

Estimation of the Heat Capacities of Organic Liquids as a Function of Temperature Using Group Additivity.

II. Compounds of Carbon, Hydrogen, Halogens, Nitrogen, Oxygen, and Sulfur

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A second-order group additivity method has been developed for the estimation of the heat capacity of liquid organic compounds containing carbon, hydrogen, halogens, nitrogen, oxygen, and sulfur. The method permits the estimation of the heat capacity as a function of temperature in the range from the melting temperature to the normal boiling temperature. Group contributions and structural corrections have been made temperature dependent by the use of a polynomial expression. The adjustable parameters in the polynomials have been calculated using a weighted least squares minimization procedure. This work has drawn information for both the development and testing of the method from a large compilation of critically evaluated heat capacity data for over 1300 organic liquids.

Key words: estimation; group contribution approach; heat capacity of liquids; compounds of carbon, hydrogen, halogens, nitrogen, oxygen, and sulfur; temperature dependence.

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1. Introduction

This paper is the second part of a communication on the group-additivity method for the estimation of the heat capacities of liquids as a function of temperature (93RUZ/DOM1). The main objective of the project was to develop a second-order group-additivity method for organic compounds including both hydrocarbons and non-hydrocarbons. The method follows the definition of groups according to Benson and coworkers (58BEN/BUS, 69BEN/CRU).

Experimental liquid heat capacities are available for a limited number of compounds. Estimation methods are an obvious choice to substitute for missing data, in particular in engineering applications. Additivity schemes (55JOH/HUA, 65MIS, 69SHA, 73CHU/SWA1, 73CHU/SWA2, 77LUR/

BEN, 81OGI/ARA, 82CHU/NGU, 88DOM/HEA, 92HUR/HAR) and methods based on the corresponding states principle (69ROW, 70YUA/STI, 75LEE/KES, 76LYM/DAN, 77TAR/DAN) are the two main and most frequently used categories of estimation techniques. Whereas the additivity schemes are empirical, methods based on the corresponding states principle have a theoretical foundation.

In the literature, there is a lack of additivity methods for the estimation of the liquid heat capacity as a function of temperature. The paper by Luria and Benson (77LUR/BEN) is the only one that presents group contributions for the calculation of the heat capacity as a function of temperature. However, group contribution parameters in 77LUR/BEN are available for the estimation of the liquid heat capacity of hydrocarbons only.

The first part of the current project has been concerned with the revision and the extension of the existing group contributions and structural corrections developed by Luria and Benson (77LUR/BEN). A total of 29 groups and 24 structural corrections has been published (93RUZ/DOM1) which includes those for families such as alkanes, alkenes, alkynes, aromatic hydrocarbons, and saturated and unsaturated cyclic hydrocarbons. This paper is an extension of the method to include organic liquids containing the elements carbon, hydrogen, oxygen, nitrogen, sulfur, and halogens. It presents 85 groups and 12 structural corrections that permit the estimation of the heat capacity of many major families of organic compounds such as alcohols, aldehydes, ketones, ethers, organic acids, esters, amines, nitriles, hydrazines, sulfides, thiols, halides, and heterocyclic compounds containing nitrogen, oxygen, and sulfur. The present second-order group-additivity method yields the heat capacity of organic liquids as a function of temperature in an analytical form. Thus, the method can be implemented readily in chemical engineering calculations to establish energy balances or to evaluate the effect of temperature on phase and reaction equilibria.

2. Development of the Method

2.1. Additivity Scheme

We have used the following expression to estimate the molar heat capacities of organic liquids, C , as a function of temperature:

$$\frac{C}{R} = \sum_{i=1}^k n_i \Delta c_i \quad (1)$$

where R is the gas constant ($R=8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$, 88COH/TAY), n_i is the number of additivity units of type i , Δc_i is the dimensionless value of the additivity unit of type i , and k is the total

number of additivity units in a molecule. The additivity units include groups and structural corrections. The following functional form for the dependence of Δc_i on temperature has been chosen:

$$\Delta c_i = a_i + b_i \frac{T}{100} + d_i \left(\frac{T}{100} \right)^2 \quad (2)$$

where T is temperature in K and a_i , b_i , d_i are adjustable parameters.

2.2. Temperature Range

The present estimation method is applicable from the melting temperature to the normal boiling temperature. It may happen, in particular for high molecular weight compounds, that the normal boiling temperature of a compound lies above the upper temperature limit of one or more groups that constitute the molecule. We have found that an extrapolation of up to about 100 K has no significant effect on the error of prediction.

The estimation method may be applied to the prediction of both the isobaric heat capacity, C_p , and the saturation heat capacity, C_{sat} over the designated temperature range. Below the normal boiling temperature, C_p and C_{sat} are almost identical within the experimental error of measurements. Even when the method is applied above the normal boiling temperature the deviations between observed and estimated heat capacities exceed the differences between C_p and C_{sat} .

When comparing recommended heat capacities and those estimated using additive contributions reported here, we have encountered only few instances where it was necessary to use temperatures outside the range of one or more groups present in the compound. It was shown by 93RUZ/DOM1 that extrapolated group values calculated outside the temperature limits are reasonable for hydrocarbons when using the eqn. (2) for the dependence of contributions Δc_i with temperature.

2.3. Group Notation

We have followed the group notation developed by Benson and coworkers (58BEN/BUS, 69BEN/CRU). A group is defined as a central atom together with its nearest-neighbor atoms and ligands. We have adopted the short form of the notation for multiple bonded atoms C_d and C_B that omits the atom at the other end of the multiple bond; C_d is a doubly bonded carbon atom attached to a second doubly bonded carbon atom and to two other monovalent ligands; C_B is a carbon atom in a benzene ring attached to two other benzene ring carbon atoms and to another monovalent ligand. Table 1 lists all groups that we have used together with a sample group assignment for some typical molecules.

In a few cases, we have assigned identical values to some groups in order to reduce the colinearity of adjustable parameters (93RUZ/DOM2); i.e., as with the methyl group, or when data for the calculation of a group

are not available. The list of equivalent groups is given in Table 2.

We have adopted the approach proposed by Benson and coworkers (69BEN/CRU, 76BEN) to estimate the heat capacity of heterocyclic compounds containing nitrogen, oxygen, or sulfur. The heat capacity of a heterocyclic compound is estimated by summing group contributions developed for acyclic compounds and a structural correction that is specific to the particular heterocyclic compound. As the corrections reflect the internal ring strain imposed on a molecule, they are denoted as ring strain corrections, or rsc. Table 3 lists all structural corrections that we have used together with typical sample group assignments.

There are two exceptions to the above procedure for the estimation of the heat capacity of heterocyclic compounds. Two groups, N-(H)(C_B)₂ (pyrrole) and S-(C_B)₂ (thiophene), include both the group contribution and the ring strain correction. The group values for the two groups have been calculated from the data on pyrrole and thiophene as there are no data on acyclic compounds that would permit the calculation of parameters for acyclic groups only.

2.4. Next-to-Nearest Neighbor Interactions

We have followed the approach adopted in our first paper (93RUZ/DOM1) and have neglected all next-to-nearest neighbor interactions. The accuracy of the available heat capacity data does not justify inclusion of next-to-nearest neighbor interactions. We found that the differences among heat capacities of structural isomers are approximately as large as the uncertainty of the present estimation method.

3. Determination of Additivity Unit Values

A multiple linear least squares method has been used for the calculation of adjustable parameters in [Eq. (2)]. The minimized objective function in this method has the following form:

$$S = \sum_{j=1}^m w_j (C_j^{\text{rec}} - C_j^{\text{estd}})^2 \quad (3)$$

where the subscript j denotes j -th data point, C_j^{rec} is the recommended liquid heat capacity, and C_j^{estd} is the estimated heat capacity. The weight, w_j , is equal to the reciprocal of the variance of the j -th data point $\sigma^2(C_j)$ that is estimated from the percentage error of the recommended data, $\sigma_r C$.

3.1. Database of Liquid Heat Capacities

The recommended heat capacities were obtained from an extensive compilation that contains all currently available calorimetrically measured heat capacities for over 1300 liquid organic compounds (88ZAB/RUZ, 93ZAB/RUZ). The compilation includes parameters of a smoothing equation obtained from a critical assessment of experimental data. Parameters are accompanied by a

rating that represents the expected overall accuracy of the data. The rating is expressed as a percentage error and serves as the input information for the calculation of weights in the least squares parameterization.

3.2. Parameter Estimation

Adjustable parameters were calculated by simultaneous minimization of the deviations from the recommended heat capacities for families of chemically similar compounds in a series of successive steps. The parameters developed in the first part of the project for hydrocarbon groups (93RUZ/DOM1) have been used in all calculations of new parameters reported here. The list of selected compounds that was used in the calculation of adjustable parameters is given in Tables 4 to 7. The tables also include the temperature ranges for the recommended data and literature references to sources of original data that served for the generation of recommended heat capacities. The adjustable parameters for the calculation of group contributions and structural corrections are given in Tables 8 and 9. The appendix gives sample calculations for 1-pentanol, 1,2-ethanediol, and pyrrolidine at different temperatures.

4. Results and Discussion

An extensive evaluation of the present method has been made by comparing recommended heat capacities with those estimated using additive contributions reported here. The recommended heat capacities were taken from the compilation 93ZAB/RUZ. A total of 558 compounds and more than 5700 data points were included in these comparisons. Deviations between recommended and estimated values were calculated for the temperature range from the lower limit of the recommended data up to the normal boiling temperature or up to the upper limit of the recommended data if it lies below the normal boiling temperature. If the recommended data extend above the normal boiling temperature, a second set of deviations was determined with data for the entire temperature range. The standard deviation and average absolute percent deviation are given for each compound in Tables 10 to 30 where compounds were divided into 21 families according to their molecular structures.

Comparison of the present method with that developed by Lee and Kesler (75LEE/KES) has been made. The Lee-Kesler method is the generalized corresponding states approach that requires data for the critical temperature, critical pressure, acentric factor, and the heat capacity of the ideal gas for the estimation of the heat capacity of the vapor and liquid as a function of temperature. We have included several representative compounds in the comparison. The input data required for the application of the Lee-Kesler method were taken from the following sources. Critical properties and acentric factors were obtained from the database of physicochemical properties of pure compounds CDATA

(92RUZ/LAB) that contains recommended values based on the critical evaluation of a wide range of literature sources and includes also some estimated values. The heat capacity of the ideal gas was taken from the compilation by Bureš *et al.* (87BUR/HOL) that presents the heat capacity as a function of temperature in an analytical form. Several reliable compilations were used to develop the parameters of the correlating equations given in 87BUR/HOL. Deviations between the recommended and the estimated heat capacities for individual compounds are given in Tables 10 to 30. Table 32 presents a comparison of the summary deviations calculated for the present group contribution method and the generalized Lee-Kesler method. Deviations are compared for identical sets of compounds belonging to different families. For some families, a slightly smaller number of data points than were included in the evaluation of the Lee-Kesler method is due to convergence problems in the calculation of density in the proximity of the critical point. Generally, deviations for the Lee-Kesler method are significantly larger than those for the present group contribution method. This is not surprising, as the Lee-Kesler method was developed to represent the volumetric and thermodynamic properties of hydrocarbons.

4.1. Organic Halogen Compounds

The organic halogen compounds include the families of bromides, iodides, chlorides, fluorides, and mixed halogen derivatives and are found in Tables 10 through 13. The quality of the recommended heat capacities of all families of organic halogen compounds is poor. This is particularly true for the data on perfluoroalkanes and is manifested in Table 12 by exceptionally large deviations for these compounds. There is a lack of data on partially substituted fluorides which resulted in a gap in the list of groups for fluorides. Therefore, the group values for the $C-(H)(C)_2(F)$ and $C-(H)_2(C)(F)$ are missing. Data on unsaturated halogen compounds are also scarce.

4.2. Organic Nitrogen Compounds

The organic nitrogen compounds consist of the following families: amines, hydrazines, nitriles, heterocyclic nitrogen compounds, and compounds of carbon, hydrogen, nitrogen, and oxygen; they are found in Tables 14 through 18. The recommended heat capacities on amines, the largest family of nitrogen compounds, are rather inconsistent which leads to large deviations for some compounds. In addition, there is a lack of reliable data on secondary amines that cover a sufficiently broad temperature interval to permit calculation of parameters for the secondary amine group $N-(H)(C)_2$. The prediction errors in the families of hydrazines and nitriles, that contain only a limited number of compounds, are reasonable with a single exception, butanenitrile (recommended data from 85GUS/MIR and 87MIR/SHA). In the heterocyclic nitrogen compounds, we have considered the ring carbon groups to be the same as benzene carbon groups.

The same approximation was also used for heterocyclic oxygen and heterocyclic sulfur compounds. The parameters for the group denoted $N-(H)(C_B)_2$ (pyrrole) were determined from the data on pyrrole. The group $N-(H)(C_B)_2$ (pyrrole) thus also includes the ring strain correction.

Therefore, the group cannot be used for compounds other than pyrrole and its substituents. The adjustable parameters for the group $N-(H)(C)_2$ have been determined from the heat capacities of heterocyclic nitrogen compounds aziridine, pyrrolidine, and piperidine. As the $N-(H)(C)_2$ is also the secondary amine group, it should be used with caution when applied to the estimation of the heat capacity of secondary amines. The pyridine group is denoted by $N_B-(C_B)_2$. The breakdown of heterocyclic nitrogen compounds into groups is clarified in Tables 1 and 3 where some typical sample group assignments are given.

4.3. Organic Oxygen Compounds

The families which comprise organic oxygen compounds are: alcohols, diols, aldehydes, ketones, ethers, organic acids, esters, and heterocyclic oxygen compounds and are found in Tables 19 through 26. The heat capacity data on oxygen compounds are the most abundant of all groups of organic compounds covered in this work. The group of oxygen compounds includes families, such as alcohols and aldehydes, that exhibit the largest prediction error of all families of organic compounds.

Primary alcohols exhibit unusual behavior in that the curve of the heat capacity as a function of temperature has an inflection point (90ZAB/RUZ). To improve the prediction accuracy for primary alcohols an approach suggested by Ambrose (78AMB) for the estimation of the critical temperature and by Ogiwara *et al.* (81OGI/ARA) for the estimation of the isochoric liquid heat capacity is examined in 93RUZ/DOM2. Ambrose and Ogiwara *et al.* note that the value for the hydroxyl group $O-(H)(C)$ is dependent on the effective carbon number or on the number of carbon atoms in the chain. Růžička and Domalski (93RUZ/DOM2) conclude that the introduction of the dependence of the group value Δc for the $O-(H)(C)$ group on the number of carbon atoms in the molecule leads to some improvement in the prediction of the heat capacity of primary alcohols. We have found that the same modification of the Δc for the $O-(H)(C)$ group results in only a marginal improvement when a joint calculation of parameters is carried out for the whole group of alcohols including both primary, secondary, and tertiary alcohols. Therefore, we have not pursued the above modification of the Δc for the $O-(H)(C)$ group further.

Large deviations, exceeding 10 %, between the recommended and the estimated heat capacities have been observed for primary alcohols higher in carbon number than 1-decanol and for a few secondary and tertiary alcohols. Deviations of primary alcohols are due to their unusual

behavior as discussed above. Large deviations for secondary and tertiary alcohols have been encountered mainly for compounds where a single experimental value, primarily from measurement of heat capacities of mixtures, is available.

We have found that better agreement between the recommended and the estimated heat capacities of diols is obtained if a separate $O-(H)(C)$ group is assigned to either alcohols or diols, rather than having a single group for both families. This separation is indicated in the list of groups (Table 1) and group parameters (Table 8). Despite the introduction of the specific group for diols, the predictions for two diols and 1,2,3-propanetriol are poor.

Aldehydes comprise another family of organic oxygen compounds that as a whole exhibit large deviations between the recommended and the estimated heat capacities. In particular, the agreement for acetaldehyde and propanal is poor due to anomalies on the curve of the heat capacity as a function of temperature that is not smooth and shows a sharp peak (93ZAB/BUR).

Heat capacities of ketones, ethers, organic acids, and esters are estimated with a reasonable accuracy when using the present estimation method. We have found that smaller deviations in the estimated heat capacities are obtained if separate $C-(H)(C)_2(O)$ and $C-(C)_3(O)$ groups are assigned to either alcohols, or ethers and esters, rather than having a single global group for all families. This separation is indicated in the list of groups (Table 1) and group parameters (Table 8). The $C-(H)(C)_2(O)$ (ether, ester) group is also used for substituted heterocyclic oxygen compounds. In the unsaturated heterocyclic compounds we have considered the ring carbon groups to be the same as benzene carbon groups.

4.4. Organic Sulfur Compounds

Organic sulfur compounds have been divided into three families: sulfides, thiols, and heterocyclic sulfur compounds and are found in Tables 27 through 29. A limited amount of experimental data on liquid heat capacities of organic sulfur compounds is available. Collectively, the data may be characterized as being of good quality. Thus, deviations between the recommended and the estimated data on all families of sulfur compounds are rather low with the largest average deviation of 1.2% for the family of thiols. In the heterocyclic sulfur compounds, we have considered the ring carbon groups to be the same as benzene carbon groups. The parameters for the group denoted by $S-(C_B)_2$ (thiophene) are determined from the data on thiophene, hence, this group also includes the ring strain correction and cannot be used for compounds other than thiophene and substituted thiophenes.

Due to the lack of data on aromatic sulfides that would cover a temperature interval broader than at least 50 K, these compounds could not be incorporated into the present estimation method.

5.0. Conclusion

The previously developed second-order additivity method that permits estimation of heat capacities of liquid hydrocarbons has been successfully extended to accommodate organic compounds containing carbon, hydrogen, halogens, nitrogen, oxygen, and sulfur. Summation of group contributions and structural corrections represented by a second order polynomial enables one to obtain an analytical expression for the heat capacity as a function of temperature.

A total of 5772 comparisons for 558 C₂ to C₄₂ organic compounds have been made between a recommended value and one calculated using the additive group contributions reported here. It has been demonstrated that the method can be used in the range from the melting temperature to the normal boiling temperature where it gives an overall average deviation of 2.9 %. A thorough testing of the present method has not revealed any problems when a group value is extrapolated almost 100 K above the upper temperature limit of the range to which the group parameters are related.

The present method has been compared with the generalized corresponding states method developed by Lee and Kesler (75LEE/KES). A test of a set of 173 compounds shows that the present additivity method is clearly superior to the Lee-Kesler method. The average absolute deviation in the set of 173 compounds for the present method is 2.8 %, whereas that for the Lee-Kesler method is 7.8 %. Collectively, deviations for the Lee-Kesler method are significantly larger at low temperatures above the melting temperature than over the entire temperature range of data.

A further development and refinement of the present additivity method is hindered by the lack of reliable data that cover a broad interval from the melting temperature to the normal boiling temperature. The unavailability of data has prohibited the calculation of group parameters for several important families of compounds; e.g., secondary amines, aromatic thiols, aromatic sulfides, and partially substituted fluorides. More reliable data are also required to improve the method for alcohols and aldehydes.

TABLE 1. List of groups

Group	Number of Atoms					X ^a	Sample Group Assignment
	C	H	N	O	S		
Halogen Groups							
C-(C)(F) ₃	1	0	0	0	0	3	hexafluoroethane: 2 C-(C)(F) ₃
C-(C) ₂ (F) ₂	1	0	0	0	0	2	octafluoropropane: 1 C-(C) ₂ (F) ₂ , 2 C-(C)(F) ₃
C-(C)(Cl) ₃	1	0	0	0	0	3	1,1,1-trichloroethane: 1 C-(C)(Cl) ₃ , 1 C-(H) ₃ (C)
C-(H)(C)(Cl) ₂	1	1	0	0	0	2	1,1,2,2-tetrachloroethane: 2 C-(H)(C)(Cl) ₂
C-(H) ₂ (C)(Cl)	1	1	2	0	0	0	1,2-dichloroethane: 2 C-(H) ₂ (C)(Cl)
C-(H)(C) ₂ (Cl)	1	1	0	0	0	1	1,2,3-trichloropropane: 1 C-(H)(C) ₂ (Cl), 2 C-(H) ₂ (C)(Cl)
C-(H) ₂ (C)(Br)	1	2	0	0	0	1	bromoethane: 1 C-(H) ₂ (C)(Br), 1 C-(H) ₃ (C)
C-(H)(C) ₂ (Br)	1	1	0	0	0	1	2-bromopropane: 1 C-(H)(C) ₂ (Br), 2 C-(H) ₃ (C)
C-(H) ₂ (C)(I)	1	2	0	0	0	1	iodoethane: 1 C-(H) ₂ (C)(I), 1 C-(H) ₃ (C)
C-(C)(Cl) ₂ (F)	1	0	0	0	0	3	1,1,2-trichloro-1,2,2-trifluoroethane: 1 C-(C)(Cl) ₂ (F), 1 C-(C)(Cl)(F) ₂
C-(C)(Cl)(F) ₂	1	0	0	0	0	3	1,2-dichloro-1,1,2,2-tetrafluoroethane: 2 C-(C)(Cl)(F) ₂
C-(C)(Br)(F) ₂	1	0	0	0	0	3	1,2-dibromo-1,1,2,2-tetrafluoroethane: 2 C-(C)(Br)(F) ₂
C _d -(H)(Cl)	1	1	0	0	0	1	chloroethene: 1 C _d -(H)(Cl), 1 C _d -(H) ₂
C _d -(F) ₂	1	0	0	0	0	2	tetrafluoroethene: 2 C _d -(F) ₂
C _d -(Cl) ₂	1	0	0	0	0	2	tetrachloroethene: 2 C _d -(Cl) ₂
C _d -(Cl)(F)	1	0	0	0	0	2	chlorotrifluoroethene: 1 C _d -(Cl)(F), 1 C _d -(F) ₂
C _B -(F)	1	0	0	0	0	1	hexafluorobenzene: 6 C _B -(F)
C _B -(Cl)	1	0	0	0	0	1	1,2,4-trichlorobenzene: 3 C _B -(Cl), 3 C _B -(H)
C _B -(Br)	1	0	0	0	0	1	bromobenzene: 1 C _B -(Br), 5 C _B -(H)
C _B -(I)	1	0	0	0	0	1	iodobenzene: 1 C _B -(I), 5 C _B -(H)
C-(C _B)(F) ₃	1	0	0	0	0	3	pentafluoro(trifluoromethyl)benzene: 1 C-(C _B)(F) ₃ , 5 C _B -(F), 1 C _B -(C)
C-(H) ₂ (C _B)(Cl)	1	2	0	0	0	1	(chloromethyl)benzene: 1 C-(H) ₂ (C _B)(Cl), 5 C _B -(H), 1 C _B -(C)
Nitrogen Groups							
C-(H) ₂ (C)(N)	1	2	0	0	0	0	1-propanamine: 1 C-(H) ₂ (C)(N), 1 N-(H) ₂ (C), 1 C-(H) ₃ (C), 1 C-(H) ₂ (C) ₂
C-(H)(C) ₂ (N)	1	1	0	0	0	0	1,2-propanediamine: 1 C-(H)(C) ₂ (N), 1 C-(H) ₂ (C)(N), 2 N-(H) ₂ (C), 1 C-(H) ₃ (C)
C-(C) ₃ (N)	1	0	0	0	0	0	2-methyl-1,2-propanediamine: 1 C-(C) ₃ (N), 2 N-(H) ₂ (C), 2 C-(H) ₃ (C), 1 C-(H) ₂ (C)(N)
N-(H) ₂ (C) ^b	0	2	1	0	0	0	methanamine: 1 N-(H) ₂ (C), 1 C-(H) ₃ (C)
N-(H)(C) ₂	0	1	1	0	0	0	ethyleneimine: 1 N-(H)(C) ₂ , 2 C-(H) ₂ (C)(N), 1 ethyleneimine rsc
N-(C) ₃	0	0	1	0	0	0	N,N-dimethylmethanamine: 1 N-(C) ₃ , 3 C-(H) ₃ (C)
N-(H)(C)(C _B)	0	1	1	0	0	0	N-methylbenzenamine: 1 N-(H)(C)(C _B), 5 C _B -(H), 1 C-(H) ₃ (C), 1 C _B -(N)

TABLE 1. List of groups — Continued

Group	Number of Atoms					X ^a	Sample Group Assignment
	C	H	N	O	S		
N-(C) ₂ (C _B)	0	0	1	0	0	0	N,N-dimethylbenzenamine: 1 N-(C) ₂ (C _B), 1 C _B -(N), 5 C _B -(H), 2 C-(H) ₃ (C)
C _B -(N)	1	0	0	0	0	0	2,6-dimethylbenzenamine ^b : 1 C _B -(N), 1 N-(H) ₂ (C), 3 C _B -(H), 2 C _B -(C), 2 C-(H) ₃ (C)
N-(H) ₂ (N)	0	2	1	0	0	0	methylhydrazine: 1 N-(H) ₂ (N), 1 N-(H)(C)(N), 1 C-(H) ₃ (C)
N-(H)(C)(N)	0	1	1	0	0	0	1,2-dimethylhydrazine: 2 N-(H)(C)(N), 2 C-(H) ₃ (C)
N-(C) ₂ (N)	0	0	1	0	0	0	1,1-dimethylhydrazine: 1 N-(C) ₂ (N), 1 N-(H) ₂ (N), 2 C-(H) ₃ (C)
N-(H)(C _B)(N)	0	1	1	0	0	0	phenylhydrazine: 1 N-(H)(C _B)(N), 1 N-(H) ₂ (N), 5 C _B -(H), 1 C _B -(N)
C-(H) ₂ (C)(CN)	2	2	1	0	0	0	propanenitrile: 1 C-(H) ₂ (C)(CN), 1 C-(H) ₃ (C)
C-(C) ₃ (CN)	2	0	1	0	0	0	2,2-dimethylpropanenitrile: 1 C-(C) ₃ (CN), 3 C-(H) ₃ (C)
C _α -(H)(CN)	2	1	1	0	0	0	2-propenenitrile: 1 C _α -(H)(CN), 1 C _α -(H) ₂
C _B -(CN)	2	0	1	0	0	0	benzonitrile: 1 C _B -(CN), 5 C _B -(H)
C-(H) ₂ (C)(NO ₂)	1	2	1	2	0	0	nitroethane: 1 C-(H) ₂ (C)(NO ₂), 1 C-(H) ₃ (C)
O-(C)(NO ₂)	0	0	1	3	0	0	methyl ester of nitric acid: 1 O-(C)(NO ₂), 1 C-(H) ₃ (C)
C _B -(NO ₂)	1	0	1	2	0	0	nitrobenzene: 1 C _B -(NO ₂), 5 C _B -(H)
N-(II)(C _B) ₂ (pyrrole)	0	1	1	0	0	0	1H-pyrrole: 1 N-(H)(C _B) ₂ , 4 C _B -(H)
N _B -(C _B) ₂	0	0	1	0	0	0	pyridine: 1 N _B -(C _B) ₂ , 5 C _B -(H)
Oxygen Groups							
O-(H)(C)	0	1	0	1	0	0	ethanol: 1 O-(H)(C), 1 C-(H) ₂ (C)(O), 1 C-(H) ₃ (C)
O-(H)(C) (diol)	0	1	0	1	0	0	1,2-ethanediol: 2 O-(H)(C) (diol), 2 C-(H) ₂ (C)(O)
O-(H)(C _B)	0	1	0	1	0	0	phenol: 1 O-(H)(C _B), 1 C _B -(C _B) ₂ (O), 5 C _B -(H)
C-(H) ₂ (C)(O)	1	2	0	0	0	0	1-methoxybutane: 1 C-(H) ₂ (C)(O), 1 O-(C) ₂ , 2 C-(H) ₃ (C), 2 C-(H) ₂ (C) ₂
C-(H) ₂ (C _B)(O)	1	2	0	0	0	0	benzenemethanol: 1 C-(H) ₂ (C _B)(O), 1 O-(H)(C), 5 C _B -(H), 1 C _B -(C)
C-(H)(C) ₂ (O) (alcohol)	1	1	0	0	0	0	2-propanol: 1 C-(H)(C) ₂ (O) (alcohol), 1 O-(H)(C), 2 C-(H) ₃ (C)
C-(H)(C) ₂ (O) (ether, ester)	1	1	0	0	0	0	2-methoxypropane: 1 C-(H)(C) ₂ (O) (ether), 1 O-(C) ₂ , 3 C-(H) ₃ (C)
C-(C) ₃ (O) (alcohol)	1	0	0	0	0	0	2-methyl-2-propanol: 1 C-(C) ₃ (O) (alcohol), 1 O-(H)(C), 3 C-(H) ₃ (C)
C-(C) ₃ (O) (ether, ester)	1	0	0	0	0	0	2-methoxy-2-methylpropane: 1 C-(C) ₃ (O) (ether), 1 O-(C) ₂ , 4 C-(H) ₃ (C)
O-(C) ₂	0	0	0	1	0	0	1-methoxypropane: 1 O-(C) ₂ , 1 C-(H) ₂ (C)(O), 2 C-(H) ₃ (C), 1 C-(H) ₂ (C) ₂
O-(C)(C _B)	0	0	0	1	0	0	ethoxybenzene: 1 O-(C)(C _B), 1 C _B -(C _B) ₂ (O), 1 C-(H) ₂ (C)(O), 1 C-(H) ₃ (C), 5 C _B -(H)
O-(C _B) ₂	0	0	0	1	0	0	1,1'-oxybisbenzene: 1 O-(C _B) ₂ , 2 C _B -(O), 10 C _B -(H)
C-(H) ₂ (O) ₂	1	2	0	0	0	0	dimethoxymethane: 1 C-(H) ₂ (O) ₂ , 2 O-(C) ₂ , 2 C-(H) ₃ (C)
C-(C) ₂ (O) ₂	1	0	0	0	0	0	2,2-dimethoxypropane: 1 C-(C) ₂ (O) ₂ , 2 O-(C) ₂ , 4 C-(H) ₃ (C)
C _B -(O)	1	0	0	0	0	0	propoxybenzene: 1 C _B -(O), 1 O-(C)(C _B), 1 C-(H) ₂ (C)(O), 1 C-(H) ₃ (C), 1 C-(H) ₂ (C) ₂ , 5 C _B -(H)
C-(H) ₂ (C)(CO)	1	2	0	0	0	0	pentanal: 1 C-(H) ₂ (C)(CO), 1 CO-(H)(C), 1 C-(H) ₃ (C), 2 C-(H) ₂ (C) ₂
C-(H)(C) ₂ (CO)	1	1	0	0	0	0	3-methyl-2-butanone: 1 C-(H)(C) ₂ (CO), 1 CO-(C) ₂ , 3 C-(H) ₃ (C)
C-(C) ₃ (CO)	1	0	0	0	0	0	2,2-dimethylpropanal: 1 C-(C) ₃ (CO), 1 CO-(H)(C), 3 C-(H) ₃ (C)
CO-(H)(C)	1	1	0	1	0	0	butanal: 1 CO-(H)(C), 1 C-(H) ₂ (C)(CO), 1 C-(H) ₃ (C), 1 C-(H) ₂ (C) ₂
CO-(H)(C _α)	1	1	0	1	0	0	2-butenal: 1 CO-(H)(C _α), 1 C _α -(H)(CO), 1 C-(H) ₃ (C), 1 C _α -(H)(C)
CO-(C) ₂	1	0	0	1	0	0	2-butanone: 1 CO-(C) ₂ , 1 C-(H) ₂ (C)(CO), 2 C-(H) ₃ (C)
CO-(C)(C _α)	1	0	0	1	0	0	4-methyl-3-penten-2-one: 1 CO-(C)(C _α), C _α -(H)(CO), 1 C _α -(C) ₂ , 3 C-(H) ₃ (C)
CO-(C)(C _B)	1	0	0	1	0	0	1-phenylethanone: 1 CO-(C)(C _B), 1 C _B -(CO), 1 C-(H) ₃ (C), 5 C _B -(H)
CO-(H)(O)	1	1	0	1	0	0	formic acid: 1 CO-(H)(O), 1 O-(H)(CO)
CO-(C)(O)	1	0	0	1	0	0	acetic acid: 1 CO-(C)(O), 1 O-(H)(CO), 1 C-(H) ₃ (C)
CO-(C _α)(O)	1	0	0	1	0	0	2-propenoic acid: 1 CO-(C _α)(O), 1 O-(H)(CO), 1 C _α -(H)(CO), 1 C _α -(H) ₂
CO-(O)(CO)	1	0	0	1	0	0	bis(2-methylpropyl) ethanedioate: 2 CO-(O)(CO), 2 O-(C)(CO), 4 C-(H) ₃ (C), 2 C-(H)(C) ₃ , 2 C-(H) ₂ (C)(O)
O-(C)(CO)	0	0	0	1	0	0	ethyl formate: 1 O-(C)(CO), 1 CO-(H)(O), 1 C-(H) ₃ (C), 1 C-(H) ₂ (C)(O)
O-(H)(CO)	0	1	0	1	0	0	propanoic acid: 1 O-(H)(CO), 1 CO-(C)(O), 1 C-(H) ₂ (C)(CO), 1 C-(H) ₃ (C)
C _α -(H)(CO)	1	1	0	0	0	0	methyl propenoate: 1 C _α -(H)(CO), 1 CO-(C _α)(O), 1 O-(C)(CO), 1 C-(H) ₃ (C), 1 C _α -(H) ₂
C _α -(C)(CO)	1	0	0	0	0	0	2-methyl-2-propenoic acid: 1 C _α -(C)(CO), 1 CO-(C _α)(O), 1 O-(H)(CO), 1 C-(H) ₃ (C), 1 C _α -(H) ₂
C _B -(CO)	1	0	0	0	0	0	benzoic acid: 1 C _B -(CO), 1 O-(H)(CO), 5 C _B -(H) 1 CO-(C _B)(O)
CO-(C _B)(O)	1	0	0	1	0	0	4-methylbenzoic acid: 1 CO-(C _B)(O), 1 C _B -(CO), 1 O-(H)(CO), 1 C-(H) ₃ (C), 4 C _B -(H), 1 C _B -(C)
Sulfur Groups							
C-(H) ₂ (C)(S)	1	2	0	0	0	0	1-(methylthio)propane: 1 C-(H) ₂ (C)(S), 1 S-(C) ₂ , 2 C-(H) ₃ (C), 1 C-(H) ₂ (C) ₂
C-(H)(C) ₂ (S)	1	1	0	0	0	0	2-(methylthio)propane: 1 C-(H)(C) ₂ (S), 1 S-(C) ₂ , 3 C-(H) ₃ (C)

TABLE 1. List of groups — Continued

Group	Number of Atoms						Sample Group Assignment
	C	H	N	O	S	X ^a	
C-(C) ₃ (S)	1	0	0	0	0	0	2-methyl-2-(methylthio)propane: 1 C-(C) ₃ (S), 1 S-(C) ₂ , 4 C-(H) ₃ (C)
C _B -(S)	1	0	0	0	0	0	benzenethiol: 1 C _B -(S), 1 S-(H)(C), 5 C _B -(H)
S-(H)(C)	0	1	0	0	1	0	ethanethiol: 1 S-(H)(C), 1 C-(H) ₂ (C)(S), 1 C-(H) ₃ (C)
S-(C) ₂	0	0	0	0	1	0	1-(ethylthio)propane: 1 S-(C) ₂ , 2 C-(H) ₂ (C)(S), 2 C-(H) ₃ (C), 1 C-(H) ₂ (C) ₂
S-(C)(S)	0	0	0	0	1	0	dipropyl disulfide: 2 S-(C)(S), 2 C-(H) ₂ (C)(S), 2 C-(H) ₃ (C), 2 C-(H) ₂ (C) ₂
S-(C _B) ₂ (thiophene)	0	0	0	0	1	0	thiophene: 1 S-(C _B) ₂ , 4 C _B -(H)

^aHalogen.^bThe approximation N-(H)₂(C_B) ≡ N-(H)₂(C) was used.

TABLE 2. List of equivalent groups

Used in the calculation of adjustable parameters
C-(H) ₃ (C) ≡ C-(H) ₃ (N) ≡ C-(H) ₃ (O) ≡ C-(H) ₃ (CO) ≡ C-(H) ₃ (S)
N-(H) ₂ (C _B) ≡ N-(H) ₂ (C)
S-(H)(C _B) ≡ S-(H)(C)
O-(H)(C _B) (diol) ≡ O-(H)(C) (diol)
CO-(H)(C _B) ≡ CO-(H)(C _d)
Used in comparisons
C-(H) ₂ (C _d)(Cl) ≡ C-(H) ₂ (C)(Cl)
C-(H) ₂ (C _B)(N) ≡ C-(H) ₂ (C)(N)
N-(C)(C _B) ₂ ≡ N-(C) ₃
C-(H) ₂ (C _d)(O) ≡ C-(H) ₂ (C _B)(O)
S-(C _B)(S) ≡ S-(C) ₂
S-(C _B) ₂ ≡ S-(C) ₂

TABLE 3. List of structural corrections

Structural Correction	Sample Group Assignment
Nitrogen Compounds	
ethyleneimine rsc	ethyleneimine: 1 N-(H)(C) ₂ , 2 C-(H) ₂ (C)(N), 1 ethyleneimine rsc
pyrrolidine rsc	pyrrolidine: 1 N-(H)(C) ₂ , 2 C-(H) ₂ (C)(N), 2 C-(H) ₂ (C) ₂ , 1 pyrrolidine rsc
piperidine rsc	piperidine: 1 N-(H)(C) ₂ , 2 C-(H) ₂ (C)(N), 3 C-(H) ₂ (C) ₂ , 1 piperidine rsc
Oxygen Compounds	
ethylene oxide rsc	ethylene oxide: 1 O-(C) ₂ , 2 C-(H) ₂ (C)(O), 1 ethylene rsc
trimethylene oxide rsc	trimethylene oxide: 1 O-(C), 2 C-(H) ₂ (C)(O), 1 C-(H) ₂ (C) ₂ , 1 trimethylene oxide rsc
1,3-dioxolane rsc	1,3-dioxolane rsc: 2 O-(C) ₂ , 2 C-(H) ₂ (C)(O), 1 C-(H) ₂ (O) ₂ , 1 1,3-dioxolane rsc
furan rsc	furan: 4 C _B -(H), 1 O-(C _B) ₂ , 1 furan rsc
tetrahydrofuran rsc	tetrahydrofuran: 1 O-(C) ₂ , 2 C-(H) ₂ (C)(O), 2 C-(H) ₂ (C) ₂ , 1 tetrahydrofuran rsc
tetrahydropyran rsc	tetrahydropyran: 1 O-(C) ₂ , 2 C-(H) ₂ (C)(O), 3 C-(H) ₂ (C) ₂ , 1 tetrahydropyran rsc
Sulfur Compounds	
thiacyclobutane rsc	thiacyclobutane: 1 S-(C) ₂ , 2 C-(H) ₂ (C)(S), 1 C-(H) ₂ (C) ₂ , 1 thiacyclobutane rsc
thiacyclopentane rsc	thiacyclopentane: 1 S-(C) ₂ , 2 C-(H) ₂ (C)(S), 2 C-(H) ₂ (C) ₂ , 1 thiacyclopentane rsc
thiacyclohexane rsc	thiacyclohexane: 1 S-(C) ₂ , 2 C-(H) ₂ (C)(S), 3 C-(H) ₂ (C) ₂ , 1 thiacyclohexane rsc

TABLE 4. List of selected compounds used for the calculation of adjustable parameters for halogen compounds

Compound	Temp. range/K		Reference
1st step of the parameterization scheme			
tetrachloroethene	253	300	86NOV/RAB
1,1-dichloroethene	157	291	59HIL/MCD
1,1,2-tetrachloroethane	234	354	48KUR, 82KOS/KOL
chloroethene	119	300	67LEB/RAB2
1,1,1-trichloroethane	243	310	44RUB/LEV, 73AND/COU
1,1-dichloroethane	177	309	48KUR, 56LI/PIT
1,2-dichloroethane	239	353	40PIT, 55RUI, 55STA/TUP, 67RAS/GAN, 69WIL/SCH, 77WIL/GRO, 79WIL/FAR, 79WIL/GRO
chloroethane	140	290	40RIE, 48GOR/GIA
1,2,3-trichloropropane	273	359	41NEL/NEW, 48KUR
1,2,4-trichlorobenzene	293	459	69WIL/ROT, 74PET/TER, 82WIL/ING, 86WIL/LAI
chlorobenzene	230	355	*81VON, *87SCH, 37STU, 88PER/AIC
(chloromethyl)benzene	246	347	*87SCH, 31SMI/AND
bromoethane	168	300	U/BAT, 12SCH, 48KUR
1,3-dibromopropane	243	358	48KUR, 50CRO/SMY
2-bromopropane	190	318	*81VON, 50KUS/CRO
bromobenzene	243	369	*81VON, 75MAS/SCO
3-bromohexane	213	420	88MEL/VER
iodoethane	243	333	*81BER/OGI, 48KUR
1-iodopropane	317	339	*81VON
iodobenzene	250	320	37STU, 61ROU
2nd step of the parameterization scheme			
tetrafluoroethene	145	210	53FUR/MCC
hexafluoroethane	175	191	48PAC/AST
1,1,1-trifluoroethane	165	221	44RUS/GOL
octafluoropropane	126	233	67PAC/PLA
hexafluorobenzene	282	350	65COU/GRE, 70MES/FIN, 82GOR/SIM
fluorobenzene	235	350	56SCO/MCC1, 84ROU/GRO
pentafluoro(trifluoromethyl)benzene	211	365	74AND/MAR
hexadecafluoroheptane	222	345	51OLI/GRI1, 57YAR/KAY
(trifluoromethyl)benzene	253	365	59SCO/DOU
1,2-dibromo-1,1,2,2-tetrafluoroethane	166	413	74GRU/SHE, 82KOS/ZHO, 88VES/ZAB
chlorotrifluoroethene	120	240	51OLI/GRI2
1,2-dichloro-1,1,2,2-tetrafluoroethane	182	296	81KOL/KOS
1,1,2-trichloro-1,2,2-trifluoroethane	241	420	40BEN/MCH, 54BUB, 81KOL/KOS, 88VES/ZAB

TABLE 5. List of selected compounds used for the calculation of adjustable parameters for nitrogen compounds

Compound	Temp.range/K		References
1st step of the parameterization scheme			
methanamine	187	259	37AST/SIL
N,N-dimethylmethanamine	161	276	44AST/SAG
1-propanamine	190	335	67SMI/GOO, 72FIN/MES
(R,S)-1,2-propanediamine	240	368	75MES/FIN
2-methyl-1,2-propanediamine	258	375	75MES/FIN
N,N-dimethyl-1,3-propanediamine	194	356	82DZH/KAR, 84LEB/GUT
benzenamine	270	453	50HOU/MAS2, 62HAT/HIL, 75NIC/WAD
N-methylbenzenamine	240	379	02LOU2, 57CRU/JOS, 87LES/LIC
N,N-dimethylbenzenamine	283	388	*81VON, *87SCH, 02LOU2, 16BRA, 57CRU/JOS
2,6-dimethylbenzenamine	285	450	86STE/CHI
hydrazine	275	464	49SCO/OLI, 50HOU/MAS1, 68AHL/YOU
methylhydrazine	221	298	51AST/FIN
1,1-dimethylhydrazine	216	298	53AST/WOO
1,2-dimethylhydrazine	264	298	51AST/JAN
trimethylhydrazine	205	294	55AST/ZOL
phenylhydrazine	293	306	81LEB/RYA
2nd step of the parameterization scheme			
2-propenenitrile	197	347	72FIN/MES
propanenitrile	185	330	00LOU, 07WAL, 62WEB/KIL
pentanedinitrile	245	347	65CLE/WUL
2,2-dimethylpropanenitrile	296	346	67WES/RIB
benzonitrile	265	377	00LOU, 83BYK/LEB, 85LAI/ROD, 85TAN/NAK
1,2-benzenedicarbonitrile	421	480	82KAR/SHV, 84RAB/KAR
3rd step of the parameterization scheme			
nitroethane	189	300	66LIN/ZIE
nitrobenzene	279	415	39MAZ1, 39MAZ2, 58LUT/PAN, 67RAS/GAN, 85LAI/ROD
methyl ester of nitric acid	194	296	53GRA/SMI
ethyl nitrate	182	293	54GRA/SMI
1-methylethyl ester of nitric acid	191	350	88BUN, 88LUS/RUB
4th step of the parameterization scheme			
ethyleneimine	197	330	77LEB/EVS2
1H-pyrrole	256	360	67SCO/BER
pyrrolidine	218	351	59HIL/SIN, 59MCC/DOU
pyridine	240	347	57MCC/DOU
3-methylpyrrolidine	170	400	86STE/CHI
piperidine	267	362	88MES/TOD
2-methylpyridine	210	369	63SCO/HUB
4-methylpyridine	283	395	88MES/TOD
2,4-dimethyl-1H-pyrrole	268	450	86STE/CHI
2,5-dimethyl-1H-pyrrole	285	384	88MES/TOD
2-methylpiperidine	273	370	88MES/TOD

TABLE 6. List of selected compounds used for the calculation of adjustable parameters for oxygen compounds

Compound	Temp. range/K		References
1st step of the parameterization scheme			
dimethoxymethane	171	308	64MCE/KIL
1-methoxypropane	138	309	75AND/MAR
2-methoxypropane	131	305	75AND/MAR
1,1'-oxybisethane	160	310	71COU/LEE, 85WIL/CHA
1-ethoxypropane	151	316	75AND/MAR
1-methoxybutane	160	316	75AND/MAR, 82VIL/CAS
2-methoxy-2-methylpropane	168	308	75AND/MAR
2,2-dimethoxypropane	273	334	86BER/GUR
1,1'-oxybispropane	161	323	75AND/COU, 83KIM/TRE
2,2'-oxybispropane	189	340	74AND/COU
ethoxybenzene	320	349	*86SCH
propoxybenzene	320	349	*86SCH
1-methoxydecane	247	349	75AND/MAR
1,1'-oxybisbenzene	301	532	51FUR/GIN
ethanol	159	352	31FIO/GIN, 66HWA/ZIE, 66KLE, 68PAZ/REC, 76FOR/ BEN1, 76FOR/BEN2, 77HAI/SUG, 79BRO/ZIE, 86OGA/MUR
1-propanol	154	371	51EUC/EIG, 68COU/LEE, 76FOR/BEN1, 76FOR/BEN2, 79GRI/YAN, 80KAL/JED, 86TAN/TOY
1-butanol	189	392	65COU/HAL, 68PAZ/REC, 75SAN, 79GRI/YAN, 86GAT/WOO, 86OGA/MUR, 86TAN/TOY, 88AND/PAT, 88PIE/SOM2
1-pentanol	206	413	68COU/LEE, 76SKO/SUU, 79GRI/YAN, 86TAN/TOY
1-hexanol	230	432	29KEL, 79GRI/YAN, 83BEN/DAR, 84BRA/PIN, 84KAL/ WOY, 85COS/PAT1, 86TAN/TOY, 88AND/PAT, 89VES/BAR
1-heptanol	240	451	56PAR/KEN, 59HUT/BAI, 79GRI/YAN, 88AND/PAT, 89VES/BAR
1-octanol	298	452	31CLI/AND, 61ROU, 79GRI/YAN, 89VES/BAR
1-nonanol	304	464	79GRI/YAN
1-decanol	283	503	75WOY/KAL, 79GRI/YAN, 79SVE, 80VAS/TRE, 85COS/PAT1, 88AND/PAT
1,2-ethanediol	262	472	25PAR/KEL, 62RAB/NIK, 67NIK/RAB, 68PAZ/REC, 77MUR/SUB, 79STE/TAM
2-propanol	185	357	48GIN/COR, 63AND/COU2, 79BRO/ZIE
1,2-propanediol	194	461	27PAR/HUF, 52CUR/JOH
(R,S)-2-butanol	188	345	71AND/CON
2-methyl-1-propanol	181	382	68COU/LEE, 77HOF/SAN, 88OKA/OGA
2-methyl-2-propanol	298	357	63OET, 76SKO/SUU, 77HOF/SAN
1,4-butanediol	296	450	79NIS/BAB
2-methyl-2-butanol	275	343	33PAR/HUF, 49LEE, 83DAP/DEL, 86BEN/DAR, 88PIE/SOM1
phenol	313	373	63AND/COU1, 67RAS/GAN
1,2-benzenediol	378	473	26AND/LYN
benzenemethanol	260	462	02LOU1, 31SMI/AND, 36PAR/TOD, 75NIC/WAD, 79GRI/YAN
2-methylphenol	304	400	67AND/COU
3-methylphenol	285	400	67AND/COU
4-methylphenol	308	400	67AND/COU
4-methyl-4-heptanol	201	299	31CLI/AND
2nd step of the parameterization scheme			
2-butenal	273	343	86BER/GUR
butanal	180	300	56PAR/KEN
2-butanone	191	353	64SIN/OET, 67RAS/GAN, 68AND/COU
2,2-dimethylpropanal	274	350	80FUC, 83KOR/DYA
3-methyl-2-butanone	184	324	68AND/COU
pentanal	192	340	83KOR/DYA
2-pentanone	201	364	65OET, 68AND/COU
4-methyl-3-penten-2-one	317	355	*81VON, *98LOU
3,3-dimethyl-2-butanone	226	363	70AND/COU
2-hexanone	221	383	70AND/COU
3-hexanone	222	322	70AND/COU
benzaldehyde	218	425	75AMB/CON
3,4-dimethylpentanal	323	428	87MIL/FEN1
2,4-dimethyl-3-pentanone	208	319	70AND/COU

TABLE 6. List of selected compounds used for the calculation of adjustable parameters for oxygen compounds — Continued

Compound	Temp. range/K		References
heptanal	230	368	*81VON, 56PAR/KEN
1-phenylethanone	298	381	00LOU, 80FUC
5-nonanone	277	320	70AND/COU
6,10-dimethyl-3,5,9-undecatriene-2-one	273	343	86BER/GUR
2-pentyl-2-nonenal	323	428	87MIL/FEN2
1,4-diphenyl-1,4-butanedione	423	463	32SPA/THO
formic acid	282	342	*81VON, *95MAS/GUI, 41STO/FIS
acetic acid	293	400	65CAM/GIE, 82MAR/AND
2-propenoic acid	289	343	83KAR/ABD
propanoic acid	255	447	78WOY/KAL, 82MAR/AND
2-methyl-2-propenoic acid	289	348	67RAB/LEB, 85KAR/ABD2
butanoic acid	273	373	71KON/WAD, 82MAR/AND
2-methylpropanoic acid	227	374	*81VON, 67RAB/LEB, 71KON/WAD
pentanoic acid	241	303	65MCD/KIL
hexanoic acid	285	392	*81VON, 26GAR/MAD
benzoic acid	396	471	26AND/LYN, 51FUR/MCC, 67PAC
2-methylbenzoic acid	377	473	26AND/LYN
4-methylbenzoic acid	453	498	26AND/LYN
ethyl formate	298	309	*81BER/OGI, 36KUR/VOS, 79FUC
methyl propenoate	196	300	67LEB/RAB1, 79FUC
propyl formate	298	310	*86SCH, 85BAL/BRA, 86JIM/ROM, 88PIN/BRA
methyl 2-methyl-2-propenoate	226	323	52ERD/JAG, 62MEL, 67LEB/RAB1, 86ZHA/BEN
butyl acetate	196	399	79BAL/PET, 80VAS/TRE, 86JIM/ROM, 87ZAB/HYN
ethyl butanoate	180	370	36KUR/VOS, 79FUC, 80BAL/VAS
ethyl 2-methylpropanoate	308	327	*86SCH
3-methylbutyl formate	309	334	*86SCH
butyl 2-propenoate	210	334	85KAR/ABD1
methyl benzoate	298	345	*86SCH, 79FUC
butyl 2-methyl-2-propenoate	197	350	52ERD/JAG, 85KAR/ABD2
butyl butanoate	182	439	79BAL/PET, 80VAS/TRE
ethyl hexanoate	210	370	80BAL/VAS
bis(2-methylpropyl) ethanedioate	318	347	*87SCH
diethyl 1,2-benzenedicarboxylate	273	353	67CHA/HOR
octyl 2-methyl-2-propenoate	230	350	85KAR/ABD2
bis(3-methylbutyl) ethanedioate	318	347	*87SCH
dibutyl butanedioate	250	400	89KHO/PUL
dibutyl 1,2-benzenedicarboxylate	177	360	70MAR/RAB, 85RAB/NOV
3rd step of the parameterization scheme			
ethylene oxide	161	284	49GIA/GOR, 77LEB/EVS1
1,2-propylene oxide	167	325	64OET, 82TAN/ZHO
trimethylene oxide	185	298	76CON/GIA, 85HAN
1,3-dioxolane	176	300	69CLE/MEL, 76CON/GIA
furan	191	299	52GUT/SCO
1,2-butylene oxide	137	322	73GOO/FIN
tetrahydrofuran	162	323	78LEB/RAB, 79KIY/DAR, 85COS/PAT2
2-methylfuran	196	307	65CAR/WES1
tetrahydropyran	298	372	64MOE/THO, 84ING/GRO, 88ING

TABLE 7. List of selected compounds used for the calculation of adjustable parameters for sulfur compounds

Compound	Temp.range/K		References
2,3-dithiabutane	192	352	50SCO/FIN
1-(methylthio)propane	167	326	57SCO/FIN
2-(methylthio)propane	177	344	55MCC/FIN
3,4-dithiahexane	168	299	52SCO/FIN
1-(ethylthio)propane	166	366	61MCC/FIN
2-methyl-2-(methylthio)propane	190	364	62SCO/GOO
methylthiocyclopentane	173	369	74MES/FIN
2,2'-thiobispropane	204	383	67MES/TOD
dipropyl disulfide	194	351	58HUB/DOU
1,1'-thiobisbutane	205	356	61MCC/FIN
ethanethiol	130	315	52MCC/SCO
1-propanethiol	168	315	56PEN/SCO
2-propanethiol	149	322	54MCC/FIN2
2-methyl-1-propanethiol	137	349	58SCO/MCC
2-methyl-2-propanethiol	281	329	53MCC/SCO
cyclopentanethiol	162	366	61BER/SCO
3-methyl-1-butanethiol	141	371	74MES/FIN
3-methyl-2-butanethiol	148	379	74MES/FIN
benzenethiol	262	375	56SCO/MCC2
cyclohexanethiol	197	365	67MES/TOD
1-hexanethiol	200	372	70FIN/MCC
thiacyclobutane	202	321	53SCO/FIN
thiophene	238	336	49WAD/KNO, 85FIG/SZW
thiacyclopentane	180	333	52HUB/FIN
2-methylthiophene	213	344	56PEN/FIN
3-methylthiophene	207	337	53MCC/SUN
2-methylthiacyclopentane	168	389	74MES/FIN
3-methylthiacyclopentane	194	337	74MES/FIN
thiacyclohexane	296	342	54MCC/FIN1
2,5-dimethylthiophene	217	304	65CAR/WES2

TABLE 8. Parameters for the dependence of group contribution Δc_i on temperature, $\Delta c_i = a_i + b_i(T/100) + d_i(T/100)^2$, T/K

Group	Adjustable Parameters			Temperature Range/K	
	a_i	b_i/K^{-1}	d_i/K^{-2}		
Halogen Groups					
C-(C)(F) ₃	1.5423E+1 ^a	-9.2464	2.8647	125	345
C-(C) ₂ (F) ₂	-8.9527	1.0550E+1	-1.9986	125	345
C-(C)(Cl) ₃ ^b	8.5430	2.6966	-4.2564E-1	245	310
C-(H)(C)(Cl) ₂	1.0880E+1	-3.5391E-1	8.4875E-2	180	355
C-(H) ₂ (C)(Cl)	9.6663	-1.8601	4.1360E-1	140	360
C-(H)(C) ₂ (Cl) ^b	-2.0600	5.3281	-8.2721E-1	275	360
C-(H) ₂ (C)(Br)	6.3944	-1.0298E-1	1.9403E-1	168	360
C-(H)(C) ₂ (Br)	1.0784E+1	-2.4754	3.3288E-1	190	420
C-(H) ₂ (C)(I)	3.7620E-2	5.6204	-9.2054E-1	245	340
C-(C)(Cl) ₂ (F) ^b	1.3532E+1	-3.2794	8.0145E-1	240	420
C-(C)(Cl)(F) ₂	7.2295	4.1759E-1	1.5892E-1	180	420
C-(C)(Br)(F) ₂ ^b	8.7956	-1.9165E-1	2.4596E-1	165	415
C _d -(H)(Cl) ^b	7.1564	-8.4442E-1	2.7199E-1	120	300
C _d -(F) ₂	7.6646	-2.0750	8.2003E-1	120	240
C _d -(Cl) ₂	9.3249	-1.2478	4.4241E-1	155	300
C _d -(Cl)(F) ^b	7.8204	-6.9005E-1	1.9165E-1	120	240
C _B -(F)	3.0794	4.6959E-1	-5.5745E-3	210	365
C _B -(Cl)	4.5479	2.2250E-1	-9.7873E-3	230	460
C _B -(Br) ^b	2.2857	2.2573	-4.0942E-1	245	370
C _B -(I) ^b	2.9033	2.9763	-6.2960E-1	250	320
C-(C _B)(F) ₃	7.4477	-9.2230E-1	3.9346E-1	210	365
C-(H) ₂ (C _B)(Cl)	1.6752E+1	-6.7938	1.2520	245	345

TABLE 8. Parameters for the dependence of group contribution Δc_i on temperature, $\Delta c_i = a_i + b_i(T/100) + d_i(T/100)^2$, T/K

Group	Adjustable Parameters			Temperature	
	a_i	b_i/K^{-1}	d_i/K^{-2}	Range/K	
Nitrogen Groups					
C-(H) ₂ (C)(N)	2.4555	1.0431	-2.4054E-1	190	375
C-(H)(C) ₂ (N) ^b	2.6322	-2.0135	4.5109E-1	240	370
C-(C) ₃ (N) ^b	1.9630	-1.7235	3.1086E-1	255	375
N-(H) ₂ (C)	8.2758	-1.8365E-1	3.5272E-2	185	455
N-(H)(C) ₂	-1.0987E+1	7.3024E-1	8.9325E-1	170	400
N-(C) ₃	4.5942	-2.2134	5.5316E-1	160	360
N-(H)(C)(C _B) ^b	4.9631E-1	3.4617	-5.7161E-1	240	380
N-(C) ₂ (C _B) ^b	-2.3640E+1	1.6260E+1	-2.52580	285	390
C _B -(N)	-7.8169E-1	1.5059	-2.5287E-1	240	455
N-(H) ₂ (N)	6.8050	-7.2563E-1	1.5634E-1	215	465
N-(H)(C)(N)	1.1411	3.5981	-6.9350E-1	205	300
N-(C) ₂ (N)	-1.0570	4.0038	-7.1494E-1	205	300
N-(H)(C _B)(N) ^b	-7.4531E-1	3.6258	-5.3306E-1	295	385
C-(H) ₂ (C)(CN)	1.1976E+1	-2.4886	5.2358E-1	185	345
C-(C) ₃ (CN) ^b	2.5774	3.5218	-5.8466E-1	295	345
C _r -(H)(CN) ^b	9.0789	-8.6929E-1	3.2986E-1	195	345
C _B -(CN)	1.9389	3.0269	-4.7276E-1	265	480
C-(H) ₂ (C)(NO ₂) ^b	1.8520E+1	-5.4568	1.0508	190	300
O-(C)(NO ₂)	-2.0181	1.0505E+1	-1.8398	180	350
C _B -(NO ₂) ^b	1.5277E+1	-4.4049	7.1161E-1	280	415
N-(H)(C _B) ₂ (pyrrole)	-7.3662	6.3622	-6.8137E-1	255	450
N _B -(C _B) ₂	8.4237E-1	1.2556	-2.0336E-1	210	395
Oxygen Groups					
O-(H)(C)	1.2952E+1	-1.0145E+1	2.6261	155	505
O-(H)(C) (diol)	5.2302	-1.5124	5.4075E-1	195	475
O-(H)(C _B)	-7.9768	8.1045	-8.7263E-1	285	400
C-(H) ₂ (C)(O)	1.4596	1.4657	-2.7140E-1	135	505
C-(H) ₂ (C _B)(O) ^b	-3.5127E+1	2.8409E+1	-4.9593	260	460
C-(H)(C) ₂ (O) (alcohol)	2.2209	-1.4350	6.9508E-1	185	460
C-(H)(C) ₂ (O) (ether, ester)	9.8790E-1	3.9403E-1	-1.6124E-2	130	170
C-(C) ₃ (O) (alcohol)	-4.4690E+1	3.1769E+1	-4.8791	200	355
C-(C) ₃ (O) (ether, ester) ^b	-3.3182	2.6317	-4.4354E-1	170	310
O-(C) ₂	5.0312	-1.5718	3.7860E-1	130	350
O-(C)(C _B)	-2.2524E+1	1.3115E+1	-1.4421	320	350
O-(C _B) ₂	-4.5788	9.4150E-1	3.1655E-1	300	535
C-(H) ₂ (O) ₂ ^b	1.0852	1.5402	-3.1693E-1	170	310
C-(C) ₂ (O) ₂ ^b	-1.2955E+1	9.1027	-1.5367	275	335
C _B -(O)	-1.0686	3.5221	-7.9259E-1	285	530
C-(H) ₂ (C)(CO)	6.6782	-2.4473	4.7121E-1	180	465
C-(H)(C) ₂ (CO)	3.9238	-2.1210	4.9646E-1	185	375
C-(C) ₃ (CO)	-2.2681	1.7558	-2.5674E-1	225	360
CO-(H)(C)	-3.8268	7.6719	-1.2711	180	430
CO-(H)(C _a)	-8.0024	3.6379	-1.5377E-1	220	430
CO-(C) ₂	5.4375	7.2091E-1	-1.8312E-1	185	380
CO-(C)(C _a)	4.1507E+1	-3.2632E+1	6.0326	275	355
CO-(C)(C _B)	-4.7211E+1	2.4368E+1	-2.8274	300	465
CO-(H)(O)	1.3118E+1	1.6120E+1	-5.1273	280	340
CO-(C)(O)	2.9246E+1	3.4261	-2.8962	180	445
CO-(C _a)(O)	4.1615E+1	-1.2789E+1	5.3631E-1	195	350
CO-(O)(CO)	2.3990E+1	6.2573	-3.2427	320	345
O-(C)(CO)	-2.1434E+1	-4.0164	3.0531	175	440
O-(H)(CO)	-2.7587E+1	-1.6485E-1	2.7483	230	500
C _r -(H)(CO)	-9.0108	1.5148E+1	-3.0436	195	355
C _r -(C)(CO)	-1.2818E+1	1.5997E+1	-3.0567	195	430
C _B -(CO)	1.2151E+1	-1.6705	-1.2758E-1	175	500
CO-(C _B)(O)	1.6586E+1	5.4491	-2.6849	175	500

TABLE 8. Parameters for the dependence of group contribution Δc_i on temperature, $\Delta c_i = a_i + b_i(T/100) + d_i(T/100)^2$, T/K

Group	Adjustable Parameters			Temperature Range/K	
	a_i	b_i/K^{-1}	d_i/K^{-2}		
Sulfur Groups					
C-(H) ₂ (C)(S)	1.5456	8.8228E-1	-8.3493E-2	130	390
C-(H)(C) ₂ (S)	-1.6430	2.3072	-3.1234E-1	150	390
C-(C) ₃ (S)	-5.3825	4.5023	-7.2356E-1	190	365
C _B -(S)	-4.4507	4.4324	-7.5674E-1	260	375
S-(H)(C)	1.0994E+1	-3.2113	4.7368E-1	130	380
S-(C) ₂	9.2306	-3.0087	4.5625E-1	165	390
S-(C)(S)	6.6590	-1.3557	1.7938E-1	170	350
S-(C _B) ₂ (thiophene)	3.8461	3.6718E-1	-6.1312E-2	205	345

^aParameter values given in the E notation. The first part of the number denotes the fractional part which is followed by the exponent to the base 10 (e.g. 1.5423E+1 means 1.5423·10¹).

^bAdjustable parameters were calculated from heat capacity data on a single compound only.

TABLE 9. Parameters for the dependence of structural correction Δc_i on temperature, $\Delta c_i = a_i + b_i(T/100) + d_i(T/100)^2$, T/K

Structural Correction	Adjustable Parameters			Temperature Range, K	
	a_i	b_i, K^{-1}	d_i, K^{-2}		
Nitrogen Compounds					
ethyleneimine rsc ^b	1.5281E+1 ^a	-2.3360	-1.3720E-1	195	330
pyrrolidine rsc	1.2703E+1	1.3109	-1.18130	170	400
piperidine rsc	2.5681E+1	-7.0966	1.4304E-1	265	370
Oxygen Compounds					
ethylene oxide rsc	6.8459	-5.8759	1.2408	135	325
trimethylene oxide rsc ^b	-7.0148	7.3764	-2.1901	185	300
1,3-dioxolane rsc ^b	2.3985	4.8585E-1	1.0253E-1	175	300
furan rsc	9.6704	-2.8138	1.1376E-1	190	305
tetrahydrofuran rsc ^b	3.2842	-5.8260	1.2681	160	320
tetrahydropyran rsc ^b	-1.3017E+1	3.7416	-1.5622E-1	295	325
Sulfur Compounds					
thiacyclobutane rsc	-7.3127E-1	-1.3426	4.0114E-1	200	320
thiacyclopentane rsc	-3.2899	3.8399E-1	8.9358E-2	170	390
thiacyclohexane rsc	-1.2766E+1	5.2886	-5.9558E-1	295	340

^aParameter values given in the E notation. The first part of the number denotes the fractional part which is followed by the exponent to the base 10 (e.g. 1.5281E+1 means 1.5281·10¹).

^bAdjustable parameters were calculated from heat capacity data on a single compound only.

TABLE 10. Deviations between recommended and estimated heat capacities of bromides and iodides. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Zábřanský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^b %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
1,2-dibromoethane	9(9)	5.2	3.6	283–346	136–143	25.5
bromoethane	16(16)	2.5	2.4	168–300	89–101	9.4
1,2,3-tribromopropane	9(9)	7.8	3.3	320–391	182–213	
1,3-dibromopropane	14(14)	4.1	2.2	243–358	155–173	
1-bromopropane	8(8)	4.5	2.9	268–323	134–139	3.8
2-bromopropane	15(15)	3.3	2.4	190–318	125–134	8.4
1-bromobutane	18(18)	4.9	2.9	177–331	142–175	6.0
1-bromo-2-methylpropane	3(3)	6.6	4.2	306–319	157–161	8.6
1,3-dibromo-2,2-bis(bromomethyl)propane	3(3)	29.1	9.2	440–460	311–317	
1-bromo-3-methylbutane	4(4)	3.7	1.9	307–330	190–199	
1-bromopentane	11(11)	11.0	5.7	190–291	172–173	
bromobenzene	15(15)	0.2	0.1	243–369	144–169	4.7
3-bromohexane	33(21)	15.5	4.0 (2.5)	213–523	196–361	
1-bromooctane	3(3)	6.0	2.2	222–234	261–261	
1-bromononane	2(2)	4.0	1.3	249–257	287–287	
iodoethane	11(11)	1.9	1.2	243–333	103–116	
1-iodopropane	4(4)	1.8	1.1	317–339	139–143	
1-iodo-2-methylpropane	4(4)	4.3	2.1	315–344	170–170	
1-iodo-3-methylbutane	6(6)	11.3	5.7	307–350	186–202	
1,2-diiodobenzene	5(5)	1.3	0.6	297–325	189–193	
1,3-diiodobenzene	3(3)	1.8	0.8	322–340	189–193	
iodobenzene ^d	9(9)	0.0	0.0	250–320	154–164	

^aStandard deviation is calculated as

$$SD = \sqrt{\frac{1}{n_p} \sum (C^{rec} - C^{std})^2}$$

where n_p is the number of data points (usually 10 K apart).

^bAverage absolute percent deviation is calculated as

$$APD = 100 \frac{1}{n_p} \sum \left| \frac{C^{rec} - C^{std}}{C^{rec}} \right|$$

^cAverage absolute percent deviation calculated by the above equation between the recommended heat capacities and those estimated by the Lee-Kesler method (75LEE/KES).

^dThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.

TABLE 11. Deviations between recommended and estimated heat capacities of chlorides. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Zábanský *et al.* (93ZAB/RUZ).

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
tetrachloroethene	7(7)	2.4	1.3	253–300	150–159	9.1
trichloroethene	2(2)	14.1	11.4	293–298	123–124	4.5
pentachloroethane	1(1)	30.9	13.7	293–	225–	
1,1-dichloroethene	15(15)	0.5	0.3	157–291	101–110	
1,2-dichloroethene	6(6)	7.8	7.1	265–307	104–113	
(E)-1,2-dichloroethene	1(1)	3.3	3.0	288–	113–	2.1
(Z)-1,2-dichloroethene	1(1)	2.1	1.9	288–	114–	
1,1,2,2-tetrachloroethane	14(14)	8.9	5.1	234–354	165–176	2.8
chloroethene	20(15)	0.6 (0.5)	0.6 (0.5)	119–300	85–90	10.9 (13.8)
1,1,1-trichloroethane ^b	9(9)	0.0	0.0	243–310	139–145	3.2
1,1,2-trichloroethane	3(3)	8.3	5.8	240–252	141–143	40.2
1,1-dichloroethane	16(16)	0.3	0.2	177–309	120–127	5.3
1,2-dichloroethane	14(14)	0.6	0.4	239–353	126–138	3.1
chloroethane	20(15)	2.7 (0.6)	1.4 (0.4)	140–318	97–114	6.3 (7.9)
1,1,1,3-tetrachloropropane	6(6)	5.1	2.6	240–289	190–195	
3-chloro-1-propene	3(3)	6.9	5.5	299–312	125–127	8.2
1,2,3-trichloropropane ^b	11(11)	0.0	0.0	273–359	180–192	
1,2-dichloropropane	7(7)	5.4	2.8	306–359	154–174	
1-chloropropane	14(14)	8.6	6.0	200–312	109–134	3.8
1,4-dichlorobutane	1(1)	5.6	3.1	298–	184–	
1-chlorobutane	3(3)	1.6	0.8	298–309	160–164	1.6
1-chloro-2-methylpropane	4(4)	14.5	8.7	292–310	137–162	8.5
1,3-dichloro-2,2-bis(chloromethyl)propane	4(4)	19.6	7.0	373–398	275–283	
1-chloro-3-methylbutane	4(4)	16.1	8.8	307–329	178–184	
1,2,4-trichlorobenzene	19(19)	0.7	0.3	293–459	191–227	
1,2-dichlorobenzene	6(6)	2.4	1.4	291–326	169–176	
1,3-dichlorobenzene	10(10)	2.1	1.2	254–327	163–176	
1,4-dichlorobenzene	4(4)	6.0	2.0	328–349	180–183	
chlorobenzene	15(15)	2.0	1.1	230–355	138–165	4.3
1,6-dichlorohexane	1(1)	9.2	3.9	298–	240–	
(chloromethyl)benzene ^b	13(13)	0.0	0.0	246–347	174–199	
1-chloro-2-methylbenzene	4(4)	3.4	1.6	317–346	184–196	11.6
3-chloroheptane	36(20)	74.1 (20.4)	13.9 (6.8)	233–573	239–531	
1-chloronaphthalene	1(1)	8.0	3.8	298–	211–	
2-chloro-1,1'-biphenyl	4(4)	21.3	8.0	305–330	263–272	
4-chloro-1,1'-biphenyl	4(4)	25.2	9.2	348–370	272–277	4.4
1-chlorooctadecane	1(1)	24.9	4.1	301–	607–	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.

^cSee footnote c at the bottom of Table 10.

TABLE 12. Deviations between recommended and estimated heat capacities of fluorides. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ).

Compound	No. data points	Std.dev. ^a		Avg.dev. ^a		Temp. range, K	Heat capacity range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler)	
		J·K ⁻¹ ·mol ⁻¹	%	%	%			%	
tetrafluoroethene ^b	8(6)	0.0	(0.0)	0.0	(0.0)	145–210	106–115	0.6	(0.8)
hexafluoroethane	3(3)	8.4		6.6		175–191	124–129		
1,1,1-trifluoroethane	7(7)	3.4		3.1		165–221	102–110		
octafluoropropane	12(12)	6.4		2.5		126–233	147–181		
hexafluorobenzene	9(9)	0.6		0.2		282–350	219–233	0.4	
pentafluorobenzene	12(12)	1.3		0.6		231–324	190–211		
1,2,3,4-tetrafluorobenzene	11(11)	1.8		0.9		235–320	174–196		
1,2,3,5-tetrafluorobenzene	11(11)	1.5		0.7		229–311	174–194		
1,2,4,5-tetrafluorobenzene	10(10)	1.3		0.7		280–353	188–206		
1,2-difluorobenzene	15(15)	2.9		1.8		229–357	142–174		
1,3-difluorobenzene	17(17)	3.0		1.8		214–355	139–175		
fluorobenzene	14(14)	0.2		0.1		235–350	133–160	1.7	
pentafluoro(trifluoromethyl)benzene	18(18)	0.3		0.1		211–365	240–283		
hexadecafluoroheptane	15(15)	13.7		2.2		222–345	376–444		
pentafluoromethylbenzene	15(15)	5.7		2.4		253–377	213–250		
(trifluoromethyl)benzene	14(14)	0.7		0.3		253–365	173–212		
1-fluoro-4-methylbenzene	16(16)	2.5		1.4		221–361	151–189		
decafluorobis(trifluoromethyl)cyclohexane	7(7)	2.0		0.3		304–360	408–438		
octadecafluorooctane	1(1)	65.3		16.8		293	389		
2,2',3,3',4,4',5,5',6,6'-decafluoro-1,1'-biphenyl	2(2)	13.5		3.3		347–350	408–408		

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.

^cSee footnote c at the bottom of Table 10.

TABLE 13. Deviations between recommended and estimated heat capacities of mixed halogen derivatives. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ).

Compound	No. data points	Std.dev. ^a		Avg.dev. ^a		Temp. range, K	Heat capacity range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler)	
		J·K ⁻¹ ·mol ⁻¹	%	%	%			%	
1,2-dibromo-1,1,2,2-tetrafluoroethane	27(17)	1.0	(0.9)	0.5	(0.5)	166–413	151–202		
chlorotrifluoroethene ^b	13(13)	0.2		0.1		120–240	113–122		
chloropentafluoroethane	15(7)	9.4	(7.2)	5.9	(5.2)	175–303	130–187		
1,2-dichloro-1,1,2,2-tetrafluoroethane	12(10)	0.1	(0.1)	0.1	(0.1)	182–296	141–163	4.0	(4.8)
1,1,1-trichloro-2,2,2-trifluoroethane	3(3)	53.7		31.4		298–318	169–173		
1,1,2-trichloro-1,2,2-trifluoroethane	24(10)	8.1	(0.3)	1.8	(0.1)	241–458	162–259	2.0	(0.6)
1,1,2,2-tetrachloro-1,2-difluoroethane	3(3)	2.8		1.6		299–310	179–181	2.6	
1-chloro-1,1-difluoroethane	18(13)	10.5	(10.6)	8.8	(9.1)	146–303	111–131	5.3	(6.1)
1-bromo-2-chloroethane	8(8)	1.3		0.8		263–322	125–132		
1-chloro-1,1,3,3,3-pentafluoropropane	15(15)	13.0		5.1		167–298	164–197		
1,1,1-trichloro-3,3,3-trifluoropropane	6(6)	35.7		17.9		246–297	190–200		
3,3-dichloro-1,1,1-trifluoropropane	12(12)	19.3		9.0		185–294	175–190		
3-chloro-1,1,1-trifluoropropane	14(14)	19.8		9.4		184–299	155–171		
bromopentafluorobenzene	5(5)	6.9		3.2		246–282	213–219		
chloropentafluorobenzene	16(12)	4.5	(5.0)	1.9	(2.2)	263–395	214–243		
1,3,5-trichloro-2,4,6-trifluorobenzene	2(2)	7.6		3.2		339–347	236–238		
1-bromo-2-chlorobenzene	4(4)	2.2		1.2		306–326	178–182		
1-bromo-3-chlorobenzene	10(10)	0.5		0.2		254–327	167–180		
1-bromo-4-chlorobenzene	1(1)	6.9		3.6		355–355	191–191		
1-bromo-2-iodobenzene	6(6)	2.1		1.0		291–326	184–189		
1-bromo-3-iodobenzene	6(6)	1.0		0.5		291–326	182–187		

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.

^cSee footnote c at the bottom of Table 10.

TABLE 14. Deviations between recommended and estimated heat capacities of amines. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ).

Compound	No. data points	Std.dev. ^a		Avg.dev. ^a		Temp. range, K	Heat capacity range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
		J·K ⁻¹ ·mol ⁻¹	%	J·K ⁻¹ ·mol ⁻¹	%			
methanamine	9(9)	0.1		0.1		186–259	99–102	1.7
ethanamine	1(1)	2.2		1.7		273	130	5.2
1,2-ethanediamine	14(11)	18.4	(12.5)	8.2	(6.4)	298–413	172–217	3.2 (1.4)
cyclopropanamine	10(10)	13.7		9.0		242–314	143–149	
N,N-dimethylmethanamine	13(13)	0.1		0.1		160–275	115–132	2.1
1-propanamine	18(16)	0.4	(0.4)	0.2	(0.2)	190–334	154–166	13.8 (14.5)
2-propanamine	19(14)	16.2	(17.0)	10.0	(10.7)	181–343	147–171	12.0 (13.4)
(R,S)-1,2-propanediamine ^b	15(15)	0.1		0.0		240–367	201–214	
1-butanamine	1(1)	4.9		2.6		298	188	1.4
2-methyl-1-propanamine	1(1)	2.8		1.5		298	194	8.7
2-methyl-2-propanamine	16(13)	15.2	(15.7)	8.0	(8.4)	209–332	178–198	11.6 (12.7)
2-methyl-1,2-propanediamine ^b	15(15)	0.0		0.0		257–374	230–246	
cyclopentanamine	17(17)	8.9		4.9		200–348	167–192	
N-ethyl-N-methylethanamine	6(6)	2.4		1.0		283–313	195–195	
1-pentanamine	1(1)	4.7		2.1		298	218	
N,N-dimethyl-1,3-propanediamine	19(19)	0.5		0.2		194–358	238–268	
benzenamine	21(21)	5.0		2.0		270–453	187–218	5.2
1,3-benzenediamine	13(13)	13.5		5.4		342–451	241–257	
N,N-diethylethanamine	10(10)	11.5		4.4		278–343	205–252	
1-hexanamine	1(1)	0.5		0.2		298	252	
N,N'-bis(2-aminoethyl)-1,2-ethanediamine	16(16)	35.4		6.7		333–473	377–427	
benzenemethanamine	1(1)	7.8		3.8		298	207	
N-methylbenzenamine ^b	16(16)	0.0		0.0		240–378	190–229	
2-methylbenzenamine	14(14)	2.2		0.9		288–392	215–238	2.4
3-methylbenzenamine	1(1)	1.2		0.5		302	216	8.3
benzeneethanamine	1(1)	2.0		0.8		298	239	
N,N-dimethylbenzenamine ^b	13(13)	0.0		0.0		283–388	210–245	
2,6-dimethylbenzenamine	19(19)	1.1		0.4		284–450	234–289	
benzenepropanamine	1(1)	5.4		2.1		298	265	
N,N,2-trimethylbenzenamine	1(1)	8.6		3.1		376	279	
2-naphthalenamine	3(3)	11.9		3.8		386–396	296–306	6.0
N,N-diethylbenzenamine	6(6)	17.8		5.2		302–347	274–313	
N-methyl-N-phenylbenzenamine	7(7)	8.5		2.4		322–375	318–351	
4,4'-methylenebisbenzenamine	7(7)	12.6		3.0		350–410	385–425	
N,N-dimethyl-2-pentyl-1-nonanamine	12(12)	18.8		3.0		323–423	534–633	

^aStandard deviation and average absolute percent deviation defined in Table 10.^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.^cSee footnote c at the bottom of Table 10.TABLE 15. Deviations between recommended and estimated heat capacities of hydrazines. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ).

Compound	No. data points	Std. dev. ^a		Avg. dev. ^a		Temp. range, K	Heat capacity range, J·K ⁻¹ ·mol ⁻¹
		J·K ⁻¹ ·mol ⁻¹	%	J·K ⁻¹ ·mol ⁻¹	%		
hydrazine	21(18)	0.9	(1.0)	0.6	(0.7)	275–464	97–113
methylhydrazine	9(9)	0.6		0.4		221–298	131–135
1,1-dimethylhydrazine	10(10)	0.3		0.2		216–298	152–164
1,2-dimethylhydrazine	5(5)	0.3		0.1		264–298	169–171
trimethylhydrazine	10(10)	7.0		3.1		205–294	181–186
phenylhydrazine	12(12)	0.0		0.0		293–386	215–239

^aStandard deviation and average absolute percent deviation defined in Table 10.

TABLE 16. Deviations between recommended and estimated heat capacities of nitriles. Recommended data are from Záborský *et al.* (93ZAB/RUZ).

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. range, K	Heat capacity range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
2-propenenitrile ^b	18	0.1	0.1	196–347	102–114	15.3
propanenitrile	18	4.3	3.5	185–330	110–124	10.4
butanedinitrile	3	2.0	1.2	334–348	160–162	
butanenitrile	24	10.9	8.1	173–383	122–151	14.8
pentanedinitrile	13	0.7	0.3	245–347	176–192	
2,2-dimethylpropanenitrile ^b	7	0.0	0.0	298–346	179–189	
pentanenitrile	1	5.2	2.9	345	181	
hexanenitrile	1	3.5	1.6	360	220	
benzonitrile	14	2.0	0.6	265–377	159–190	3.9
1,2-benzenedicarbonitrile	8	4.5	1.8	421–480	217–232	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.

^cSee footnote c at the bottom of Table 10.

TABLE 17. Deviations between recommended and estimated heat capacities of heterocyclic nitrogen compounds. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ).

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. range, K	Heat capacity range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
aziridine ^b	16(15)	0.0 (0.0)	0.0 (0.0)	197–330	93–115	
1H-pyrrole	13(13)	7.8	5.2	256–360	117–143	
pyrrolidine	16(16)	2.6	1.5	218–351	150–162	15.7
pyridine	13(13)	0.4	0.2	240–347	122–143	4.6
1-methylpyrrolidine	1(1)	68.4	42.5	298–	161–	
3-methylpyrrolidine	25(23)	4.9 (4.9)	2.0 (2.0)	170–400	154–206	
piperidine	12(12)	6.4	3.4	267–362	178–191	10.7
2-methylpyridine	18(18)	0.5	0.3	210–369	142–178	4.8
3-methylpyridine	16(16)	0.4	0.1	258–388	150–182	2.4
4-methylpyridine	14(14)	0.2	0.1	283–395	156–185	1.6
2,4-dimethyl-1H-pyrrole	21(19)	4.8 (5.0)	2.2 (2.2)	268–450	180–243	
2,5-dimethyl-1H-pyrrole	12(12)	9.6	4.6	285–384	190–229	
1-methylpiperidine	1(1)	71.8	38.8	298–	185–	
2-methylpiperidine	12(12)	9.3	4.0	273–370	213–229	
4-methylpiperidine	1(1)	40.2	19.2	298–	209–	
2,3-dimethylpyridine	22(19)	4.8 (5.0)	2.3 (2.4)	259–450	180–238	
2,4-dimethylpyridine	27(24)	1.2 (1.3)	0.6 (0.6)	209–450	165–235	
2,5-dimethylpyridine	22(19)	0.9 (0.9)	0.4 (0.4)	259–450	175–234	
2,6-dimethylpyridine	20(17)	2.6 (2.4)	1.1 (1.0)	267–440	176–234	1.7 (1.7)
3,4-dimethylpyridine	21(19)	5.9 (6.2)	2.8 (3.0)	263–450	184–236	
3,5-dimethylpyridine	21(19)	0.7 (0.6)	0.3 (0.3)	267–450	176–234	
isoquinoline	12(12)	4.6	2.1	300–400	197–233	6.2
quinoline	22(22)	4.6	2.1	258–450	181–251	7.5
5,6,7,8-tetrahydroquinoline	25(25)	15.5	6.1	223–450	189–286	
benzo[h]quinoline	13(13)	7.0	2.2	328–440	271–327	
phenanthridine	8(8)	2.1	0.6	377–440	304–333	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.

^cSee footnote c at the bottom of Table 10.

TABLE 18. Deviations between recommended and estimated heat capacities of compounds of carbon, hydrogen, nitrogen, and oxygen. Recommended data are from Zábanský *et al.* (93ZAB/RUZ).

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. range, K	Heat capacity range, J·K ⁻¹ ·mol ⁻¹
3-(dimethylamino)-propanenitrile	9	9.0	4.3	228–298	202–212
3-methoxy-1-propanamine	12	3.3	1.5	200–300	214–226
2-Amino-2-methyl-1,3-propanediol	2	50.5	14.9	388–394	338–342
2-(ethylmethylamino)ethanol	3	5.8	2.2	321–341	257–271
2-nitrophenol	9	12.1	4.2	335–409	239–289
3-nitrophenol	5	14.2	5.4	370–408	249–265
4-nitrophenol	3	7.6	2.8	391–410	262–271
2-nitrobenzenamine	9	15.3	5.6	343–423	257–287
3-nitrobenzenamine	11	6.5	2.3	385–483	264–297
4-nitrobenzenamine	6	4.6	1.4	421–468	277–286
2-nitrobenzoic acid	11	52.6	17.0	419–513	281–320
3-nitrobenzoic acid	10	15.1	3.5	415–498	340–374
4-nitrobenzoic acid	2	75.4	24.0	512–518	314–314
1-methyl-4-nitrobenzene	4	8.5	3.8	315–340	219–225
1-methoxy-2-nitrobenzene	12	7.4	2.5	298–408	254–287
1-methoxy-3-nitrobenzene	7	8.5	3.1	349–404	263–283
1-methoxy-4-nitrobenzene	8	8.3	3.0	348–408	261–287
methyl ester of nitric acid	11	9.4	6.0	194–296	131–156
ethyl nitrate	12	5.8	2.8	182–293	163–169
1-methylethyl ester of nitric acid	18	10.3	5.1	191–350	167–206
nitroethane ^b	13	0.2	0.1	189–300	132–134
1,2-dinitrobenzene	14	16.6	4.8	390–513	273–302
1,4-dinitrobenzene	5	11.6	3.9	446–483	277–294
nitrobenzene ^b	16	0.8	0.4	279–415	176–218
1-methyl-4-nitrobenzene	4	8.5	3.8	315–340	219–225
1-nitronaphthalene	5	7.9	2.8	332–367	268–283

^aStandard deviation and average absolute percent deviation defined in Table 10.^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.TABLE 19. Deviations between recommended and estimated heat capacities of alcohols. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Zábanský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. range, K	Heat capacity range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
methanol	35(17)	41.7 (10.0)	26.3 (11.6)	180–503	71–251	47.7 (66.8)
ethanol	24(21)	6.8 (4.9)	4.3 (3.5)	159–378	88–155	49.5 (55.1)
1-propanol	33(23)	15.6 (2.4)	4.1 (1.8)	154–463	106–243	29.3 (37.0)
1-butanol	30(22)	19.9 (2.5)	3.9 (0.9)	188–467	136–278	14.3 (14.4)
1-pentanol	28(22)	19.1 (4.7)	3.6 (1.4)	205–463	165–321	12.1 (11.0)
1-hexanol	26(22)	23.0 (10.5)	4.5 (2.7)	229–462	198–354	10.4 (9.4)
1-heptanol	25(22)	26.5 (15.5)	5.4 (3.9)	240–462	234–388	9.8 (9.1)
1-octanol	23(23)	23.0	5.0	246–452	243–423	10.9
1-nonanol	17(17)	33.5	6.5	304–464	342–465	14.1
1-decanol	24(24)	60.6	9.1	283–503	353–503	12.5
1-undecanol	24(23)	83.5 (75.1)	11.8 (10.7)	298–523	406–552	13.9 (14.2)
1-dodecanol	20(20)	57.6	8.2	298–486	438–572	13.0
1-tridecanol	26(25)	126. (116.)	15.1 (14.0)	305–553	485–633	11.6 (11.9)
1-tetradecanol	28(25)	160. (128.)	17.7 (14.2)	312–573	524–687	10.6 (11.4)
1-pentadecanol	28(26)	182. (160.)	19.3 (16.9)	318–583	553–727	7.9 (8.3)
1-hexadecanol	4(4)	29.0	4.5	323–346	582–635	10.4
1-octadecanol	28(26)	249. (220.)	23.0 (20.6)	353–623	735–887	8.6 (9.0)
2-propen-1-ol	4(4)	7.1	4.5	304–331	147–160	9.1
2-propanol	31(19)	45.5 (6.0)	11.8 (3.0)	185–473	108–280	23.5 (28.7)
(R,S)-2-butanol	18(18)	5.0	1.9	188–345	131–244	15.4
(S)-2-butanol	15(15)	4.1	1.7	180–310	130–210	
2-methyl-1-propanol	34(22)	31.7 (7.8)	7.1 (3.0)	180–493	129–300	17.7 (18.3)

TABLE 19. Deviations between recommended and estimated heat capacities of alcohols. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Zábanský *et al* (93ZAB/RUZ) — Continued

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. range, K	Heat capacity range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
2-methyl-2-propanol	17(6)	13.8 (1.8)	3.9 (0.6)	298–453	219–301	15.5 (12.5)
2-methyl-1-butanol	4(4)	7.3	2.6	313–343	227–241	
2-methyl-2-butanol	9(9)	1.5	0.6	275–343	225–291	
3-methyl-1-butanol	15(15)	6.4	2.3	224–353	168–260	
2-pentanol	9(9)	14.6	5.3	298–362	239–296	11.4
3-pentanol	6(6)	13.5	4.9	298–343	240–272	
3,3-dimethyl-1-butanol	1(1)	9.1	3.9	298	236	
2-ethyl-1-butanol	1(1)	18.7	7.4	298	253	
2-hexanol	1(1)	6.5	2.5	298	256	3.8
3-hexanol	1(1)	19.4	7.2	298	269	
2-methyl-1-pentanol	1(1)	14.3	5.8	298	248	
2-methyl-2-pentanol	1(1)	10.0	3.4	298	289	
3-methyl-2-pentanol	1(1)	27.9	10.1	298	276	
3-methyl-3-pentanol	6(6)	20.6	6.4	283–323	275–332	
4-methyl-2-pentanol	1(1)	24.8	9.1	298	273	9.7
3-ethyl-3-pentanol	1(1)	45.0	12.7	298	354	
2-heptanol	1(1)	4.7	1.7	298	275	
4-heptanol	1(1)	38.0	12.0	298	318	
2-ethyl-1-hexanol	8(8)	34.9	9.8	293–353	315–391	15.2
2-methyl-1-heptanol	8(8)	19.9	6.0	260–311	280–335	
2-methyl-2-heptanol	10(10)	4.1	1.1	232–311	261–352	
2-methyl-4-heptanol	12(12)	15.1	4.7	201–299	243–332	
3-methyl-2-heptanol	16(16)	15.4	5.4	167–299	247–299	
4-methyl-2-heptanol	14(14)	7.5	2.7	184–299	230–315	
4-methyl-3-heptanol	16(16)	7.1	2.4	167–299	235–309	
4-methyl-4-heptanol	12(12)	14.9	3.6	201–299	240–369	
5-methyl-1-heptanol	14(14)	5.9	1.4	184–299	234–306	
5-methyl-2-heptanol	16(16)	6.0	2.0	167–299	231–299	
6-methyl-2-heptanol	9(9)	8.8	3.0	232–299	260–315	
6-methyl-3-heptanol	12(12)	6.1	1.9	232–323	255–329	
2-octanol	9(9)	16.4	4.8	246–314	269–344	
3-octanol	11(11)	27.6	9.0	217–299	269–339	
4-octanol	12(12)	23.4	7.3	217–311	276–351	
5-decanol	1(1)	36.8	9.1	298	406	
3,7-dimethyl-1-octanol	1(1)	15.7	4.3	298	367	
4-propyl-4-heptanol	1(1)	48.4	10.8	298	447	
5-butyl-5-nonanol	1(1)	61.0	11.1	298	549	
cyclopentanol	6(6)	1.3	0.7	260–300	155–186	
cyclohexanol	15(15)	28.7	6.4	298–428	211–320	17.8
cycloheptanol	6(6)	14.9	5.8	283–316	233–271	
1-methylcyclohexanol	1(1)	10.3	3.7	298	279	
2-methylcyclohexanol	1(1)	29.7	11.1	298	267	
phenol	7(7)	5.3	2.5	313–373	200–214	8.5
benzenemethanol ^b	23(23)	0.9	0.3	260–462	191–272	1.7
2-methylphenol	11(11)	2.7	1.0	304–400	233–252	10.1
3-methylphenol	14(14)	0.8	0.3	285–400	219–256	10.7
4-methylphenol	11(11)	1.8	0.6	308–400	227–258	7.3
benzeneethanol	1(1)	24.5	9.7	298	253	
benzenepropanol	1(1)	22.8	8.1	298	281	
1-naphthol	10(10)	58.1	18.5	368–453	275–317	
2-naphthol	10(10)	80.0	24.9	394–478	289–320	
2-methyl-5-(1-methylethyl)phenol	1(1)	8.0	2.2	402	363	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.

^cSee footnote c at the bottom of Table 10.

TABLE 20. Deviations between recommended and estimated heat capacities of diols. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Zábanský *et al.* (93ZAB/RUZ).

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^b (Lee-Kesler) %
1,2-ethanediol	26(22)	3.9 (2.1)	1.5 (1.0)	262–493	138–206	32.4 (32.0)
1,2-propanediol	29(29)	23.9	6.4	194–461	151–263	
1,2,3-propanetriol	18(18)	51.9	16.9	293–453	216–257	5.2
1,3-butanediol	1(1)	2.0	0.9	303–	227–	6.1
1,4-butanediol	18(18)	8.1	2.8	296–450	199–291	7.6
2,3-butanediol	6(6)	32.7	13.2	316–358	227–259	
2,2-dimethyl-1,3-propanediol	4(4)	31.0	9.3	410–440	325–336	
1,5-pentanediol	3(3)	27.4	13.4	270–287	197–209	
1,2-benzenediol	11(11)	0.0	0.0	378–473	239–263	
1,3-benzenediol	10(10)	2.2	0.7	383–473	240–267	
1,4-benzenediol	4(4)	1.5	0.5	446–473	259–264	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bSee footnote c at the bottom of Table 10.

TABLE 21. Deviations between recommended and estimated heat capacities of aldehydes. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Zábanský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
acetaldehyde ^b	11(11)	26.0	20.1	150–240	60–150	31.5
acetaldehyde	6(4)	14.7 (15.4)	17.1 (18.2)	260–300	82–89	28.4 (30.1)
propanal ^b	13(13)	16.4	11.1	171–286	129–158	5.2
propanal	7(5)	24.6 (27.9)	14.4 (16.6)	286–335	170–148	10.0 (12.3)
2-butenal	10(10)	2.6	1.2	273–343	145–152	
butanal	14(14)	4.1	2.2	180–300	147–165	4.0
2,2-dimethylpropanal	10(10)	3.7	1.7	274–350	180–201	
pentanal	17(17)	14.2	7.6	192–340	168–183	
benzaldehyde	23(23)	0.4	0.2	218–425	156–205	5.8
3,4-dimethylpentanal	12(6)	21.1 (25.7)	7.7 (10.6)	323–428	235–296	
heptanal	16(16)	2.3	0.8	230–368	231–268	
3-methylhexanal	12(8)	9.6 (10.4)	3.3 (3.7)	323–428	246–303	
octanal	13(13)	20.4	7.7	248–350	248–278	
3-phenyl-2-propenal	1(1)	4.8	2.0	298	233	
nonanal	11(11)	20.9	7.1	254–340	276–302	
3,7,-dimethyl-2,6-octadienal	7(7)	20.8	7.3	233–293	263–305	
decanal	9(9)	24.9	7.8	269–338	304–331	
2-(1,2-dimethylpropyl)-5,6-dimethyl-2-heptenal	12(12)	19.8	46.0	9.9	323–428	421–509
2-pentyl-2-nonenal	12(12)	19.8	3.7	323–428	439–521	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bThe dependence of the heat capacity with temperature is discontinuous; two sets of parameters are given in 93ZAB/RUZ for two different temperature ranges.

^cSee footnote c at the bottom of Table 10.

TABLE 22. Deviations between recommended and estimated heat capacities of ketones. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^b (Lee-Kesler) %
2-propanone	18(16)	1.8 (1.1)	1.0 (0.6)	180-333	117-134	4.2 (4.4)
2-butanone	19(18)	3.4 (3.4)	2.1 (2.1)	191-353	149-169	4.1 (4.3)
cyclopentanone	1(1)	8.0	5.2	298-	155-	7.1
2,4-pentanedione	7(7)	5.2	2.2	255-300	191-209	
3-methyl-2-butanone	16(16)	0.5	0.2	184-324	163-186	10.7
2-pentanone	19(19)	0.8	0.4	201-364	173-200	4.2
3-pentanone	11(11)	5.7	3.0	238-319	183-194	
cyclohexanone	8(8)	4.5	2.2	246-301	159-178	6.4
4-methyl-3-pentan-2-one	5(5)	3.9	1.7	317-355	200-215	
3,3-dimethyl-2-butanone	16(16)	0.3	0.1	226-363	190-224	
2-hexanone	19(19)	2.0	0.8	221-383	203-236	3.4
3-hexanone	12(12)	1.9	0.9	222-322	205-223	2.3
4-methyl-2-pentanone	3(3)	1.4	0.6	298-318	212-217	0.4
cycloheptanone	1(1)	11.5	5.4	298-	212-	
2-methylcyclohexanone	1(1)	7.6	3.7	290-	205-	
3-methylcyclohexanone	1(1)	6.8	3.3	290-	207-	
4-methylcyclohexanone	1(1)	6.8	3.3	290-	207-	
2,4-dimethyl-3-pentanone	14(14)	0.9	0.3	208-319	209-243	
2-heptanone	1(1)	0.8	0.3	298-	244-	
4-heptanone	1(1)	1.9	0.8	298-	246-	
2-methyl-3-hexanone	1(1)	1.9	0.8	298-	242-	
1-phenylethanone	10(10)	5.4	2.1	298-381	205-238	2.5
6-methyl-5-hepten-2-one	9(9)	4.0	1.3	273-343	262-279	
2-octanone	15(15)	3.5	0.9	258-380	264-300	
1-phenyl-1-propanone	1(1)	13.7	5.6	298-	244-	
2,6-dimethyl-4-heptanone	3(3)	3.4	1.1	298-318	298-306	
5-nonanone	7(7)	0.8	0.2	277-320	298-311	
1-(4-ethylphenyl)ethanone	1(1)	4.5	1.7	298-	261-	
6,10-dimethyl-3,5,9-undecatriene-2-one	10(10)	18.5	3.6	273-343	375-404	
4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	9(9)	12.5	2.7	273-334	365-395	
6,10-dimethyl-2-undecanone	10(10)	1.3	0.3	273-343	402-453	
2-tetradecanone	4(4)	4.5	0.8	313-338	469-482	
2-pentadecanone	4(4)	4.1	0.6	318-343	504-516	
1,4-diphenyl-1,4-butanedione	5(5)	1.9	0.3	423-463	504-516	
6,10,14-trimethyl-3,5-pentadecadien-2-one	9(9)	38.4	6.8	273-334	538-583	
6,10,14-trimethyl-2-pentadecanone	9(9)	38.1	6.2	273-334	574-646	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bSee footnote c at the bottom of Table 10.

TABLE 23. Deviations between recommended and estimated heat capacities of ethers. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
oxybismethane	12(12)	5.5	5.5	137-245	98-103	4.1
dimethoxymethane ^b	15(15)	0.1	0.0	171-308	144-163	
2-methoxy-1-propene	5(5)	3.7	2.3	273-302	155-162	
1-methoxypropane	20(20)	0.3	0.2	138-309	141-168	
2-methoxypropane	21(19)	0.6 (0.6)	0.4 (0.4)	130-311	136-166	
1,1'-oxybisethane	33(16)	55.7 (7.1)	13.9 (4.3)	160-460	148-329	3.9 (2.0)
1-ethoxypropane	19(19)	3.1	1.6	151-316	168-202	12.1
1-methoxybutane	18(18)	1.5	0.7	160-316	169-198	
2-methoxy-2-methylpropane ^b	16(16)	0.0	0.0	168-308	155-191	1.3
2,2-dimethoxypropane ^b	9(9)	0.0	0.0	273-334	208-232	
1,2-dimethoxyethane	1(1)	1.1	0.6	298-	193-	
1-ethoxy-2-methoxyethane	1(1)	1.9	0.8	298-	225-	
2-ethoxy-2-methylpropane	1(1)	2.1	1.0	298-	218-	
2-methoxy-2-methylbutane	1(1)	5.0	2.3	298-	222-	
1,1'-oxybispropane	19(19)	1.9	0.9	161-323	192-230	3.1
2,2'-oxybispropane	18(18)	0.7	0.3	188-340	184-233	1.2
1,2-diethoxyethane	1(1)	8.5	3.3	298-	260-	
1-methoxy-2-propoxyethane	1(1)	3.7	1.5	298-	249-	
1,1'-oxybis(2-methoxyethane)	16(16)	5.9	1.8	210-350	269-284	
methoxybenzene	6(6)	8.4	3.7	305-350	209-214	8.4
2-ethoxy-2-methylbutane	1(1)	2.6	1.1	298-	243-	
1-butoxy-2-methoxyethane	1(1)	0.4	0.1	298-	282-	
ethoxybenzene	4(4)	1.5	0.6	320-349	240-252	
1-methoxy-4-methylbenzene	5(5)	9.5	4.0	312-350	226-240	
1,2-dipropoxyethane	1(1)	1.8	0.6	298-	309-	
1,1'-oxybis(2-ethoxyethane)	5(5)	9.0	2.6	283-313	345-352	
2,5,8,11-tetraoxadodecane	14(14)	7.2	1.5	230-350	368-378	
1-ethoxy-4-methylbenzene	4(4)	3.3	1.2	320-350	268-282	
1-methoxy-2,4-dimethylbenzene	4(4)	3.7	1.3	322-351	262-276	
propoxybenzene	4(4)	1.8	0.7	320-349	267-282	
1,1'-[1,2-ethanediybis(oxy)]bisbutane	1(1)	18.4	5.3	293-	350-	
2,5,8,11,14-pentaoxapentadecane	16(16)	5.3	0.9	293-426	455-509	
1-methoxydecane	13(13)	5.1	1.2	247-349	355-397	
1,1'-oxybisbenzene ^b	28(22)	0.0 (0.0)	0.0 (0.0)	300-570	268-390	2.8 (3.3)
1-(ethenyloxy)butane	1(1)	21.1	9.1	298-	232-	
1-(ethenyloxy)-2-methylpropane	1(1)	23.7	10.2	298-	233-	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.

^cSee footnote c at the bottom of Table 10.

TABLE 24. Deviations between recommended and estimated heat capacities of organic acids. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^b (Lee-Kesler) %
formic acid	8(8)	1.1	1.0	282–342	98–101	6.1
Acetic acid	13(11)	0.8 (0.9)	0.5 (0.6)	293–400	122–149	7.6 (8.7)
2-propenoic acid	8(8)	0.4	0.2	289–343	142–158	6.0
propanoic acid	22(17)	1.8 (2.0)	1.0 (1.2)	255–447	142–204	9.0 (11.2)
(E)-2-butenic acid	1(1)	13.9	7.7	345	180	
2-methyl-2-propenoic acid	8(8)	7.1	3.9	289–348	158–196	8.0
butanoic acid	13(13)	2.8	1.4	273–373	169–209	12.6
2-methylpropanoic acid	17(17)	6.7	3.7	227–374	145–201	
3-methylbutanoic acid	9(9)	7.5	2.9	314–385	205–241	
pentanoic acid	8(8)	1.3	0.6	241–303	190–213	
hexanedioic acid	4(4)	34.5	9.6	430–460	348–351	3.4
hexanoic acid	13(13)	8.3	3.0	285–392	248–281	
benzoic acid	9(9)	2.7	1.0	396–471	251–299	14.5
heptanoic acid	5(5)	4.9	1.9	275–305	255–268	
2-methylbenzoic acid	11(11)	6.9	2.0	377–473	284–324	
3-methylbenzoic acid	8(8)	25.3	7.5	382–443	312–327	
4-methylbenzoic acid	6(6)	4.2	1.1	453–498	322–357	
octanoic acid	3(3)	2.0	0.7	290–305	294–302	
nonanoic acid	3(3)	3.9	1.2	290–305	322–330	
decanoic acid	5(5)	4.7	1.2	310–345	364–386	
undecanoic acid	4(4)	3.6	0.9	305–330	391–408	
dodecanoic acid	3(3)	2.0	0.4	325–345	438–455	
tridecanoic acid	3(3)	2.9	0.5	320–340	466–480	
tetradecanoic acid	2(2)	1.4	0.3	335–345	510–520	
pentadecanoic acid	3(3)	1.3	0.2	330–345	538–551	
hexadecanoic acid	5(5)	36.7	4.8	340–373	575–672	5.6
heptadecanoic acid	2(2)	0.5	0.1	340–350	612–624	
(Z)-9-octadecenoic acid	1(1)	4.6	0.8	290	583	
octadecanoic acid	2(2)	0.5	0.1	350–355	656–661	2.5
nonadecanoic acid	2(2)	3.0	0.4	345–355	686–697	
eicosanoic acid	3(3)	4.1	0.6	350–361	726–731	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bSee footnote c at the bottom of Table 10.

TABLE 25. Deviations between recommended and estimated heat capacities of esters. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^b (Lee-Kesler) %
methyl formate	3(3)	3.8	2.6	293–299	115–120	2.5
ethyl formate	3(3)	13.4	6.9	298–309	144–161	5.4
methyl acetate	5(5)	3.9	2.4	283–313	136–147	2.9
methyl propanoate	13(13)	1.9	1.2	196–300	148–160	3.4
ethyl acetate	17(17)	4.9	2.5	196–340	160–182	3.6
methyl propanoate	17(17)	8.1	4.4	205–348	168–182	4.2
propyl formate	3(3)	1.1	0.4	298–310	172–175	
methyl 2-methyl-2-propenoate	12(12)	3.6	1.5	226–323	167–201	
2-propenyl acetate	4(4)	5.2	2.3	309–338	193–203	
butyl formate	1(1)	3.3	1.6	298–	200–	
ethyl propanoate	8(8)	3.4	1.6	294–349	200–211	4.2
methyl butanoate	4(4)	2.4	1.2	298–323	199–206	
methyl 2-methylpropanoate	3(3)	6.5	3.2	309–322	202–207	
1-methylethyl acetate	1(1)	4.1	2.1	298–	197–	4.1
2-methylpropyl formate	2(2)	2.4	0.8	310–318	204–208	
propyl acetate	5(5)	4.3	1.8	298–338	196–209	2.5
2-propenyl propanoate	4(4)	4.7	1.9	308–333	222–232	

TABLE 25. Deviations between recommended and estimated heat capacities of esters. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ) — Continued

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^b (Lee-Kesler) %
1,2-ethanediyl diacetate	1(1)	12.7	4.7	298-	269-	
butyl acetate	23(23)	1.8	0.7	196-399	207-257	3.0
1,1-dimethylethyl acetate	1(1)	12.4	5.4	298-	231-	
ethyl butanoate	21(21)	1.9	0.6	180-370	213-248	4.8
ethyl 2-methylpropanoate	3(3)	6.7	2.8	308-327	230-237	
methyl 2,2-dimethylpropanoate	1(1)	7.4	3.3	298-	227-	
methyl pentanoate	5(5)	1.4	0.5	298-332	226-240	
3-methylbutyl formate	4(4)	3.3	1.2	309-334	231-243	
2-methylpropyl acetate	4(4)	3.9	1.6	307-332	229-240	
Propyl propanoate	10(10)	4.0	1.7	294-367	228-248	2.7
butyl 2-propenoate	15(15)	2.1	0.8	210-334	226-261	
2-propenyl butanoate	4(4)	5.8	1.8	308-332	249-260	
2-propenyl 2-methylpropanoate	4(4)	4.4	1.5	308-332	248-259	
ethyl 2,2-dimethylpropanoate	1(1)	3.5	1.4	298-	251-	
ethyl 3-methylbutanoate	4(4)	15.1	5.3	313-343	271-288	
ethyl pentanoate	4(4)	2.4	0.8	308-332	258-269	
3-methylbutyl acetate	4(4)	1.7	0.6	308-333	258-269	
2-methylpropyl propanoate	4(4)	3.1	1.1	310-334	258-270	
propyl butanoate	4(4)	3.3	1.0	318-346	262-276	
propyl 2-methylpropanoate	4(4)	4.3	1.6	309-333	258-269	
methyl benzoate	6(6)	1.5	0.6	298-345	221-238	
di-2-propenyl ethanedioate	4(4)	13.3	3.3	319-348	316-329	
butyl 2-methyl-2-propenoate	18(18)	5.5	1.7	197-350	246-288	
2-propenyl pentanoate	4(4)	5.9	1.8	318-347	282-296	
diethyl butanedioate	7(7)	22.2	6.3	298-349	331-355	
dipropyl ethanedioate	4(4)	4.5	1.3	319-347	328-343	
butyl butanoate	28(28)	3.4	1.1	182-439	259-346	
ethyl hexanoate	18(18)	1.0	0.3	210-370	264-314	
hexyl acetate	17(17)	2.5	0.8	220-370	263-311	
3-methylbutyl propanoate	17(17)	2.8	0.7	220-370	266-315	
2-methylpropyl butanoate	4(4)	1.2	0.4	318-345	290-305	
2-methylpropyl 2-methylpropanoate	4(4)	2.3	0.7	318-346	289-305	
propyl pentanoate	4(4)	1.3	0.4	318-346	290-304	
ethyl benzoate	8(8)	2.0	0.7	293-346	243-270	7.6
phenylmethyl acetate	1(1)	16.7	6.7	298-	248-	
butyl pentanoate	20(20)	4.6	1.4	190-370	285-344	
3-methylbutyl butanoate	4(4)	2.1	0.5	318-343	319-334	
3-methylbutyl 2-methylpropanoate	4(4)	1.1	0.3	317-346	319-336	
2-methylpropyl pentanoate	4(4)	1.7	0.4	318-347	319-336	
pentyl butanoate	19(19)	3.8	1.2	200-370	286-343	
2-propenyl benzoate	4(4)	5.4	1.7	319-348	277-291	
dimethyl 1,2-benzenedicarboxylate	11(11)	11.7	3.2	274-360	295-324	
dimethyl 1,4-benzenedicarboxylate	7(7)	33.4	8.8	416-466	360-385	
propyl benzoate	4(4)	0.8	0.2	318-347	286-301	
di-2-propenyl butanedioate	4(4)	24.2	5.4	320-348	384-400	
bis(2-methylpropyl) ethanedioate	4(4)	0.5	0.1	318-347	386-403	
dipropyl butanedioate	4(4)	17.0	4.1	319-347	396-413	
hexyl butanoate	19(19)	12.1	3.6	200-370	308-366	
3-methylbutyl pentanoate	5(5)	5.4	1.5	310-346	342-364	
ethyl 3-phenyl-2-propenoate	8(8)	6.8	2.0	316-380	305-337	
diethyl 1,2-benzenedicarboxylate	11(11)	0.6	0.2	273-353	355-394	
diethyl 1,4-benzenedicarboxylate	5(5)	3.8	1.0	316-348	376-396	
nonyl 2-propenoate	12(12)	23.5	4.7	237-334	353-462	
octyl 2-methyl-2-propenoate	15(15)	10.8	2.3	230-350	355-410	
bis(3-methylbutyl) ethanedioate	4(4)	0.7	0.2	318-347	447-467	
bis(2-methylpropyl) butanedioate	4(4)	12.5	2.7	319-348	455-474	
dibutyl butanedioate	17(17)	2.8	0.5	250-400	424-488	
nonyl 2-methyl-2-propenoate	10(10)	4.5	1.0	244-315	399-429	
decyl 2-methyl-2-propenoate	12(12)	2.6	0.4	251-350	421-489	
bis(3-methylbutyl) butanedioate	4(4)	13.4	2.5	319-348	517-539	
dibutyl 1,2-benzenedicarboxylate	21(21)	9.4	1.9	177-360	427-515	
dibutyl decanedioate	11(11)	10.4	1.3	312-412	613-735	

TABLE 25. Deviations between recommended and estimated heat capacities of esters. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ) — Continued

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^b (Lee-Kesler) %
bis(2-ethylhexyl) hexanedioate	14(14)	20.6	2.8	180–300	642–701	
dihexyl decanedioate	13(13)	15.6	1.6	303–414	703–874	
butyl octadecanoate	2(2)	12.3	1.5	302–305	711–726	
bis(2-ethylhexyl)-1,2-benzenedicarboxylate	19(19)	16.5	2.1	190–360	635–768	
bis(2-ethylhexyl) nonanedioate	19(19)	16.8	2.0	170–336	738–844	
dihexadecyl decanedioate	8(8)	9.3	0.6	353–418	1460–1595	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bSee footnote c at the bottom of Table 10.

TABLE 26. Deviations between recommended and estimated heat capacities of heterocyclic oxygen compounds. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Záborský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
oxirane	14(13)	2.0 (2.1)	2.4 (2.4)	161–284	83–87	7.5 (7.6)
methyloxirane	18(16)	5.2 (5.4)	4.4 (4.7)	167–325	109–127	4.9 (5.2)
oxetane ^b	13(13)	0.0	0.0	185–298	99–100	
1,3-dioxolane ^b	15(15)	0.0	0.0	176–300	109–118	
furan	13(13)	0.6	0.5	191–299	100–115	6.8
ethyloxirane	21(21)	2.6	1.7	137–322	134–153	
tetrahydrofuran	19(19)	0.3	0.2	162–323	107–131	8.9
2-methylfuran	13(13)	3.0	2.2	196–307	129–146	
tetrahydropyran ^b	5(5)	0.0	0.0	298–327	150–162	
benzofuran	23(23)	11.2	4.4	245–450	165–228	
2,3-dihydrobenzofuran	22(22)	15.5	7.0	251–450	175–242	
3,4-dihydro-1H-2-benzopyran	20(20)	46.9	13.4	278–450	210–282	
3,4-dihydro-2H-1-benzopyran	21(21)	12.5	4.8	270–450	203–279	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.

^cSee footnote c at the bottom of Table 10.

TABLE 27. Deviations between recommended and estimated heat capacities of sulfides. Recommended data are from Zábanský *et al.* (93ZAB/RUZ).

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^b (Lee-Kesler) %
thiobismethane	12	5.6	4.9	181–287	113–117	3.9
2,3-dithiabutane	19	0.2	0.1	192–352	144–152	
(methylthio)ethane	13	3.1	2.2	172–298	135–144	8.6
1-(methylthio)propane	18	1.1	0.6	167–326	158–177	6.4
2-(methylthio)propane	19	2.9	1.7	177–344	158–183	5.8
1,1'-thiobisethane	16	1.8	0.9	182–316	157–175	4.4
3,4-dithiahexane	15	0.6	0.2	168–299	192–204	
1-(ethylthio)propane	23	1.0	0.4	166–366	180–216	5.6
2-methyl-2-(methylthio)propane	20	0.9	0.5	190–364	178–220	5.4
1-(methylthio)butane	20	0.7	0.3	187–358	184–217	4.1
methylthiocyclopentane	22	3.7	1.8	173–369	170–217	
1,1'-thiobispropane	17	3.5	1.6	174–315	204–230	5.0
2,2'-thiobispropane	20	3.8	1.5	204–383	209–260	
dipropyldisulfide	18	0.4	0.1	194–351	245–277	
1,1'-thiobisbutane	18	4.0	1.4	205–356	258–309	2.9

^aStandard deviation and average absolute percent deviation defined in Table 10.^bSee footnote c at the bottom of Table 10.TABLE 28. Deviations between recommended and estimated heat capacities of thiols. Numbers of data points and values of standard and average deviations in parentheses apply to data up to the normal boiling temperature only. Temperature and heat capacity ranges correspond to the entire range of available data. Recommended data are from Zábanský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
methanethiol	13(13)	2.2	2.1	154–271	89–88	6.6
ethanethiol	21(19)	2.8 (2.4)	1.9 (1.6)	130–315	114–120	11.6 (12.8)
1-propanethiol	17(17)	1.2	0.8	168–315	137–147	6.9
2-propanethiol	20(20)	1.5	0.8	149–322	131–150	9.3
1-butanethiol	18(18)	1.6	0.9	160–314	164–176	8.9
2-butanethiol	19(19)	1.8	1.0	136–307	160–173	13.4
2-methyl-1-propanethiol	24(24)	1.8	0.9	137–349	157–183	10.7
2-methyl-2-propanethiol	7(7)	1.1	0.6	281–329	172–181	3.4
cyclopentanethiol	23(23)	5.0	2.7	162–366	149–185	
2-methyl-2-butanethiol	20(20)	4.9	2.4	172–347	179–211	
3-methyl-1-butanethiol	25(25)	1.3	0.5	141–371	182–222	
3-methyl-2-butanethiol	26(26)	4.3	1.8	148–379	181–222	
1-pentanethiol	15(15)	1.8	0.9	200–321	187–207	4.7
benzenethiol ^b	14(14)	0.0	0.0	262–375	168–188	6.9
cyclohexanethiol	19(19)	1.0	0.5	197–365	172–214	11.1
1-hexanethiol	20(20)	1.8	0.7	200–372	215–254	3.8
1-heptanethiol	15(15)	2.7	1.0	232–359	244–282	2.9
1-decanethiol	14(14)	2.5	0.6	255–375	337–389	3.1

^aStandard deviation and average absolute percent deviation defined in Table 10.^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.^cSee footnote c at the bottom of Table 10.

TABLE 29. Deviations between recommended and estimated heat capacities of heterocyclic sulfur compounds. Recommended data are from Záborský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^c (Lee-Kesler) %
thietane ^b	14	0.1	0.1	202–321	102–117	
thiophene	12	1.0	0.7	238–336	114–131	5.3
tetrahydrothiophene	18	2.2	1.5	180–333	121–149	11.6
1,3-dithiane	4	11.1	6.2	340–370	174–185	
1,4-dithiane	2	4.0	1.8	390–400	202–203	
2-methylthiophene	16	0.7	0.5	213–344	137–159	6.0
3-methylthiophene	16	0.3	0.2	207–337	137–159	7.9
2-methyltetrahydrothiophene	25	0.8	0.3	168–389	144–200	
3-methyltetrahydrothiophene	17	2.9	1.7	194–337	148–184	
tetrahydro-2H-thiopyran ^b	7	0.0	0.0	296–342	162–178	
2,5-dimethylthiophene	11	1.9	1.1	217–304	165–180	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bThe heat capacity values for the compound were used as a single source of data to determine the adjustable parameters.

^cSee footnote c at the bottom of Table 10.

TABLE 30. Deviations between recommended and estimated heat capacities of compounds of carbon, hydrogen, halogen, nitrogen, and oxygen. Recommended data are from Záborský *et al.* (93ZAB/RUZ)

Compound	No. data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^a %	Temp. Range, K	Heat capacity Range, J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^b (Lee-Kesler) %
pentafluorophenol	8	8.8	2.7	315–376	279–277	
2,4-dibromophenol	1	6.0	2.3	329	256	
4-bromophenol	1	4.3	1.9	343	228	
2-chlorophenol	8	10.8	5.0	298–351	210–223	3.4
2-chlorobenzoic acid	8	6.8	2.0	414–472	289–303	
3-chlorobenzoic acid	22	24.9	10.7	288–478	184–303	
4-chlorobenzoic acid	4	14.8	3.8	512–538	358–358	
pentafluoronitrobenzene	8	18.1	6.7	249–300	265–273	
2,3,4,5,6-pentafluorobenzeneamine	2	9.6	3.8	309–317	256–256	
1-bromo-3-nitrobenzene	1	14.3	6.4	340	223	
1-chloro-3-nitrobenzene	1	11.9	5.4	338	220	
1-chloro-4-nitrobenzene	13	15.8	5.7	354–466	239–239	
3-chlorobenzeneamine	5	8.1	3.9	298–323	199–207	

^aStandard deviation and average absolute percent deviation defined in Table 10.

^bSee footnote c at the bottom of Table 10.

TABLE 31. Summary deviations between recommended heat capacities and those estimated by the present group contribution method. Values in parentheses apply to data up to the normal boiling temperature only

Family	No. cmpds.	No. Data points	Std. dev. ^a J·K ⁻¹ ·mol ⁻¹	Avg. dev. ^b %	Temp. range, K	Heat capacity range, J·K ⁻¹ ·mol ⁻¹
bromides and iodides C ₂ to C ₉	22	205 (193)	8.5 (6.3)	2.7 (2.5)	168–523	89–361
chlorides C ₂ to C ₁₂	37	304 (278)	26.4 (8.9)	3.7 (2.6)	119–573	85–607
fluorides C ₂ to C ₁₂	20	217 (215)	6.5 (6.6)	1.3 (1.3)	126–377	102–444
mixed halogen derivatives C ₂ to C ₆	21	220 (177)	12.5 (13.3)	4.1 (4.3)	120–458	111–259
amines C ₁ to C ₁₆	28	230 (228)	6.5 (6.5)	1.2 (1.2)	161–453	99–633
hydrazines C ₁ to C ₆	6	67 (64)	2.8 (2.8)	0.7 (0.8)	97–239	205–464
nitriles C ₃ to C ₇	10	105 (105)	5.7	2.8	173–480	102–232
heterocyclic nitrogen compounds C ₄ to C ₉	26	404 (383)	7.9 (8.0)	2.1 (2.2)	170–450	93–333
compounds of carbon, hydrogen, nitrogen, and oxygen C ₃ to C ₇	26	221 (221)	17.2	4.2	182–518	130–374
alcohols C ₁ to C ₁₈	74	903 (807)	71.0 (62.8)	7.8 (6.1)	71–887	154–623
diols C ₂ to C ₆	11	130 (126)	24.7 (25.0)	5.7 (5.8)	138–336	194–493
aldehydes C ₁ to C ₆	19	216 (202)	18.7 (19.1)	6.4 (6.4)	60–521	150–428
ketones C ₃ to C ₁₈	36	281 (278)	11.0(11.0)	1.6 (1.6)	180–463	117–646
ethers C ₂ to C ₆	36	336 (311)	17.9 (4.6)	2.4 (1.3)	98–509	130–570
organic acids C ₁ to C ₂₀	31	204 (197)	10.1 (10.3)	2.1 (2.1)	227–498	98–731
esters C ₂ to C ₄₂	85	692 (692)	9.5	1.8	170–466	115–1595
heterocyclic oxygen compounds C ₂ to C ₄	13	217 (214)	16.1 (16.2)	3.7 (3.8)	137–450	81–282
sulfides C ₂ to C ₈	15	270 (270)	2.6	1.1	166–383	112–309
thiols C ₁ to C ₁₀	18	330 (328)	2.7 (2.7)	1.2 (1.2)	130–379	87–389
heterocyclic sulfur compounds C ₄ to C ₅	11	142 (142)	2.4	0.9	168–400	102–203
compounds of carbon, hydrogen, halogen, nitrogen, and oxygen C ₆ to C ₆	13	78 (78)	16.6	6.0	250–538	184–359

^aStandard deviation is calculated as

$$SD = \sqrt{\frac{1}{n_c} \sum \frac{1}{n_p} \sum (C^{rec} - C^{estd})^2}$$

where n_c is the number of compounds and n_p is the number of data points for each compound (usually 10 K apart).

^bAverage absolute percent deviation is calculated as

$$APD = 100 \cdot \frac{1}{n_c} \sum \frac{1}{n_p} \sum \left| \frac{C^{rec} - C^{estd}}{C^{rec}} \right|$$

TABLE 32. Summary deviations between recommended heat capacities and those estimated by the Lee-Kesler method (75LEE/KES). Values in parentheses apply to data up to the normal boiling temperature only

Family	No. compds.	No. data points	Std. dev. ^a J·K ⁻¹ mol ⁻¹	Avg. dev. ^a %	Temp. range, K	Heat capacity range, J·K ⁻¹ mol ⁻¹
bromides and iodide						
C ₂ to C ₆	7	84 (84)	3.8	2.3	168–369	89–175
Lee-Kesler	7	84 (84)	15.1	8.8		
chlorides C ₂ to C ₁₂	17	153 (143)	6.6 (6.7)	2.4 (2.4)	119–370	85–277
Lee-Kesler	17	153 (143)	12.9 (13.3)	6.4 (6.7)		
fluorides C ₂ to C ₇	4	46 (44)	7.8 (8.0)	0.8 (0.9)	145–350	106–444
Lee-Kesler	4	46 (44)	11.5 (11.8)	2.3 (2.4)		
mixed halogen derivatives						
C ₂ to C ₂	4	57 (36)	8.0 (6.5)	3.6 (3.5)	146–458	11–259
Lee-Kesler	4	54 (36)	7.2 (7.9)	3.4 (3.9)		
amines C ₂ to C ₁₀	13	126 (113)	10.4 (9.1)	3.9 (3.5)	161–453	99–307
Lee-Kesler	13	126 (113)	15.8 (15.7)	7.1 (7.0)		
nitriles C ₂ to C ₇	4	73 (73)	6.7	3.7	173–383	102–190
Lee-Kesler	4	73 (73)	16.8	11.8		
heterocyclic nitrogen compounds						
C ₄ to C ₉	9	143 (140)	3.2 (3.2)	1.2 (1.2)	210–450	122–251
Lee-Kesler	9	143 (140)	14.4 (14.5)	6.0 (6.1)		
alcohols C ₁ to C ₁₈	32	627 (531)	83.8 (75.5)	9.0 (6.6)	154–623	71–887
Lee-Kesler	32	614 (531)	49.5 (51.6)	16.0 (16.7)		
diols C ₂ to C ₄	4	63 (59)	28.2 (29.1)	6.3 (6.4)	262–493	138–291
Lee-Kesler	4	63 (59)	39.5 (36.5)	17.1 (15.9)		
aldehydes C ₂ to C ₁₂	6	74 (70)	15.0 (15.1)	8.2 (8.0)	150–425	60–205
Lee-Kesler	6	74 (70)	16.6 (16.7)	11.4 (11.2)		
ketones C ₃ to C ₈	10	125 (122)	2.7 (2.7)	1.1 (1.1)	180–383	117–239
Lee-Kesler	10	125 (122)	11.2 (11.3)	4.7 (4.7)		
ethers C ₂ to C ₁₂	8	151 (128)	26.2 (3.8)	4.0 (1.6)	137–570	98–390
Lee-Kesler	8	145 (128)	13.4 (13.1)	4.1 (4.2)		
organic acids						
C ₁ to C ₁₈	10	92 (85)	11.5 (11.9)	1.7 (1.8)	254–471	98–672
Lee-Kesler	10	92 (85)	21.8 (22.6)	8.7 (9.3)		
esters C ₂ to C ₉	13	134 (134)	4.5	1.9	180–399	115–270
Lee-Kesler	13	134 (134)	9.8	3.9		
heterocyclic oxygen compounds						
C ₂ to C ₄	4	64 (61)	2.9 (3.0)	1.9 (1.9)	161–325	81–131
Lee-Kesler	4	64 (61)	11.0 (11.2)	7.0 (7.2)		
sulfides C ₂ to C ₈	10	176 (176)	2.7	1.3	166–366	112–309
Lee-Kesler	10	176 (176)	13.0	5.2		
thiols C ₁ to C ₁₀	14	236 (234)	1.9 (1.8)	0.9 (0.9)	130–375	87–389
Lee-Kesler	14	236 (234)	19.8 (19.9)	7.9 (8.0)		
heterocyclic sulfur compounds						
C ₄ to C ₅	4	62 (62)	1.3	0.8	180–344	114–159
Lee-Kesler	4	62 (62)	14.9	8.0		

^a Standard deviation and average absolute percent deviation defined in Table 31.

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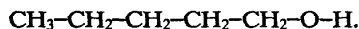
Appendix

Sample calculations for the estimation of the heat capacities of 1-pentanol, 1,2-ethanediol, and pyrrolidine

Sample calculation for the estimation of the heat capacity of 1-pentanol at 350 K.

- (1) Kind and number of additive groups.

The structural formula for 1-pentanol is:



The following groups are needed for the calculation of adjustable parameters necessary to estimate the heat capacity of 1-pentanol in the liquid phase at an arbitrary temperature in the range from the melting to the boiling temperature; let us choose 350 K.

Molecular fragment	Group	No. of groups
CH ₃ -	C-(H) ₃ (C)	1
C-CH ₂ -C	C-(H) ₂ (C) ₂	3
C-CH ₂ -O	C-(H) ₂ (C)(O)	1
C-O-H	O-(H)(C)	1

- (2) Group additivity representation for 1-pentanol:

$$(1 \times \text{C-(H)}_3\text{(C)}) + (3 \times \text{C-(H)}_2\text{(C)}_2) + (1 \times \text{C-(H)}_2\text{(C)(O)}) + (1 \times \text{O-(H)(C)})$$

- (3) Equations (1) and (2) are used to perform the calculation.

$C/R = \sum n_i \Delta c_i$, and $\Delta c_i = a_i + b_i(T/100) + d_i(T/100)^2$, respectively, where $R = 8.31451 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ and T is in kelvin.

- (4) Selection of groups and adjustable parameters.

Adjustable parameters for C-(H)₃(C) and C-(H)₂(C)₂ are obtained from Table 5 in (93RUZ/DOM1). Those for C-(H)₂(C)(O) and O-(H)(C) are obtained from Table 8 in this paper.

Group	a_i	b_i	d_i	Temp. range, K
C-(H) ₃ (C)	3.8452	-3.3997E-1	1.9489E-1	80-490
C-(H) ₂ (C) ₂	2.7972	-5.4967E-2	1.0679E-1	80-490
C-(H) ₂ (C)(O)	1.4596	1.4657	-2.7140E-1	135-505
O-(H)(C)	1.2952E+1	-1.0145E+1	2.6261	195-475

- (5) Calculation of the estimated value and comparison with the recommended value.

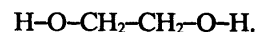
$$C/R = 29.663 \text{ and } C = 246.6 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$$

This result may be compared with the recommended value for the heat capacity of liquid 1-pentanol at 350 K given in 90ZAB/RUZ equal to 255.45 J·mol⁻¹·K⁻¹. The estimated value differs by 8.85 J·mol⁻¹·K⁻¹ or by 3.5 %.

Sample calculation for the estimation of the heat capacity of 1,2-ethanediol (ethylene glycol) at 400 K

- (1) Kind and number of additive groups.

The structural formula for 1,2-ethanediol is :



The following groups are needed for the calculation of adjustable parameters necessary to estimate the heat capacity of 1,2-ethanediol in the liquid phase at an arbitrary temperature in the range from the melting to the boiling temperature; let us choose 400 K.

Molecular fragment	Group	No. of groups
C-CH ₂ -O	C-(H) ₂ (C)(O)	2
C-O-H	O-(H)(C)(diol)	2

- (2) Group additivity representation for 1,2-ethanediol:

$$(2 \times \text{C-(H)}_2\text{(C)(O)}) + (2 \times \text{O-(H)(C)(diol)})$$

- (3) Equations (1) and (2) are used to perform the calculation.

- (4) Selection of groups and adjustable parameters.

Adjustable parameters for C-(H)₂(C)(O) and O-(H)(C)(diol) are obtained from Table 8 in this paper.

Group	a_i	b_i	d_i	Temp. range, K
C-(H) ₂ (C)(O)	1.4596	1.4657	-2.7140E-1	135-505
O-(H)(C)(diol)	5.2302	-1.5124	5.4075E-1	195-475

- (5) Calculation of the estimated value and comparison to the recommended value.

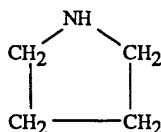
$$C/R = 21.625 \text{ and } C = 179.8 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$$

This result may be compared with the recommended value for the heat capacity of liquid 1,2-ethanediol at 400 K in 93ZAB/RUZ equal to 180.5 J·mol⁻¹·K⁻¹. The estimated value differs by 0.7 J·mol⁻¹·K⁻¹ or 0.4 %.

Sample calculation for the estimation of the heat capacity of pyrrolidine at 250 K

(1) Kind and number of additive groups

The structural formula for pyrrolidine is:



The following groups are needed for the calculation of adjustable parameters necessary to estimate the heat capacity of pyrrolidine in the liquid phase at an arbitrary temperature; let us choose 250 K.

Molecular Group	No. of fragment groups
C-CH ₂ -CC-(H) ₂ (C) ₂	2
C-CH ₂ -NC-(H) ₂ (C)(N)	2
C-NH-CN-(H)(C) ₂	1
ring strain correction (rsc)	1

(2) Group additivity representation for pyrrolidine:

$$(2 \times \text{C}-(\text{H})_2(\text{C})_2) + (2 \times \text{C}-(\text{H})_2(\text{C})(\text{N})) + (1 \times \text{N}-(\text{H})(\text{C})_2) + (1 \times \text{pyrrolidine rsc})$$

(3) Equations (1) and (2) are used to perform the calculation.

(4) Selection of groups and adjustable parameters.

Adjustable parameters for C-(H)₂(C)₂ are obtained from Table 5 in (93RUZ/DOM1). Those for C-(H)₂(C)(N) and N-(H)(C)₂ are found in Table 8. Adjustable parameters for the ring strain correction in pyrrolidine is given in Table 9.

Group	a_i	b_i	d_i	Temp. range, K
C-(H) ₂ (C) ₂	2.7972	-5.4967E-2	1.0679E-1	80-490
C-(H) ₂ (C)(N)	2.4555	1.0431	-2.4054E-1	190-375
N-(H)(C) ₂	-1.0987E+1	7.3024E-1	8.9325E-1	170-400
pyrrolidine rsc	-1.2703E+1	1.3109	1.1813	170-400

(5) Calculation of the estimated value and comparison with the recommended value.

$$C/R = 18.792 \text{ and } C = 156.3 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$$

This result may be compared with the recommended value for the heat capacity of liquid pyrrolidine at 250 K given in 93ZAB/RUZ equal to 154.5 J·mol⁻¹·K⁻¹. The estimate value differs by 1.8 J·mol⁻¹·K⁻¹ or by 1.2 %.