origin of data unclear								

Table 62.141.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	5	5	0.272	1.38−1	0.54	7.90−4	1
Temp. range K		A_1	A_2				Level of uncertainty
293.1–333.1		3.62591	6.78168				VI

Name: Methyl ester *N*,*N*-dimethylglycine
Formula: $C_5H_{11}NO_2$

CAS-RN: 7148-06-3
Group No.: 62-142
Molar Mass: 117.15

Table 62.142.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92VER/BEC	298.15	2.427	nosp	99.995	chrom	*p*	BDHT	69PER/COM

Name: *N*,*N*-Diethylurea
Formula: $C_5H_{12}N_2O$

CAS-RN: 634-95-7
Group No.: 62-143
Molar Mass: 116.16

Table 62.143.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86KRA/KOZ	380.0–400.0	2	2.00	99.97	anal	*p*	BDHT	92KAB/KOZ

Table 62.143.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
380.0–400.0		2.12881+1	3.00678				V

Name: 2-(Propylamino)ethanol
Formula: $C_5H_{13}NO$

CAS-RN: 16369-21-4
Group No.: 62-144
Molar Mass: 103.16

Table 62.144.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97MAH/HEP	299.1–397.8	5	nosp	98.	anal	*p*	BDCT	91BAN/GAR

Table 62.144.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	5	5	0.822	2.90–1	0.82	2.79–3	1
Temp. range K		A_1	A_2				Level of uncertainty
299.1–397.8		9.35863	7.31011				IV

Name: 2,2′-(Methylimino)bisethanol
Formula: $C_5H_{13}NO_2$

CAS-RN: 105-59-9
Group No.: 62-145
Molar Mass: 119.16

Table 62.145.1. Experimental heat capacities

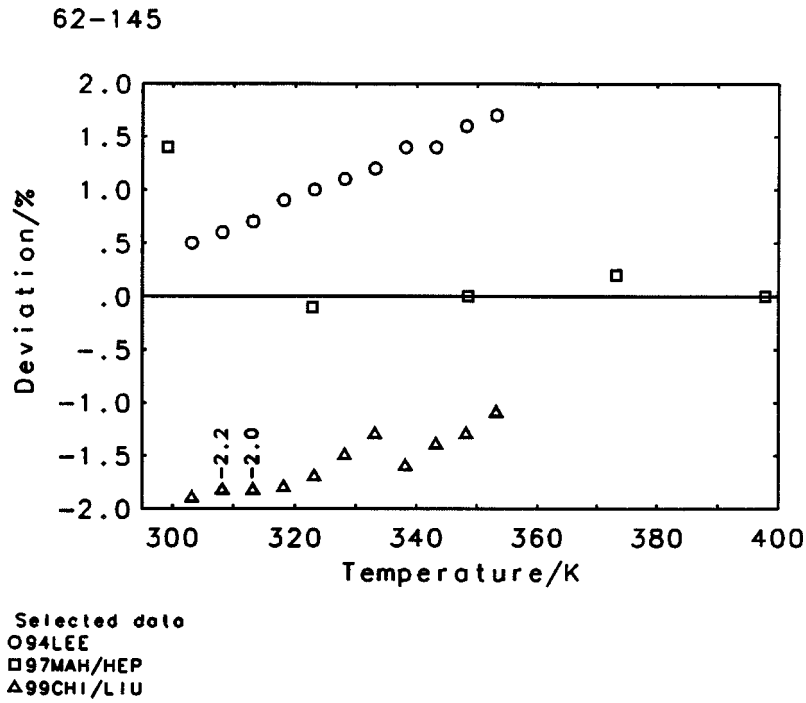
Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94LEE	303.1–353.1	11 S	nosp	not specified		p	not specified	
97MAH/HEP	299.1–397.8	5	nosp	99.0	anal	p	BDCT	91BAN/GAR
99CHI/LIU	303.1–353.1	11	1.00	98.5	anal	p	BDHT	99CHI/LIU

Table 62.145.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
94LEE	303.1–353.1	11	1.00 #	1.161	4.13–1	1.16	3.85–1	11
97MAH/HEP	299.1–397.8	5	0.50 #	1.267	2.07–1	0.63	1.06–1	1
99CHI/LIU	303.1–353.1	11	1.00	1.658	5.53–1	1.66	−5.45–1	−11

Table 62.145.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	27	27	1.457	4.67–1	1.37	−4.53–2	1
Temp. range K		A_1	A_2				Level of uncertainty
299.1–397.8		9.45850	7.57912				V



Name: 1-Ethenyl-2-pyrrolidinone
Formula: C_6H_9NO

CAS-RN: 88-12-0
Group No.: 62-146
Molar Mass: 111.14

Table 62.146.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97KUL/LEB2	288.8–328.1	12	0.20	99.42	melpt	*p*	BSAO	76LEB/LIT

Table 62.146.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	12	12	0.976	4.59–2	0.20	1.51–4	2
Temp. range K		A_1	A_2				Level of uncertainty
288.8–328.1		1.51598+1	2.78914				III

Name: Ethyl ester 2-cyanopropanoic acid
Formula: $C_6H_9NO_2$

CAS-RN: 1572-99-2
Group No.: 62-147
Molar Mass: 127.14

Table 62.147.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95VER/BEC	298.00	2.400	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: Tetrahydro-5,5-dimethyl-2*H*-1,3-oxazin-2-one
Formula: $C_6H_{11}NO_2$

CAS-RN: 54953-79-6
Group No.: 62-148
Molar Mass: 129.16

Table 62.148.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96LEB/SMI	395.1–499.0	23	2.50	not specified		*p*	BDHT	92KAB/KOZ

Table 62.148.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	23	23	0.496	9.28–1	1.24	−2.23–2	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
395.1–420.0	6.66400+5	−4.75603+5	1.13159+5	−8.97485+3	V
420.0–499.0	5.31153+3	−3.39671+3	7.28556+2	−5.18270+1	V

Name: Ethyl ester *N*,*N*-dimethylglycine
Formula: $C_6H_{13}NO_2$

CAS-RN: 33229-89-9
Group No.: 62-149
Molar Mass: 131.17

Table 62.149.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92VER/BEC	298.15	1.862	nosp	99.995	chrom	*p*	BDHT	69PER/COM

Name: Methyl ester *N*,*N*-dimethyl-*L*-alanine
Formula: $C_6H_{13}NO_2$

CAS-RN: 42293-86-7
Group No.: 62-150
Molar Mass: 131.17

Table 62.150.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92VER/BEC	298.15	2.046	nosp	99.995	chrom	*p*	BDHT	69PER/COM

Name: 2-(Diethylamino)ethanol
Formula: $C_6H_{15}NO$

CAS-RN: 100-37-8
Group No.: 62-151
Molar Mass: 117.19

Table 62.151.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97MAH/HEP	299.1–397.8	5	nosp	99.0	chrom	*p*	BDCT	91BAN/GAR

Table 62.151.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	5	5	0.326	1.19–1	0.33	3.56–4	0

Temp. range K	A_1	A_2	Level of uncertainty
299.1–397.8	1.65621+1	5.67486	IV

Name: 2,2′-(Ethylimino)bisethanol
Formula: $C_6H_{15}NO_2$

CAS-RN: 139-87-7
Group No.: 62-152
Molar Mass: 133.19

Table 62.152.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97MAH/HEP	299.1–397.8	5	nosp	98.	anal	*p*	BDCT	91BAN/GAR

Table 62.152.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	5	5	0.930	3.75–1	0.93	2.76–3	−1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
299.1–397.8		4.22183+1	−9.15515	2.41072			IV

Name: 1,1′-Iminobis-2-propanol
Formula: $C_6H_{15}NO_2$

CAS-RN: 110-97-4
Group No.: 62-153
Molar Mass: 133.19

Table 62.153.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99CHI/LIU	323.1–353.1	7	3.00	95.	anal	*p*	BDHT	99CHI/LIU

Table 62.153.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	7	7	0.000	2.41–6	0.00	−1.09–6	0
Temp. range K		A_1	A_2				Level of uncertainty
323.1–353.1		1.34736+1	9.61145				VI

Name: 2,2′-(1,2-Ethanediyldiimino)bisethanol
Formula: $C_6H_{16}N_2O_2$

CAS-RN: 4439-20-7
Group No.: 62-154
Molar Mass: 148.21

Table 62.154.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97STE/CHI3	N	395.0–475.0	5	1.00	99.95	chrom	sat	BDHT	89KNI/ARC
97STE/CHI3	an equation in 97STE/CHI4								

Table 62.154.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	5	5	0.222	1.21−1	0.22	2.43−4	−1

Temp. range K	A_1	A_2	Level of uncertainty
395.0−475.0	2.26299+1	7.11464	IV

Name: Isocyanatobenzene
Formula: C_7H_5NO

CAS-RN: 103-71-9
Group No.: 62-155
Molar Mass: 119.12

Table 62.155.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
85BYK/LEB		241.6−330.0	4 S	0.30	99.86	melpt	p	BSAO	76LEB/LIT
93STE/CHI2	N	300.0−480.0	10	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

93STE/CHI2 same data in 96STE/CHI2

Table 62.155.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
85BYK/LEB	241.6−330.0	4	0.30	1.477	1.00−1	0.44	−4.17−2	0
93STE/CHI2	300.0−480.0	10	1.00	1.252	2.93−1	1.25	1.97−1	6

Table 62.155.3. Parameters of regression polynomial

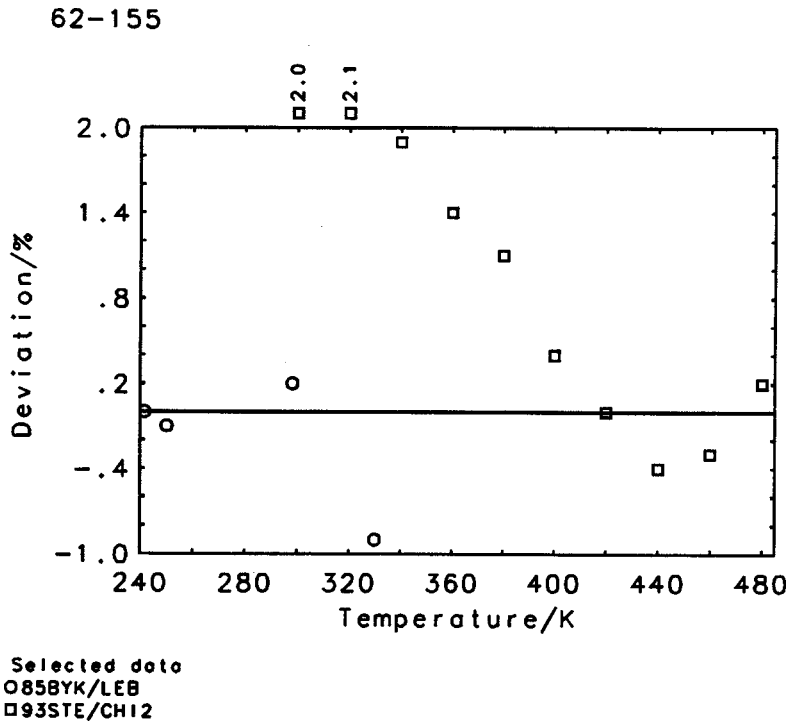
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	14	14	1.562	3.00−1	1.28	1.28−1	6
sat	14	14	1.564	3.00−1	1.28	1.29−1	6

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
241.6−480.0	3.13347+1	−1.14257+1	3.60368	−2.79514−1	IV
241.6−480.0	3.16554+1	−1.17483+1	3.71041	−2.91140−1	IV

Table 62.155.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	14	14	2.384	2.30−1	0.98	3.69−2	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
241.6−480.0	675.00	−4.98547	1.07345	1.47947+1	5.78858	IV



Name: 2-Propenyl ester 2-cyano-2-propenoic acid
Formula: $C_7H_7NO_2$

CAS-RN: 7324-02-9
Group No.: 62-156
Molar Mass: 137.14

Table 62.156.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93KIP/BYK	265.3–330.0	4 S	0.20	99.50	melpt	*p*	BSAO	76LEB/LIT

Table 62.156.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	4	4	0.821	4.92–2	0.16	9.63–5	0

Temp. range K	A_1	A_2	Level of uncertainty
265.3–330.0	2.16035+1	2.77940	III

Name: 2-Methoxy-3,3-dimethylbutanenitrile
Formula: $C_7H_{13}NO$

CAS-RN: 162047-91-8
Group No.: 62-157
Molar Mass: 127.19

Table 62.157.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95VER/BEC	298.00	2.220	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 2-Methoxy-2-methylpentanenitrile
Formula: $C_7H_{13}NO$

CAS-RN: 162047-90-7
Group No.: 62-158
Molar Mass: 127.19

Table 62.158.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95VER/BEC	298.00	1.670	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 2-Piperidineethanol
Formula: $C_7H_{15}NO$

CAS-RN: 1484-84-0
Group No.: 62-159
Molar Mass: 129.20

Table 62.159.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99CHI/LIU	303.1–353.1	11	3.00	95.	anal	*p*	BDHT	99CHI/LIU

Table 62.159.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	11	11	0.047	5.20−2	0.14	1.11−4	−1
Temp. range K		A_1	A_2				Level of uncertainty
303.1–353.1		8.39210	8.84639				VI

Name: Methyl ester *N*,*N*,2-trimethylalanine
Formula: $C_7H_{15}NO_2$

CAS-RN: 140653-59-4
Group No.: 62-160
Molar Mass: 145.20

Table 62.160.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92VER/BEC	298.15	2.176	nosp	99.91	chrom	*p*	BDHT	69PER/COM

Name: 4-Ethoxybenzenamine
Formula: $C_8H_{11}NO$

CAS-RN: 156-43-4
Group No.: 62-161
Molar Mass: 137.18

Table 62.161.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
74OVC/BAT	333.1–343.1	2 S	nosp	not specified		*p*	not specified	

Table 62.161.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	3.82−6	0
Temp. range K		A_1	A_2				Level of uncertainty
333.1–343.1		8.08714+1	−1.17386+1				VI

Name: 2-[Bis(1-methylethyl)amino] ethanol
Formula: $C_8H_{19}NO$

CAS-RN: 96-80-0
Group No.: 62-162
Molar Mass: 145.24

Table 62.162.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97MAH/HEP	299.1–397.8	5	nosp	not specified		*p*	BDCT	91BAN/GAR

Table 62.162.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	5	5	0.396	1.69−1	0.40	4.90−4	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
299.1–397.8		6.51355+1	−1.79996+1	3.37172			IV

Name: 2,2′-(Butylimino)bisethanol
Formula: $C_8H_{19}NO_2$

CAS-RN: 102-79-4
Group No.: 62-163
Molar Mass: 161.24

Table 62.163.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97MAH/HEP	299.1–397.8	5	nosp	not specified		*p*	BDCT	91BAN/GAR

Table 62.163.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	5	5	0.597	2.80−1	0.60	2.62−3	1
Temp. range K		A_1	A_2				Level of uncertainty
299.1–397.8		1.92073+1	8.32587				IV

Name: 2,2′-[(1,1-Dimethylethyl)imino]bisethanol
Formula: $C_8H_{19}NO_2$

CAS-RN: 2160-93-2
Group No.: 62-164
Molar Mass: 161.24

Table 62.164.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97MAH/HEP	322.8–397.8	4	nosp	not specified		*p*	BDCT	91BAN/GAR

Table 62.164.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	4	4	0.286	1.37−1	0.29	1.89−4	−2
Temp. range K		A_1	A_2				Level of uncertainty
322.8–397.8		1.36217+1	9.83623				IV

Name: 4-(Dimethylamino)benzaldehyde
Formula: $C_9H_{11}NO$

CAS-RN: 100-10-7
Group No.: 62-165
Molar Mass: 149.19

Table 62.165.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99MEN/LIA	N	349.0–361.7	4	0.50	99.74	melpt	*p*	BSAO	83TAN/ZHO
99MEN/LIA	same data in 99MEN/TAN								

Table 62.165.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	4	4	0.029	5.29–3	0.01	−3.72–5	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
349.0–361.7	2.93632+2	−1.54963+2	2.32568+1	IV

Name: Ethyl ester 2-cyano-3-methyl-2-(1-methylethyl)butanoic acid
Formula: $C_{11}H_{19}NO_2$

CAS-RN: 62391-95-1
Group No.: 62-166
Molar Mass: 197.28

Table 62.166.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95VER/BEC	298.00	1.820	nosp	99.99	chrom	*p*	BDHT	69PER/COM

Name: 1-Oxide diphenyldiazene
Formula: $C_{12}H_{10}N_2O$

CAS-RN: 495-48-7
Group No.: 62-167
Molar Mass: 198.22

Table 62.167.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	326.15	1.100	nosp	not specified		avg	DSIO	*94BRU
*94BRU	average value in temperature range 318–334 K								

Name: 4,4′-Oxybis-1,2-benzenediamine
Formula: $C_{12}H_{14}N_4O$

CAS-RN: 2676-59-7
Group No.: 62-168
Molar Mass: 230.27

Table 62.168.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
77KAR/RAB	N	435.7–512.8	8	1.50	99.25	melpt	*p*	BDAO	51POP/GAL
77KAR/RAB	data from a graph only								

Table 62.168.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	8	8	0.166	1.70−1	0.25	5.17−4	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
435.7–512.8		−2.50428+1	3.65322+1	−3.52386			V

Name: α-[(Cyclohexyloxy)methyl]-4-morpholineethanol
Formula: $C_{13}H_{25}NO_3$

CAS-RN: 95639-17-1
Group No.: 62-169
Molar Mass: 243.35

Table 62.169.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
88GEI/MEK	213.7–306.4	49	nosp	not specified		p	BSAO	54STR/ICK

Table 62.169.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	49	49	0.893	3.43−1	0.63	4.21−3	−5
Temp. range K		A_1	A_2				Level of uncertainty
213.7–306.4		3.59073+1	6.81549				V

Name: 1-Anilino-3-piperidino-2-propanol
Formula: $C_{14}H_{22}N_2O$

CAS-RN: 14585-29-6
Group No.: 62-170
Molar Mass: 234.34

Table 62.170.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
88DZH/MEK	402.4–420.5	10	nosp	not specified		p	BSAO	54STR/ICK

Table 62.170.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	10	10	0.426	1.87−1	0.30	8.90−4	0
Temp. range K		A_1	A_2				Level of uncertainty
402.4–420.5		5.29539+1	2.37712				V

Name: Decyl ester 2-cyano-2-propenoic acid
Formula: $C_{14}H_{23}NO_2$

CAS-RN: 3578-07-2
Group No.: 62-171
Molar Mass: 237.34

Table 62.171.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93BYK/KIP	294.5–330.0	4 S	0.20	99.54	melpt	p	BSAO	76LEB/LIT

Table 62.171.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	4	4	0.112	1.35–2	0.02	4.77–6	0
Temp. range K		A_1	A_2				Level of uncertainty
294.5–330.0		3.91839+1	7.24141				III

Name: α-[(Cyclohexyloxy)methyl]-1-piperidineethanol
Formula: $C_{14}H_{27}NO_2$

CAS-RN: 96450-92-9
Group No.: 62-172
Molar Mass: 241.37

Table 62.172.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
89GEI/ZEI	209.4–302.7	32	nosp	not specified		p	BSAO	54STR/ICK

Table 62.172.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	32	32	0.967	4.23–1	0.77	5.78–3	5
Temp. range K		A_1	A_2				Level of uncertainty
209.4–302.7		2.89235+1	1.02756+1				IV

Name: (1-Methylethylidene)di-1,4-phenylene ester cyanic acid
Formula: $C_{17}H_{14}N_2O_2$

CAS-RN: 1156-51-0
Group No.: 62-173
Molar Mass: 278.31

Table 62.173.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
75LEB/ARO	N	355.8–420.0	3 S	nosp	not specified		p	BSAO	68LEA
77LEB/RAB1	N	355.9–420.0	8 S	0.30	not specified		p	BSAO	76LEB/LIT

75LEB/ARO data above 380 K obtained by extrapolation; experim. data drop down at 380 K due to polymerization
77LEB/RAB1 only a graph given in the paper; smoothed values provided by the authors

Table 62.173.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
77LEB/RAB1	355.9–420.0	8	0.30	0.131	2.25–2	0.04	−1.67–5	−1
Rejected data								
75LEB/ARO	(1.81–2,0.03,−1.72–2,−2)							

Table 62.173.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	11	8	0.151	2.59−2	0.05	−1.67−5	−1

Temp. range K	A_1	A_2	Level of uncertainty
355.9–420.0	6.67944	1.33918+1	IV

Name:
(*E*,*E*)-*N*,*N*′-Bis[[4-(octyloxy)phenyl]methylene]-1,4-benzenediamine
Formula: $C_{36}H_{48}N_2O_2$

CAS-RN: 29273-90-3
Group No.: 62-174
Molar Mass: 540.79

Table 62.174.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
92CHE/JIN	530.0–550.0	3	nosp	not specified		*p*	BDHT	90JIN/WUN

Table 62.174.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	3	3	0.031	9.57−2	0.06	3.05−5	1

Temp. range K	A_1	A_2	Level of uncertainty
530.0–550.0	1.72376+2	−3.70858	VI

Name: Sulfinylbismethane
Formula: C_2H_6OS

CAS-RN: 67-68-5
Group No.: 63-001
Molar Mass: 78.14

Table 63.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
60KEN/LIN		298.1–343.1	2	nosp	not specified		*p*	BSIO	57KEN
62MUR/YAM	N	315.6	1	nosp	not specified		avg	not specified	
62SHE/NIN	N	288.1	1	nosp	not specified		*p*	not specified	
70CLE/WES		295.8–348.0	12	0.15	99.96	chrom	*p*	BSAO	68WES/FUR
78DEV/HEU		298.1	1	1.00	99.8	chrom	*p*	BSIO	70LKB/COM
79DEV/SOM		298.1	1	1.00	99.8	chrom	*p*	BSIO	70LKB/COM
86KOR/KUK		298.0	1	0.20	not specified		*p*	BSAO	83KUK/KOR
87LAN/CRI	N	298.1–353.1	3	nosp	not specified		*p*	FSIO	87LAN/CRI
88ROD/MAR	N	298.1	1	nosp	not specified		*p*	BSIO	88ROD/MAR
89BAR/KOO1		298.1	1	nosp	not specified		*p*	FSIT	71PIC/LED
91GRO/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
92MIY/TAM1		298.1	1	nosp	99.6	chrom	*p*	FSIO	85OGA/MUR
93BAS/VOL	N	298.1	1	nosp	99.5	chrom	*p*	DDCT	71KON/SUU
93CON/GIR1		298.0–356.0	eqn	5.00	not specified		sat	BDHT	93CON/GIR1
93GRO/ROU		298.1	1	nosp	99.5	anal	*p*	FSIT	71PIC/LED
93NAK/CHU		298.1	1	0.50	99.97	chrom	*p*	FSIO	85OGA/MUR
94GRO/ROU		298.1	1	nosp	99.0	anal	*p*	FSIT	71PIC/LED

62MUR/YAM	average value in temperature range 298–333 K
62SHE/NIN	very unreliable data under melting point temperature
87LAN/CRI	C_p at 298.15 K measured by Picker calorimeter (71PIC/LED)
88ROD/MAR	water content 0.009% (Karl Fisher method)
93BAS/VOL	content of water less than 0.05 mol.% by Karl Fischer method

Name: Tetrahydrothiophene 1,1-dioxide
Formula: $C_4H_8O_2S$

CAS-RN: 126-33-0
Group No.: 63-004
Molar Mass: 120.17

Table 63.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
59DEA/EVA	N	303.1–473.1	3 S	nosp	not specified		*p*	not specified	
69TOM/LIN		303.1	1	nosp	not specified		*p*	BSIO	69TOM/LIN
81CAS/ING		303.1	1	1.00	not specified		*p*	BDCT	68WAD
97STE/CHI2		315.1–555.1	13	nosp	99.95	chrom	sat	BDHT	89KNI/ARC

59DEA/EVA data of firm Shell Development Company, Emeryville, Calif.

Table 63.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
81CAS/ING	303.1	1	1.00	0.853	1.83–1	0.85	−1.83–1	−1
97STE/CHI2	315.1–555.1	13	1.00 #	0.407	1.05–1	0.41	1.51–2	1
Rejected data								
59DEA/EVA	(3.48,15.24,−3.47,−2)		69TOM/LIN	(2.73,14.45,−2.73,−1)				

Table 63.4.3. Parameters of regression polynomial

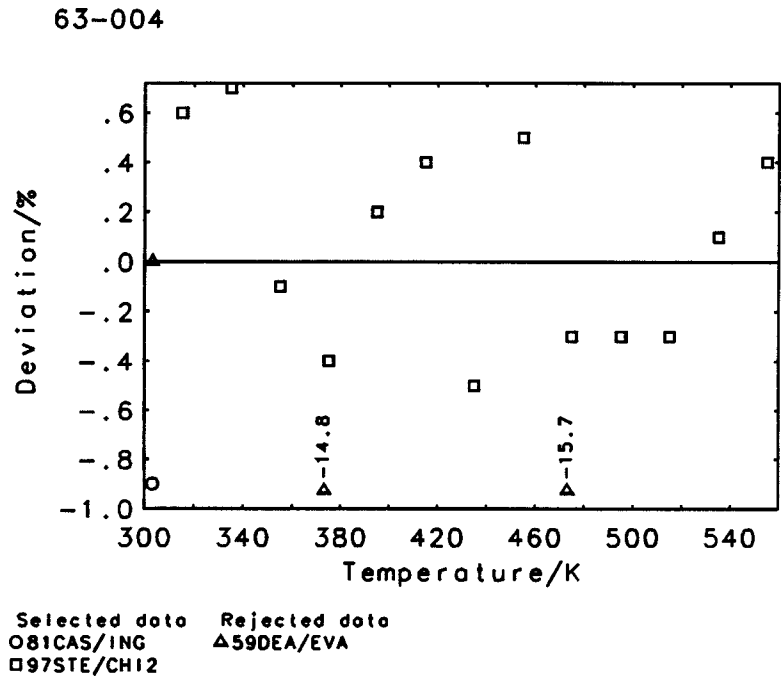
Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	18	14	0.512	1.27–1	0.51	9.90–4	0
sat	18	14	0.509	1.26–1	0.51	9.78–4	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
303.1–555.1	8.56005	4.63641	−1.10798–1	IV
303.1–555.1	8.49829	4.66945	−1.15118–1	IV

Table 63.4.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	18	14	0.483	1.18–1	0.48	8.04–4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
303.1–555.1	855.00	3.52775+1	7.60354	−6.30495	1.10818+2	−8.11499+1	5.42525+1	IV



Name: Phenoxathiin
Formula: $C_{12}H_8OS$

CAS-RN: 262-20-4
Group No.: 63-007
Molar Mass: 200.26

Table 63.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93STE/CHI1	313.3–439.8	15	0.10	99.987	melpt	sat	BSAO	88STE/ARC
93STE/CHI1	360.0–700.0	18 S	1.00	99.987	melpt	sat	BDHT	89KNI/ARC

Table 63.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
93STE/CHI1	313.3–439.8	15	0.10	0.267	9.76–3	0.03	−1.04–4	0
93STE/CHI1	360.0–700.0	18	1.00	0.101	4.89–2	0.10	9.08–3	0

Table 63.7.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	33	33	0.211	3.98–2	0.08	4.90–3	0
sat	33	33	0.214	4.11–2	0.08	4.80–3	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
313.3–450.0	8.14990	1.18499+1	−1.68434	1.44824−1	II
450.0–700.0	−1.48416+1	2.71775+1	−5.09048	3.97130−1	IV
313.3–450.0	8.01977	1.19561+1	−1.71307	1.47396−1	II
450.0–700.0	−1.34246+1	2.62524+1	−4.89003	3.82726−1	IV

Table 63.7.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	33	33	0.677	1.57−1	0.30	−1.45−2	−12

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
313.3–700.0	863.00	4.44839	5.22453	8.60034	6.24508+1	−3.76148+1	1.46917+1	IV

Name: S-(4-Pentylphenyl) ester 4-(heptyloxy)benzenecarbothioic acid
Formula: $C_{25}H_{34}O_2S$

CAS-RN: 61519-00-4
Group No.: 63-008
Molar Mass: 398.61

Table 63.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
81CHR/RIC	N	356.3–364.3	2 S	nosp	not specified		sat	BDHT	69PER/COM

81CHR/RIC data from a graph only

Table 63.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
356.3–364.3	1.55114+2	−1.57256+1	VI

Name: 1-Chloro-3-nitrobenzene
Formula: $C_6H_4ClNO_2$

CAS-RN: 121-73-3
Group No.: 64-017
Molar Mass: 157.56

Table 64.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	332.1	1	nosp	not specified		avg	DSIO	*94BRU
08BOG/WIN	N	338.1	1	nosp	not specified		avg	DSIO	08BOG/WIN

*94BRU average value in temperature range 326–338 K
08BOG/WIN average value in temperature range 318–358 K

Table 64.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*94BRU	332.1	1	3.00 #	4.810	4.98	14.43	4.98	1
08BOG/WIN	338.1	1	3.00 #	3.704	2.95	11.11	−2.95	−1

Table 64.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
C	2	2	6.071	5.79	18.21	1.01	0
Temp. range K		A_1					Level of uncertainty
332.1–338.1		2.95121+1					VI

Name: 1-Chloro-4-nitrobenzene
Formula: $C_6H_4ClNO_2$

CAS-RN: 100-00-5
Group No.: 64-018
Molar Mass: 157.56

Table 64.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
*94BRU	N	364.6	1	nosp	not specified		avg	DSIO	*94BRU
78MAR/ClO1	N	354.6–466.9	2	nosp	not specified		*p*	DSIO	71MAR/CIO

*94BRU average value in temperature range 361–368 K
78MAR/CIO1 constant value calculated from temperature dependence of enthalpy by the authors

Table 64.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
*94BRU	364.6	1	3.00 #	0.000	0.00	0.00	0.00	0

Table 64.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
364.6–364.6		2.74325+1					VI

Name: 2,2,2-Trifluoroacetamide
Formula: $C_2H_2F_3NO$

CAS-RN: 354-38-1
Group No.: 64-031
Molar Mass: 113.04

Table 64.31.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00DI/TAN	N	353.9–403.7	86	0.50	99.3	melpt	*p*	BSAO	95TAN/SUN

#00DI/TAN at 389.9 K transition from liquid crystalline phase to fully liquid phase

Table 64.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	86	16	0.623	8.10−2	0.31	4.39−4	3
Temp. range K		A_1	A_2				Level of uncertainty
393.5–403.6		−1.95732+1	1.14535+1				IV

Name: 2-Bromothiophene
Formula: C_4H_3BrS

CAS-RN: 1003-09-4
Group No.: 64-032
Molar Mass: 163.04

Table 64.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93FUJ/OGU1	209.2–298.8	38	0.20	99.92	melpt	sat	BSAO	93FUJ/OGU1

Table 64.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	38	38	0.176	5.98−3	0.04	4.01−6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
209.2–298.8		2.00145+1	−4.88687	1.92123	−1.96639−1		II

Table 64.32.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	38	38	0.227	7.70−3	0.05	7.13−6	−1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
209.2–298.8	677.00	1.05779+1	7.94730	7.70953	3.51984		III

Name: 2-Chlorothiophene
Formula: C_4H_3ClS

CAS-RN: 96-43-5
Group No.: 64-033
Molar Mass: 118.59

Table 64.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93FUJ/OGU2	204.4–300.3	33	0.30	99.98	melpt	sat	BSAO	93FUJ/OGU1

Table 64.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	33	33	0.133	6.55−3	0.04	1.94−6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
204.4–300.3		2.77198+1	−1.55850+1	6.37486	−7.98042−1		III

Table 64.33.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
sat	33	33	0.376	1.84−2	0.11	3.74−5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
204.4–300.3	635.00	2.41804−1	2.93863	1.14067+1	4.97420−3		III

Name: *O*-Ethyl ester 2,3,3-trichloro-2-propenethioic acid
Formula: $C_5H_5Cl_3OS$

CAS-RN: 76619-92-6
Group No.: 64-034
Molar Mass: 219.52

Table 64.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
81SHA/AND	243.0–300.0	5 S	0.50	99.57	melpt	*p*	BSAO	80SHA/LYU

Table 64.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	5	5	0.136	2.17−2	0.07	2.02−5	−1
Temp. range K		A_1	A_2				Level of uncertainty
243.0–300.0		2.35333+1	3.09908				IV

Name: 4-Chlorobenzenamine
Formula: C_6H_6ClN

CAS-RN: 106-47-8
Group No.: 64-035
Molar Mass: 127.57

Table 64.35.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter reference
*94BRU	N	356.15	1.699	nosp	not specified		avg	DSIO	*94BRU

*94BRU average value in temperature range 344–388 K

Name: 2-Fluorobenzenamine
Formula: C_6H_6FN

CAS-RN: 348-54-9
Group No.: 64-036
Molar Mass: 111.12

Table 64.36.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91LIC	244.15	1.713	2.00	99.	anal	*p*	BDCT	89BRE/LIC

Name: 2,2,3,3-Tetrafluoropropyl ester 2-cyano-2-propenic acid
Formula: $C_7H_5F_4NO_2$

CAS-RN: 27827-91-4
Group No.: 64-037
Molar Mass: 211.12

Table 64.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95LEB/BYK	287.4–330.0	4 S	0.20	98.3	melpt	*p*	BSAO	76LEB/LIT

Table 64.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	4	4	0.213	1.57–2	0.04	5.72–6	0

Temp. range K	A_1	A_2	Level of uncertainty
287.4–330.0	3.19867+1	1.65816	III

Name: *O*-Butyl ester 2,3,3-trichloro-2-propenethioic acid
Formula: $C_7H_9Cl_3OS$

CAS-RN: 79886-21-8
Group No.: 64-038
Molar Mass: 247.57

Table 64.38.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
81SHA/AND	232.9–300.0	5 S	0.50	98.7	melpt	*p*	BSAO	80SHA/LYU

Table 64.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	5	5	0.052	1.01–2	0.03	3.05–6	−1

Temp. range K	A_1	A_2	Level of uncertainty
232.9–300.0	2.97555+1	3.43239	IV

Name: *O*-Pentyl ester 2,3,3-trichloro-2-propenethioic acid
Formula: $C_8H_{11}Cl_3OS$

CAS-RN: 76619-94-8
Group No.: 64-039
Molar Mass: 261.60

Table 64.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
81SHA/AND	219.4–300.0	5 S	0.50	98.8	melpt	*p*	BSAO	80SHA/LYU

Table 64.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	5	5	1.033	2.26−1	0.52	1.34−3	−3

Temp. range K	A_1	A_2	Level of uncertainty
219.4–300.0	3.36753+1	3.55386	IV

Name: 2-[[3-(Trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid
Formula: $C_{13}H_9F_3N_2O_2$

CAS-RN: 4394-00-7
Group No.: 64-040
Molar Mass: 282.22

Table 64.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
89PIN/GON	483.0–499.0	2	nosp	not specified		*p*	BDHT	69PER/COM

Table 64.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	−7.63−6	0

Temp. range K	A_1	A_2	Level of uncertainty
483.0–499.0	−1.35028+2	4.28468+1	VI

Name: 2-(4-Morpholinyl)ethyl ester 2-[[3-trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid
Formula: $C_{19}H_{20}F_3N_3O_3$

CAS-RN: 65847-85-0
Group No.: 64-041
Molar Mass: 395.38

Table 64.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
89PIN/GON	356.0–439.0	eqn	nosp	not specified		*p*	BDHT	69PER/COM

Table 64.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	10	10	0.000	6.61−6	0.00	4.58−6	0

Temp. range K	A_1	A_2	Level of uncertainty
356.0–438.8	1.70786+1	1.68380+1	V

Name: Ethenyltrimethylsilane
Formula: $C_5H_{12}Si$

CAS-RN: 754-05-2
Group No.: 71-010
Molar Mass: 100.24

Table 71.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
73LEB/TSV		141.6–300.0	6 S	0.50	99.67	melpt	*p*	BSAO	66NIK/LEB
75RAB/LEB	N	141.6–300.0	5 S	0.50	99.67	melpt	*p*	BSAO	66NIK/LEB

75RAB/LEB smoothed value at 298.15 K in 81LEB/LEB

Table 71.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
73LEB/TSV	170.0–300.0	5	0.50	0.632	6.93–2	0.32	−1.99–2	1
75RAB/LEB	141.6–300.0	5	0.50	0.768	8.25–2	0.38	2.11–2	3

Table 71.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w %	s/R %	s_r %	s_b/R %	±
p	11	10	0.786	8.52–2	0.39	6.14–4	4

Temp. range K	A_1	A_2	Level of uncertainty
141.6–300.0	1.82178+1	1.87339	III

Name: Tetraethylsilane
Formula: $C_8H_{20}Si$

CAS-RN: 631-36-7
Group No.: 71-022
Molar Mass: 144.33

Table 71.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
54STA/WAR	190.0–220.0	4 S	1.00	99.9	melpt	*p*	BSAO	49STA/GUP
72MAS/RAB	200.0–300.0	12 S	0.40	99.8	melpt	*p*	BSAO	56POP/KOL
91STE/CHI2	300.0–600.0	16	1.00	99.95	chrom	sat	BDHT	89KNI/ARC

Table 71.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w %	d/R %	d_r %	d_b/R %	±
Selected data								
72MAS/RAB	200.0–300.0	12	0.40	0.574	8.12–2	0.23	1.95–2	0
91STE/CHI2	300.0–600.0	16	1.00	1.357	9.38–1	1.36	−5.77–2	−3
Rejected data								
54STA/WAR	(3.61–1,1.12,3.46–1,3)							

Table 71.22.3. Parameters of cubic spline polynomials

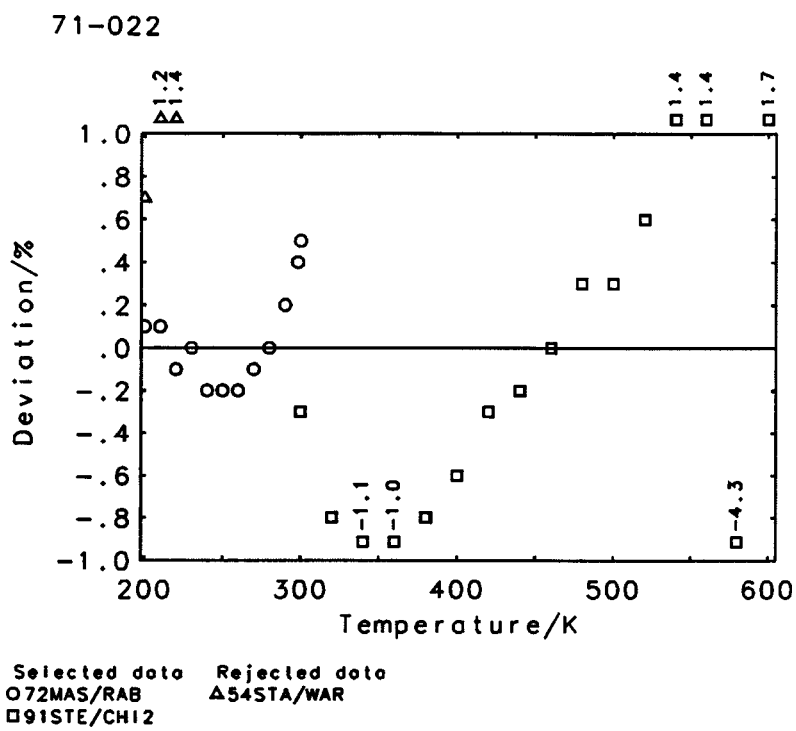
Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
total	used						
p	32	28	1.232	8.02−1	1.17	−2.46−2	−3
sat	32	28	0.837	4.42−1	0.75	−3.59−2	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
200.0–320.0	3.61385+1	−1.16417+1	6.10923	−7.55797−1	III
320.0–540.0	−3.44614+1	5.45457+1	−1.45743+1	1.39874	IV
540.0–600.0	−2.12986+4	1.18680+4	−2.20224+3	1.36440+2	V
200.0–320.0	3.73895+1	−1.30576+1	6.63202	−8.18748−1	III
320.0–540.0	−3.50669+1	5.48703+1	−1.45954+1	1.39245	IV
540.0–600.0	−1.15081+4	6.42880+3	−1.19495+3	7.42540+1	V

Table 71.22.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	32	28	2.291	1.07	2.02	−1.39−1	−6

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
200.0–600.0	606.00	−6.28270	3.30397−1	2.56973+1	5.66748	7.42802	2.14298	V



Name: 1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane
Formula: $C_{16}H_{22}OSi_2$

CAS-RN: 56-33-7
Group No.: 71-039
Molar Mass: 286.52

Table 71.39.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
83DZH/KUL		250.0–300.0	7 S	0.20	not specified		*p*	BSAO	54STR/ICK
86DZH/KUL2	N	170.0–300.0	eqn	0.20	not specified		*p*	BSAO	54STR/ICK
96FUJ/MIZ		228.9–302.3	30	0.30	99.78	melpt	*p*	BSAO	93FUJ/OGU1

86DZH/KUL2 low temperature limit is below n.m.t.; undercooled liquid

Table 71.39.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
96FUJ/MIZ	228.9–302.3	30	0.30	0.101	1.60–2	0.03	8.77–6	0
Rejected data								
83DZH/KUL	(4.39,7.42,4.37,7)		86DZH/KUL2		(4.07,7.03,4.05,8)			

Table 71.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	51	30	0.106	1.69–2	0.03	8.77–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
228.9–302.3		4.39628+1	−3.62630−1	1.49525			III

Name: 1-[2-(Trimethylsilyl)ethyl]aziridine
Formula: $C_7H_{17}NSi$

CAS-RN: 18387-12-7
Group No.: 71-043
Molar Mass: 143.30

Table 71.43.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
74LEB/TSV	N	182.8–299.5	21	0.50	98.93	melpt	*p*	BSAO	66NIK/LEB

74LEB/TSV smoothed values in 75LEB/TSV2 and data given graphically in 74LEB/RAB

Table 71.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	21	21	0.378	6.35–2	0.19	1.96–4	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
182.9–299.5		3.21177+1	−4.08928	1.81095			IV

Name: Trichloromethylsilane
Formula: CH_3Cl_3Si

CAS-RN: 75-79-6
Group No.: 71-057
Molar Mass: 149.48

Table 71.57.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
71SAM/KOS1	N	198.0–300.0	eqn	1.00	99.2	melpt	*p*	BSAO	54STR/ICK
71SAM/KOS1	data deposited in VINITI No.2423-71								

Table 71.57.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	11	11	0.005	9.76−4	0.01	−1.73−7	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
198.0–300.0		2.15114+1	−5.00141	2.15425	−2.31398−1		IV

Name: Dichlorodimethylsilane
Formula: $C_2H_6Cl_2Si$

CAS-RN: 75-78-5
Group No.: 71-058
Molar Mass: 129.06

Table 71.58.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
71SAM/KOS1	N	199.0–300.0	eqn	1.00	98.7	melpt	*p*	BSAO	54STR/ICK
71SAM/KOS1	data deposited in VINITI No. 2423-71								

Table 71.58.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	11	11	0.013	2.60−3	0.01	2.60−6	−1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
199.0–300.0		3.35295+1	−1.64664+1	5.98363	−6.41334−1		IV

Name: Dichloroethenylmethylsilane
Formula: $C_3H_6Cl_2Si$

CAS-RN: 124-70-9
Group No.: 71-059
Molar Mass: 141.07

Table 71.59.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
71GEI/DZH	176.6–298.1	14 S	nosp	99.42	melpt	*p*	BSAO	54STR/ICK

Table 71.59.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	14	14	0.004	1.78−3	0.01	−8.17−7	−2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
176.6–298.1		2.33206+1	4.59459−1	1.78626−1	−3.72401−2		V

Name: Chlorotrimethylsilane
Formula: C_3H_9ClSi

CAS-RN: 75-77-4
Group No.: 71-060
Molar Mass: 108.64

Table 71.60.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
71SAM/KOS2	N	218.0–300.0	eqn	1.00	99.41	melpt	p	BSAO	54STR/ICK
71SAM/KOS2	data deposited in VINITI No. 2501-71								

Table 71.60.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	10	10	0.005	9.84−4	0.00	1.91−6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
218.0–299.9		3.31456+1	−1.48170+1	5.45709	−5.63069−1		IV

Name: 1-(Trimethylsilyl)aziridine
Formula: $C_5H_{13}NSi$

CAS-RN: 2116-90-7
Group No.: 71-061
Molar Mass: 115.25

Table 71.61.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99KUL/LEB	197.8–310.0	27	0.20	99.17	melpt	p	BSAO	97VAR/DRU1

Table 71.61.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	27	27	1.363	7.23−2	0.27	3.39−4	−2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
197.8–310.0		3.55947+1	−1.03354+1	2.54277			IV

Name: Trimethyl-1-propynylsilane
Formula: $C_6H_{12}Si$

CAS-RN: 6224-91-5
Group No.: 71-062
Molar Mass: 112.25

Table 71.62.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97LEB/KUL	216.9–328.0	32	0.20	99.968	melpt	*p*	BSAO	76LEB/LIT

Table 71.62.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	32	32	0.347	1.83–2	0.07	2.25–5	−1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
216.9–328.0	1.12663+1	1.34470+1	−4.04028	4.27377−1	III

Name: Octamethyltrisiloxane
Formula: $C_8H_{24}O_2Si_3$

CAS-RN: 107-51-7
Group No.: 71-063
Molar Mass: 236.53

Table 71.63.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
86DZH/KUL1	190.8–300.5	23	nosp	not specified		*p*	BSAO	54STR/ICK

Table 71.63.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	23	23	0.241	2.34–1	0.48	2.15–3	1

Temp. range K	A_1	A_2	Level of uncertainty
190.8–300.5	3.20853+1	7.63582	V

Name: 1-Methyl-1-phenylsilacyclobutane
Formula: $C_{10}H_{14}Si$

CAS-RN: 3944-08-9
Group No.: 71-064
Molar Mass: 162.31

Table 71.64.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78LEB/RAB1	298.15	1.683	0.20	99.	chrom	*p*	BSAO	76LEB/LIT

Name: Bicyclo[2.2.1]hept-5-en-2-yltrimethylsilane
Formula: $C_{10}H_{18}Si$

CAS-RN: 17985-13-6
Group No.: 71-065
Molar Mass: 166.34

Table 71.65.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94LEB/SMI1	204.6–326.5	41	0.20	99.8	chrom	*p*	BSAO	76LEB/LIT

Table 71.65.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	41	40	3.389	2.25−1	0.68	2.81−3	−4

Temp. range K	A_1	A_2	A_3	Level of uncertainty
204.6–326.5	1.89811+1	3.64358	5.62335−1	III

Name: Hexamethyl phosphoric triamide
Formula: $C_6H_{18}N_3OP$

CAS-RN: 680-31-9
Group No.: 72-011
Molar Mass: 179.20

Table 72.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
73MOS/NIK		280.0–298.1	2 S	nosp	97.7	melpt	p	BSAO	66NIK/LEB
81CAS/ING		298.1	1	1.00	not specified		p	BDCT	68WAD
82VOR/YAK		298.1	1	nosp	not specified		p	BSAO	77VOR/PRI
85KOL/KUL		283.1–298.1	4 S	nosp	not specified		p	BSAO	75VYU/ZVE
92KOL/KUL2	N	283.1–328.1	4	0.05	not specified		p	BSAO	75VYU/ZVE

92KOL/KUL2 content of water 0.01%–0.02% by Karl Fischer method

Table 72.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
81CAS/ING	298.1	1	0.50 #	0.125	2.42–2	0.06	2.42–2	1
82VOR/YAK	298.1	1	0.50 #	0.454	8.77–2	0.23	−8.77–2	−1
85KOL/KUL	283.1–298.1	4	0.50 #	0.428	8.39–2	0.21	−2.92–2	−2
92KOL/KUL2	283.1–328.1	4	0.30 #	0.585	6.77–2	0.18	1.67–2	0
Rejected data								
73MOS/NIK	(1.73,4.27,1.73,1)							

Table 72.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	12	10	0.539	8.28–2	0.21	−1.14–2	−2

Temp. range K	A_1	A_2	Level of uncertainty
283.1–328.1	5.24323+1	−4.59506	III

Name: Trimethyl ester boric acid (H_3BO_3)
Formula: $C_3H_9BO_3$

CAS-RN: 121-43-7
Group No.: 72-016
Molar Mass: 103.91

Table 72.16.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
59HAN/HUG	N	249.6–298.2	10	nosp	not specified		p	not specified	
59HAN/HUG		273.1–353.1	9 S	nosp	not specified		p	FSIO	59HAN/HUG

59HAN/HUG private communication from D. White, Ohio State University, USA

Table 72.16.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
				%				
Selected data								
59HAN/HUG	249.6–298.2	10	1.00 #	0.220	4.90–2	0.22	1.68–3	4
59HAN/HUG	273.1–353.1	9	1.00 #	0.028	6.37–3	0.03	−1.60–3	−2

Table 72.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	19	19	0.170	3.79–2	0.17	1.27–4	2
Temp. range K	A_1	A_2					Level of uncertainty
249.6–353.1	1.51339+1	2.65342					V

Table 72.16.4. Parameters of quasipolynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	19	19	0.170	3.81–2	0.17	−1.27–4	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
249.6–353.1	502.00	−7.36017–1	1.18954–2	1.55823+1	1.13851+1		V

Name: 1-Ethyl-3-methyl-1*H*-imidazolium tetrafluoroborate
Formula: $C_6H_{11}BF_4N_2$

CAS-RN: 143314-16-3
Group No.: 72-017
Molar Mass: 197.97

Table 72.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98MUT/WIL	283.1–403.1	12	nosp	not specified		p	BDHT	98MUT/WIL

Table 72.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	12	12	0.728	6.72–1	2.18	2.43–2	2
Temp. range K		A_1	A_2				Level of uncertainty
283.1–403.1		2.78640+1	8.34830–1				VI

Name: Triethylphosphine
Formula: $C_6H_{15}P$

CAS-RN: 554-70-1
Group No.: 72-018
Molar Mass: 118.16

Table 72.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99SHE/KAM	191.4–298.3	27	0.20	99.95	melpt	p	BSAO	85RAB/SHE

Table 72.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	27	27	0.845	4.47−2	0.17	1.36−4	−2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
191.4–298.3		2.39175+1	−1.21834	9.17147−1			III

Name: Tributyl ester phosphoric acid
Formula: $C_{12}H_{27}O_4P$

CAS-RN: 126-73-8
Group No.: 72-019
Molar Mass: 266.32

Table 72.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
81NAZ/RUD	283.1–383.1	11	nosp	not specified		p	BDAO	51POP/GAL

Table 72.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	11	11	0.018	8.82−3	0.02	1.25−5	1
Temp. range K		A_1	A_2				Level of uncertainty
283.1–383.1		6.95364	1.29716+1				V

Name: Tris(anhydrosulfide) with phosphorotrithious acid dibutylcarbamodithioic acid
Formula: $C_{27}H_{54}N_3PS_6$

CAS-RN: 69267-83-0
Group No.: 72-020
Molar Mass: 644.12

Table 72.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
89AIR/DE	385.0–395.0	2	nosp	not specified		p	BDHT	87PER/COM

Table 72.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
385.0–395.0		1.32539+2					VI

Name: 1,6-Hexanediyl[diphenylphosphine]
Formula: $C_{30}H_{32}P_2$

CAS-RN: 19845-69-3
Group No.: 72-021
Molar Mass: 454.53

Table 72.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98ZHA/TAN	N	425.0–715.0	23	2.00	99.8	chrom	*p*	BDHT	96KAB/BLO
98ZHA/TAN	decomposition of the substance starts at 650 K and ends at 700 K in a single step								

Table 72.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	23	23	0.194	4.29–1	0.39	2.78–3	−1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
425.0–645.0		−1.58642+2	1.41973+2	−2.54006+1	1.54019		V

Name: [[(4*R*,5*R*)-2,2-Dimethyl-1,3-dioxolane-4,5-diyl]bis(methylene)]bis[diphenylphosphine]
Formula: $C_{31}H_{32}O_2P_2$

CAS-RN: 32305-98-9
Group No.: 72-022
Molar Mass: 498.54

Table 72.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00WU/TAN	366.4–378.2	7	nosp	98.37	melpt	*p*	BSAO	83TAN/ZHO

Table 72.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	7	7	0.159	1.84–1	0.16	3.97–4	1
Temp. range K		A_1	A_2				Level of uncertainty
366.4–378.2		−3.11252+1	3.94756+1				IV

Name: [1,1′-Binaphthalene]-2,2′-diylbis[bis(4-methylphenyl)phosphine]
Formula: $C_{48}H_{40}P_2$

CAS-RN: 153305-67-0
Group No.: 72-023
Molar Mass: 678.79

Table 72.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
97ZHA/GAO	540.0–660.0	13	2.00	99.8	chrom	*p*	BDHT	96KAB/BLO

Table 72.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	13	13	1.308	5.83	2.62	2.55−1	1

Temp. range K	A_1	A_2	Level of uncertainty
540.0–660.0	1.46177+2	1.28362+1	VI

Name: Tripropylaluminium
Formula: $C_9H_{21}Al$

CAS-RN: 102-67-0
Group No.: 73-027
Molar Mass: 156.25

Table 73.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
84SHE/NIS	150.0–298.1	4 S	0.20	99.9	chrom	p	BSAO	80GUR/GAV
91SHE/RAB	155.2–302.8	44	0.20	99.9	chrom	p	BSAO	76LEB/LIT

Table 73.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r	d_b/R	±
						%		
Selected data								
84SHE/NIS	200.0–298.1	3	0.20	0.452	3.31–2	0.09	1.03–2	1
91SHE/RAB	155.2–302.8	44	0.30 #	0.965	1.05–1	0.29	−9.48–4	2

Table 73.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	48	47	0.984	1.06–1	0.29	−2.27–4	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
155.2–302.8	1.47041+1	1.98606+1	−8.55031	1.62260	III

Name: (*E*)-(2-Chloroethenyl)arsonous dichloride
Formula: $C_2H_2AsCl_3$

CAS-RN: 50361-05-2
Group No.: 73-033
Molar Mass: 207.32

Table 73.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96LEB/KUL1	274.8–330.1	18	1.00	99.02	melpt	p	BSAO	76LEB/LIT

Table 73.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	18	18	0.358	8.01–2	0.36	4.73–4	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
274.8–330.1	4.88424+1	−1.83803+1	3.19521	IV

Name: Tellurobismethane
Formula: C_2H_6Te

CAS-RN: 593-80-6
Group No.: 73-034
Molar Mass: 157.67

Table 73.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
98SHE/NIS	207.1–308.2	31	0.20	99.99	chrom	*p*	BSAO	85RAB/SHE

Table 73.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	31	31	0.851	2.60−2	0.17	8.25−5	7
Temp. range K		A_1	A_2	A_3			Level of uncertainty
207.1–308.2	2.69744+1	−8.66157	1.56589				III

Name: 1,1′-Tellurobisethene
Formula: C_4H_6Te

CAS-RN: 63000-06-6
Group No.: 73-035
Molar Mass: 181.69

Table 73.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
99NIS/SHE	182.9–297.4	37	0.20	99.03	melpt	*p*	BSAO	85RAB/SHE

Table 73.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	37	37	0.500	2.02−2	0.10	3.65−5	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
182.9–297.4	2.97850+1	−7.41503	1.38528				III

Name: Diethyltelluride
Formula: $C_4H_{10}Te$

CAS-RN: 627-54-3
Group No.: 73-036
Molar Mass: 185.72

Table 73.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96SHE/KAM	169.1–298.2	34	0.20	99.9	melpt	*p*	BSAO	85RAB/SHE

Table 73.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	34	34	0.611	2.61−2	0.12	5.58−5	−8
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
169.1–298.2	2.75767+1	−5.63965	1.06938	6.71560−2			III

Name: Dimethyl[thiobis[methane]]zinc
Formula: $C_4H_{12}SZn$

CAS-RN: 91071-61-3
Group No.: 73-037
Molar Mass: 157.60

Table 73.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93LEB/KUL1	246.8–330.0	26	0.20	99.26	melpt	*p*	BSAO	76LEB/LIT

Table 73.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	26	26	3.463	2.38–1	0.69	2.93–3	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
246.8–330.0		4.92411+1	−1.17334+1	2.32236			IV

Name: Hydrobis(2-methylpropyl)aluminum
Formula: $C_8H_{19}Al$

CAS-RN: 1191-15-7
Group No.: 73-038
Molar Mass: 142.22

Table 73.38.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91SHE/RAB	148.8–327.3	49	0.20	99.9	chrom	*p*	BSAO	76LEB/LIT

Table 73.38.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	49	49	1.011	6.51–2	0.20	2.44–4	−13
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
148.8–250.0		1.20466+1	1.84300+1	−7.49220	1.47464		III
250.0–327.3		1.16517+2	−1.06935+2	4.26537+1	−5.21148		III

Name: Diethyl[1,1′-oxybis(ethane)]zinc
Formula: $C_8H_{20}OZn$

CAS-RN: 58482-38-5
Group No.: 73-039
Molar Mass: 197.64

Table 73.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93LEB/KUL2	174.1–310.0	45	0.20	99.77	melpt	*p*	BSAO	76LEB/LIT

Table 73.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	45	44	1.084	9.59–2	0.22	3.85–4	4
Temp. range K		A_1	A_2				Level of uncertainty
174.1–310.0		3.14930+1	5.21300				III

Name: Diethyl[1,1′-tellurobis(ethane)]zinc
Formula: $C_8H_{20}TeZn$

CAS-RN: 132851-15-1
Group No.: 73-040
Molar Mass: 309.24

Table 73.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
91LEB/KUL1	189.7–306.0	38	0.20	99.82	melpt	*p*	BSAO	76LEB/LIT

Table 73.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	38	37	0.892	2.16−1	0.45	1.76−3	−6
Temp. range K		A_1	A_2	A_3			Level of uncertainty
192.1–306.0		5.42256+1	−4.72502	8.81089−1			IV

Name: 1,1′-Tellurobispentane
Formula: $C_{10}H_{22}Te$

CAS-RN: 71475-88-2
Group No.: 73-041
Molar Mass: 269.88

Table 73.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94TEL/SHE	215.4–300.0	10 S	0.30	99.5	melpt	*p*	BSAO	94TEL/SHE

Table 73.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	10	10	0.071	8.47–3	0.02	1.14–6	−1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
215.4–300.0		3.25636+1	1.52939	4.95319−1			IV

Name: Pentaethoxyuranium
Formula: $C_{10}H_{25}O_5U$

CAS-RN: unknown
Group No.: 73-042
Molar Mass: 463.33

Table 73.42.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
65FER/SCO	257.5–400.0	31 S	0.10	not specified		sat	BSAO	45SCO/MEY

Table 73.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
sat	31	31	0.966	5.48–2	0.10	7.15–5	−4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
257.5–400.0		2.33039+2	−1.60560+2	4.66049+1	−4.31516		III

Name: Diphenyltelluride
Formula: $C_{12}H_{10}Te$

CAS-RN: 1202-36-4
Group No.: 73-043
Molar Mass: 281.81

Table 73.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96TEL/SHE	269.6–294.1	10	0.30	99.95	chrom	*p*	BSAO	85RAB/SHE

Table 73.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	10	10	0.679	7.28−2	0.20	2.10−4	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
269.6–294.1	1.12644+2	−5.98342+1	1.15425+1	III

Name: Tri(diethylcarbamodithioato-*S*,*S*′)indium
Formula: $C_{15}H_{30}InN_3S_6$

CAS-RN: 15741-07-8
Group No.: 73-044
Molar Mass: 559.64

Table 73.44.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00SOU/OLI	N	567.00	1.547	nosp	not specified		avg	BDHT	87PER/COM

#00SOU/OLI average value between 523–611 K

Name: Bis[(1,2,3,4,5,6-η)-ethylbenzene]chromium
Formula: $C_{16}H_{20}Cr$

CAS-RN: 12212-68-9
Group No.: 73-045
Molar Mass: 264.33

Table 73.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
72NIK/SAF	275.6–298.1	3 S	0.30	99.5	anal	*p*	BSAO	66NIK/LEB

Table 73.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	3	3	0.041	5.67−3	0.01	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
275.6–298.1	1.90417+1	9.47767	V

Name: Tris[2,3,4,5,6-pentafluorophenyl]germane
Formula: $C_{18}HF_{15}Ge$

CAS-RN: 42371-50-6
Group No.: 73-046
Molar Mass: 574.79

Table 73.46.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
96SMI/LEB	409.2–499.3	27	1.50	99.0	chrom	*p*	BDHT	69YAG

Table 73.46.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	27	27	0.821	1.29	1.23	−3.17−2	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
409.2–430.0	1.94454+6	−1.35537+6	3.14937+5	−2.43948+4	V
430.0–499.3	2.02597+4	−1.28490+4	2.72358+3	−1.92213+2	V

Name: Tris[bis(1-methylethyl)carbamodithioato-*S*,*S*′]indium
Formula: $C_{21}H_{42}InN_3S_6$

CAS-RN: 85883-33-6
Group No.: 73-047
Molar Mass: 643.80

Table 73.47.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00SOU/OLI	N	651.00	1.056	nosp	not specified		avg	BDHT	87PER/COM

#00SOU/OLI average value between 561–741 K

Name: Tris(dipropylcarbamodithiato-*S*,*S*′)indium
Formula: $C_{21}H_{42}InN_3S_6$

CAS-RN: 87052-01-5
Group No.: 73-048
Molar Mass: 643.80

Table 73.48.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00SOU/OLI	N	530.50	3.075	nosp	not specified		avg	BDHT	87PER/COM

#00SOU/OLI average value between 472–589 K

Name: Bis[(1,2,3,4,5,6-η)-bis(1-methylethyl)benzene]chromium
Formula: $C_{24}H_{36}Cr$

CAS-RN: 38744-20-6
Group No.: 73-049
Molar Mass: 376.55

Table 73.49.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
72NIK/SAF	200.0–298.1	4 S	0.30	99.5	anal	*p*	BSAO	66NIK/LEB

Table 73.49.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	4	4	0.375	7.40−2	0.11	−2.21−4	−2

Temp. range K	A_1	A_2	Level of uncertainty
200.0–298.1	2.28146+1	1.79239+1	IV

Name: Tris(dibutylcarbamodithioato-S,S')arsenic
Formula: $C_{27}H_{54}AsN_3S_6$

CAS-RN: 48233-55-2
Group No.: 73-050
Molar Mass: 688.06

Table 73.50.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
89AIR/DE	405.0–415.0	2	nosp	not specified		p	BDHT	87PER/COM

Table 73.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
405.0–415.0	1.28931+2	VI

Name: Tris(dibutylcarbamodithioato-S,S')bismuth
Formula: $C_{27}H_{54}BiN_3S_6$

CAS-RN: 34410-99-6
Group No.: 73-051
Molar Mass: 822.12

Table 73.51.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
89AIR/DE	375.0–385.0	2	nosp	not specified		p	BDHT	87PER/COM

Table 73.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	±
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
375.0–385.0	1.84497+2	VI

Name: Tris[bis(2-methylpropyl)carbamodithiato-S,S']indium
Formula: $C_{27}H_{54}InN_3S_6$

CAS-RN: 85129-27-7
Group No.: 73-052
Molar Mass: 727.96

Table 73.52.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00SOU/OLI	N	519.00	1.657	nosp	not specified		avg	BDHT	87PER/COM
#00SOU/OLI	average value between 444 and 594 K								

Name: Tris(dibutylcarbamodithioato-S,S')indium
Formula: $C_{27}H_{54}InN_3S_6$

CAS-RN: 23467-56-3
Group No.: 73-053
Molar Mass: 727.96

Table 73.53.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
#00SOU/OLI	N	526.00	2.675	nosp	not specified		avg	BDHT	87PER/COM
#00SOU/OLI	average value between 444–607 K								

Name: Tris(dibutylcarbamodithioato-S,S')antimony
Formula: $C_{27}H_{54}N_3S_6Sb$

CAS-RN: 14907-93-8
Group No.: 73-054
Molar Mass: 734.89

Table 73.54.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
89AIR/DE	355.0–365.0	2	nosp	not specified		p	BDHT	87PER/COM

Table 73.54.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
355.0–365.0	1.57917+2	VI

Name: Lithium salt formic acid
Formula: $CHLiO_2$

CAS-RN: 556-63-8
Group No.: 74-023
Molar Mass: 51.96

Table 74.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94FER/KEN	545.0–580.0	6	2.00	99.88	melpt	p	BDHT	69PER/COM

Table 74.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	6	6	0.055	1.82–2	0.11	2.54–6	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
545.0–580.0	−1.41473+2	5.38037+1	−4.58065	V

Name: Lithium salt acetic acid
Formula: $C_2H_3LiO_2$

CAS-RN: 546-89-4
Group No.: 74-024
Molar Mass: 65.99

Table 74.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94FER/KEN	570.0–580.0	3	2.00	99.91	melpt	p	BDHT	69PER/COM

Table 74.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	3	3	0.163	7.35−2	0.33	1.58−4	−1

Temp. range K	A_1	A_2	Level of uncertainty
570.0–580.0	1.44382+1	1.40369	V

Name: Lithium salt 2-methylpropanoic acid
Formula: $C_4H_7LiO_2$

CAS-RN: 25179-23-1
Group No.: 74-025
Molar Mass: 94.04

Table 74.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
93NGE/ABH	520.0–535.0	2	nosp	not specified		*p*	BDHT	93NGE/ABH

Table 74.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	1.91−6	0

Temp. range K	A_1	A_2	Level of uncertainty
520.0–535.0	3.58325+1	−1.33330	V

Name: Thallium(1+) salt butanoic acid
Formula: $C_4H_7O_2Tl$

CAS-RN: 63424-49-7
Group No.: 74-026
Molar Mass: 291.48

Table 74.26.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
94CHE/FER	460.00	0.7103	3.00	99.85	melpt	*p*	BDHT	94CHE/FER

Name: Thallium(1+) salt octanoic acid
Formula: $C_8H_{15}O_2Tl$

CAS-RN: 18993-50-5
Group No.: 74-027
Molar Mass: 347.59

Table 74.27.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
95CHE/UGA	500.00	1.309	3.00	99.76	melpt	*p*	BDHT	94CHE/FER

Name: Lead(2+) salt heptanoic acid
Formula: $C_{14}H_{26}O_4Pb$

CAS-RN: 16180-10-2
Group No.: 74-028
Molar Mass: 465.56

Table 74.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78ADE/SIM	413.0–453.0	2	2.00	not specified		*p*	BDHT	76MET/COM

Table 74.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
413.0–453.0	7.19224+1	VI

Name: Lead(2+) salt nonanoic acid
Formula: $C_{18}H_{34}O_4Pb$

CAS-RN: 63400-08-8
Group No.: 74-029
Molar Mass: 521.67

Table 74.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78ADE/SIM	413.0–463.0	2	2.00	not specified		*p*	BDHT	76MET/COM

Table 74.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
413.0–463.0	8.80389+1	VI

Name: Lead(2+) salt undecanoic acid
Formula: $C_{22}H_{42}O_4Pb$

CAS-RN: 63400-07-7
Group No.: 74-030
Molar Mass: 577.77

Table 74.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78ADE/SIM	413.0–463.0	2	2.00	not specified		*p*	BDHT	76MET/COM

Table 74.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
					%		
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
413.0–463.0	1.04636+2	VI

Name: Lead(2+) salt tridecanoic acid
Formula: $C_{26}H_{50}O_4Pb$

CAS-RN: 50354-80-8
Group No.: 74-031
Molar Mass: 633.88

Table 74.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capac	Calorimeter Type	Calorimeter Reference
78ADE/SIM	413.0–463.0	2	2.00	not specified		*p*	BDHT	76MET/COM

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r	s_b/R	±
			%				
p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
413.0–463.0	1.14258+2	VI