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Estimation of the Thermodynamic Properties of C–H–N–O–S–Halogen Compounds at 298.15 K

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An estimation method, which was developed by S.W. Benson and coworkers for calculating the thermodynamic properties of organic compounds in the gas phase, has been extended to the liquid and solid phases for organic compounds at 298.15 K and 101,325 Pa. As with a previous paper dealing with hydrocarbon compounds, comparisons of estimated enthalpies of formation, heat capacities, and entropies with literature values show that extension of the Benson's group additivity approach to the condensed phase is easy to apply and gives satisfactory agreement. Corresponding values for the entropy of formation, Gibbs energy of formation and natural logarithm of the equilibrium constant for the formation reaction are also calculated provided necessary auxiliary data are available. This work covers 1512 compounds containing the elements: carbon, hydrogen, oxygen, nitrogen, sulfur, and halogens in the gas, liquid, and solid phases. About 1000 references are provided for the literature values which are cited.

Keywords: enthalpy of formation; entropy; estimation; heat capacity; organic compounds; thermodynamic properties.

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1. Introduction

The purpose of this paper is to demonstrate that the estimation of thermodynamic properties of organic compounds in the condensed phase at 298.15 K and 101,325 Pa can be carried out in a satisfactory manner using established second-order group-additivity methods. The second-order group-additivity method, originally introduced by S.W. Benson and coworkers (58BEN/BUS, 68BEN, 69BEN/CRU, 69SHA, 71SHA, 73EIG/GOL, 76BEN, 77LUR/BEN, 77SHA/GOL, 77STE/GOL) for estimating the thermodynamic properties of organic compounds, was developed and used primarily for the gas phase. This work includes a re-examination of the capabilities for estimation of the thermodynamic properties of the gas phase to maintain continuity with the condensed phase and also to introduce changes in group values necessitated by more recent thermodynamic data available in the literature.

The coverage of organic compounds includes those substances containing the elements: carbon, C; hydrogen, H; oxygen, O; nitrogen, N; sulfur, S; fluorine, F; chlorine Cl; bromine, Br; and iodine, I. The particular thermodynamic properties for which groups and group values have been determined are: enthalpy of formation, $\Delta_f H°$; heat capacity, $C_p°$; and entropy, $S°$. The entropy of formation ($\Delta_f S°$), Gibbs energy of formation ($\Delta_f G°$), and the natural logarithm of the equilibrium constant ($\ln K_f$) for the formation reaction, are calculated as auxiliary properties.

The second-order group-additivity approach has been generally accepted by physical chemists and chemical engineers because of the simple basis of additivity, clarity of notation, second-order character, i.e., inclusion of nearest-neighbor interactions, ease of application, and satisfactory agreement between the thermodynamic value reported in the literature and its estimated value. The ASTM Chemical Thermodynamic and Energy Release Program, CHETAH, (74SEA/FRE)) uses these methods for the estimation of the thermodynamic properties of organic compounds in the gas phase and for the classification of chemicals or compositions depending upon whether they are likely to be impact sensitive. The AIChE Design Institute for Physical Property Data (DIPPR) Manual for Predicting Chemical Process Design Data (83DAN/DAU) recommends the second-order group-additivity method (76BEN) for the estimation of enthalpy of formation, heat capacity, and entropy of organic compounds at 298.15 K in the gas phase. DIPPR Project 871 is an experimental project begun to determine accurate enthalpies of formation and vaporization of key organic compounds so that reliable gas phase enthalpies of formation can be calculated at 298.15 K. The latter data would then permit either the calculation of new second-order group-additivity values or the replacement of group values which are based on poor quality data. The improved or new group values would be used to upgrade both the DIPPR Data Prediction Manual and the ASTM CHETAH Program.

With such broad needs for thermodynamic property estimation in ASTM and AIChE, we felt that the successful application of this approach for the gas phase merited an intensive examination of its application into the condensed phase. The approach taken for the evaluation of thermodynamic data and the path of development of groups and group values for hydrocarbon compounds came from our previous paper (88DOM/HEA) in which a systematic procedure was followed for the selection of group values which gave minimum residuals between the literature and calculated values. The *n*-alkanes from C_2 to C_{18} make up one of the most studied families of compounds and have some of the most pristine values for $\Delta_f H°$, $C_p°$, and $S°$ of all the families of organic compounds. They form the basis for the development of the C–(H)$_3$(C) and C–(H)$_2$(C)$_2$ group values. From this point, the group and group value development proceeds to branched alkanes, alkenes, alkynes, aromatic and alicyclic compounds, CHO compounds (alcohols, ethers, etc.), CHN compounds (amines, nitriles, etc.), and on to CHNO, CHS, CHSO, and organic halogen compounds. Care is needed in the development of group values because experimental or recommended data have different degrees of quality and are not homogeneous. Reduction of data to as common a basis as possible is required. For combustion data, some previously established guidelines were used (71DOM). A global least squares, least sums, or regression-type fit of all the group values was not performed because of the differences in the quality of the data, and because of the limited amount of data available for the generation of certain groups and group values. The generation of groups and the calculation of group values was in part manual and in part computer-assisted. Some computations for average values, average deviations, or standard deviation were performed using a desk-top calculator. Others were made using computer spread-sheet analysis.

The group values generated for the hydrocarbons were held fixed for the generation of non-hydrocarbon values. Most of the group values for non-hydrocarbon compounds were generated using the THERM/EST Program (NIST Standard Reference Database 18) (90DOM/HEA2) by having the group value being sought initially become part of the residual value. In this procedure, an unknown group value is calculated, then a value is assigned to the unknown group, and a final or true residual value is calculated which excludes the new group value, but minimizes the final residual value. When a large number of experimental values were available to calculate a group value, as with *n*-alkanes, *n*-alkanols or *n*-alkanethiols, final adjustments were examined with computer spread-sheet software. Care was taken to accommodate the adjusted group values when the same groups were needed for different families of compounds. For example, the C–(H)$_2$(C)(O) group and its group values are required for alcohols, ethers, esters, and peroxides. Group values for some families or compounds were generated simply by calculating simple arithmetic averages because the experimental data were limited to 2 or 3 values. The group C–(H)$_3$(C) is used freely in the molecular structure representation of compounds because the value of the methyl group does not change except for the physical phase no matter to what it is attached. Hence, C–(H)$_3$(C) = C–(H)$_3$(O) = C–(H)$_3$(N) = C–(H)$_3$(S), etc., and consequently, methanol can be represented by: C–(H)$_3$(C) + O–(H)(C) rather than: C–(H)$_3$(O) + O–(H)(C). Appendix 1 lists unique groups derived from data on individual compounds as their source.

The compounds for which estimated properties have been calculated are divided into various organic families as shown in Table 1. The number of compounds within each family is indicated. A total of 1512 compounds have had thermodynamic properties estimated and compared with a literature value. This total is not exhaustive, but does represent a sufficiently broad array of organic structures to demonstrate the applicability of the group additivity method to the condensed phase. Compounds are listed according to the increasing number of carbon atoms within each family, but sometimes the carbon number reverts back to lower values because of the inclusion of certain compounds with secondary or tertiary substitution, unsaturation, multiple functional groups, aromatic substitution, or cyclic structures. Table 2 provides a listing of over 600 groups and energy corrections, and their corresponding values for $\Delta_f H°$, $C_p°$, and $S°$ for the gas, liquid, and solid phases. Table 3 offers some guidance to the definition and interpretation of organic groups for persons not accustomed to the notation in Table 2.

Thermodynamic properties for 1512 compounds are shown in Tables 4 through 54 and contain the following information: the title of the organic family, the number of compounds included in that family, individual compound name(s), formula of the compound, the organic groups which comprise the structure of the compound, symmetry number, σ, and optical isomers, η. Thereafter, each phase is treated separately, gas, liquid, and solid. Property symbols $\Delta_f H°$ (in kJ/mol), $C_p°$ (in J/mol·K), and $S°$ (in J/mol·K) appear in the extreme left column. Next, the experimental or recommended values are also given, when available, and entered under the column, "Literature". The property value derived from summing the group values is given under the column, "Calculated", so that a difference or residual value may be calculated and shown under the column, "Residual". The residual offers an indication of how close the estimated value comes to the one determined experimentally or to the one derived from an evaluation of a collection of literature data. If the appropriate group values are available so that the enthalpy of formation and entropy can be estimated, we also provide the entropy of formation, $\Delta_f S^\circ$ (in J/mol·K), Gibbs energy of formation, $\Delta_f G^\circ$ (in kJ·mol^{-1}), and the logarithm of the equilibrium constant for the formation process, $\ln K_f$. In order to calculate the entropies of formation at 298.15 K and 101,325 Pa, the entropies of the elements in their standard states are needed as well as the entropies of the respective compounds. The entropies of the elements at 298.15 K and at 101,325 Pa have been obtained from (89COX/WAG) and are as follows in J/mol·K: carbon (cr,graphite), 5.740; H_2 (gas), 130.571; O_2 (gas), 205.043; N_2 (gas), 191.500; S (cr, rhombic), 32.054; F_2 (gas), 202.682; Cl_2 (gas), 222.972; Br_2 (liquid), 152.21; I_2 (cr), 116.14. Estimation of the entropy in the gas phase requires a $-R\ln\sigma$ term where σ is the total symmetry number of the molecule and R is the universal gas constant (R = 8.31451 J/mol·K). The total symmetry number of the molecule is divided into two parts: the internal symmetry number and the external symmetry number. The definitions of the latter symmetry numbers and several example calculations of symmetry numbers can be found in (88DOM/HEA). Estimation of the gas phase entropy also requires accounting for optical isomers as the molecular structure dictates with a $R\ln\eta$ term, where η indicates the number of such isomers. Since this work deals with data at only one temperature, 298.15 K, no distinction is made between the heat capacity at constant pressure, C_p°, and the saturation heat capacity, C_{sat}.

Reference squibs appear in the extreme right column of the tables under the heading "References"; The squibs are of the type XXAAA/BBBN for each property in each of the phases and correspond to entries under the column "Literature". In this squib notation, XX denotes the last two digits of the year of publication of the paper, AAA, the first three letters of the last name of the first author, and BBB, those of the last name of the second author (if present). Authors after the first two are not noted. The numeral, N, at the end of the squib is present only when the authors have more than one paper published in a given year. Table 55 provides a summary of the residuals for each family which offers some global insight into the agreement realized between literature and calculated values. The residuals have been divided into those for $\Delta_f H^\circ$ which were $< \pm 4$, $> \pm 4$ but $< \pm 8$, and $> \pm 8$ kJ·mol^{-1}. Similarly, for C_p° and S°, the residuals have been divided into those which were $< \pm 4$, $> \pm 4$ but $< \pm 8$, and $> \pm 8$ J/mol·K. Table 56 shows an alphabetical compound name-formula index which provides the CAS registry number, family in which the compounds may be found, its listing or rank within the given family, and the page on which data for the compound appears. A bibliography given in Table 57 with about 1000 references links reference squibs in Tables 4 through 54 to literature citations.

We have examined the original reference sources for data on the enthalpies of formation, heat capacities, and entropies for almost all of the compounds. The thermodynamic tables compiled by Stull, Westrum, and Sinke (69STU/WES, 69STU/WES2) have been used for many of the literature gas phase heat capacities and entropies. We have also used some general thermodynamic reference sources to find original sources in certain cases (70COX/PIL, 71ZWO/WIL, 72DOM, 77PED/RYL, 84DOM/EVA, 85MAJ/SVO, 86TRC, 86TRC2, 86PED/NAY, 90DOM/HEA). Over 3700 comparisons between literature and calculated values are shown for $\Delta_f H^\circ$, C_p°, and S° in the gas, liquid, and solid phases. Approximately half of the comparisons are for the condensed phase.

Interpretation is occasionally required when a reference squib is designated for a specific property. For example, a reference squib denoted for $\Delta_f H^\circ$ in the gas phase may not actually provide that specific property, but will report an enthalpy of vaporization at 298.15 K which when added to $\Delta_f H^\circ$ in the liquid phase, will then be equal to the designated experimental or recommended $\Delta_f H^\circ$(gas) value. Similarly, a reference squib denoted for $\Delta_f H^\circ$(solid) may not contain the actual $\Delta_f H^\circ$ property for the solid phase, but does report the ΔH° for the fusion or melting of the compound. When the latter is corrected from the melting temperature to 298.15 K and combined with $\Delta_f H^\circ$(liq) at 298.15 K, one obtains the $\Delta_f H^\circ$(solid) value. Despite concerns related to the estimation of thermodynamic properties for solid substances, we typically find good agreement between literature and calculated values. Common doubts about the ability to develop a predictive scheme for solid substances arise because some organic compounds have many crystalline forms in the proximity of the melting point. The second-order group-additivity approach does have its limits. We expect that the predicted solid phase at 298.15 K is the same as the stable form encountered experimentally at 298.15 K. For organic compounds with multiple crystalline phases and solid-solid transitions, as found with the C_{13}, C_{14}, and C_{15} 1-alkanols, the group additivity approach provides only a limited value for the thermodynamic property. We do not feel that this limitation diminishes the overall usefulness of prediction of this method for solid organic substances. Appendix 2 shows that internal consistency does exist when comparisons are made between literature values for enthalpies and entropies of fusion and enthalpies of vaporization and the estimated differences for [$\Delta_f H^\circ$(solid) $-$ $\Delta_f H^\circ$(liq)], [S°(solid) $-$ S°(liq)], and [$\Delta_f H^\circ$(liq) $-$ $\Delta_f H^\circ$(g)], at 298.15 K. Differences between literature values for enthalpies and entropies of fusion corrected from the melting temperature to 298.15 K and [$\Delta_f H^\circ$(solid) $-$ $\Delta_f H^\circ$(liq)] and [S°(solid) $-S^\circ$(liq)] yield average deviations of ± 2.7 kJ.mol^{-1} and ± 4.7 J/mol·K, respectively. A similar comparison between literature values for the enthalpy of vaporization corrected to 298.15 K and [$\Delta_f H°$(liq) − $\Delta_f H°$(g)] gives an average deviation of ±1.6 kJ·mol^{-1}.

The quality of the groups and group values can be evaluated by examining the magnitude of the difference (or residual) which is observed between the literature and calculated values for a specific property in a given physical phase. For $\Delta_f H°$, differences within ±4 kJ/mol constitutes very good or satisfactory agreement, those which are between ±4 and ±8 kJ/mol are at the limits of acceptability, and differences which are greater than ±8 kJ/mol are symptomatic of a problem. The occurrence of differences larger than ±8 kJ/mol are usually due to poor quality literature data or to a neglected molecular interaction, both of which can lead to the incorrect assignment for a group value. A similar situation applies to heat capacity and entropy differences. When differences within ±4 J/mol·K occur, the agreement is considered very good, when they are between ±4 and ±8 J/mol·K, the agreement is acceptable, and when the differences are greater than ±8 J/mol·K, they reflect a problem, which similarly can be related to poor quality data or to a neglected molecular interaction, and can lead to the selection of an incorrect group value.

Certain molecules such as methane, methanal, acetonitrile, nitromethane, and the methyl halides are precluded from the rules of group additivity because they are structurally comprised of only one group and, hence, their group value is equivalent to the corresponding property value in each of the phases. We have included a number of such substances at the beginning of some of the organic families for comparison purposes. When needed for various calculations, the 1989 table of atomic weights was used (91DEL/HEU).

2. Discussion of Results

2.1. Hydrocarbon Compounds

The hydrocarbon compounds and thermodynamic properties appearing in 88DOM/HEA are also presented here as well as the calculation of the entropy of formation, Gibbs energy of formation, and equilibrium constant for the formation reaction. A total of 48 hydrocarbon compounds has been added which have created more groups and group values. A small number of groups and group values appearing in 88DOM/HEA have also been modified. Hydrocarbons comprise the most studied single famly of organic compounds from a thermodynamic standpoint and form the foundation for the development of groups and group values not only within hydrocarbons themselves but also for non-hydrocarbon compounds. Thermodynamic property comparisons between hydrocarbons and non-hydrocarbons permit one to test whether additivity is being preserved, whether molecular forces are interacting, or whether the literature values may be suspect.

The hydrocarbon compounds examined have been divided into eleven families: *n*-alkanes, *t*-alkanes, *q*-alkanes, *n*-alkenes, *s*-alkenes, alkynes, aromatic CH–01, aromatic CH–02, cyclic CH–01, cyclic CH–02, and cyclic CH–03. These families contain thermodynamic property estimates for a total of 427 hydrocarbon compounds and are found in Tables 4 through 14. An examination of the 532 comparisons between literature and calculated values for $\Delta_f H°$ shows that 70 percent of the residuals are <±4 kJ/mol, 17 percent are >±4 but <±8 kJ/mol, and 13 percent are >±8 kJ/mol. For C_p° with 361 comparisons, we find 85 percent of the residuals <±4 J/mol·K, 8 percent >±4 but <±8 J/mol·K, and 7 percent >±8 J/mol·K. Similarly, for $S°$ with 338 comparisons, we find 76 percent of the residuals <±4 J/mol·K, 16 percent >±4 but <±8 J/mol·K, and 8 percent >±8 J/mol·K.

A novel approach for dealing with branched alkanes has been described in (88DOM/HEA) for tertiary and quaternary carbon atoms in hydrocarbon compounds. It corrects for the repulsive interactions of hydrogen atoms on methyl groups attached to tertiary or quaternary carbon atoms and improves the agreement between literature and estimated values. The corrections for methyl repulsion in branched hydrocarbons have been developed only for $\Delta_f H°$ at 298.15 K. It accommodates the observation that as branching increases for an isomeric hydrocarbon, the $\Delta_f H°$value becomes more negative (e.g., $\Delta_f H°$'s for isomeric pentanes). A summary of this approach can be found in (88DOM/HEA).

Except for *n*-hexacosane, residuals calculated from literature and calculated values for C_p° and $S°$ for *n*-alkanes with carbon atoms C_{20} and higher are large, but do not come from recent calorimetric investigations. We suggest that some re-determination and confirmation is needed for the C_p° and $S°$ values for these hydrocarbon compounds.

2.2. Organic Oxygen Compounds

After hydrocarbon compounds, organic oxygen compounds are the next most abundant category of organic substances for which thermodynamic data are available. The CHO compounds have been divided into 11 families: alcohols, ethers, aldehydes, ketones, acids, anhydrides, esters, peroxides, hydroperoxides, peroxyacids, and carbonates, and are found in Tables 15 through 25. These tables contain thermodynamic property estimates for 381 CHO compounds. An examination of 570 comparisons of literature and calculated values for $\Delta_f H°$ shows that 62 percent have residuals which are <±4 kJ/mol, 18 percent are >±4 but <±8 kJ/mol, and 20 percent are >±8 kJ/mol. Residuals for C_p° show that 72 percent are <±4 J/mol·K, 15 percent are between >±4 and <±8 J/mol·K, and 13 percent are >±8 J/mol·K. For $S°$, 72 percent of the residuals are <±4 J/mol·K, 16 percent are >±4 but <±8 J/mol·K, 12 percent are >±8 J/mol·K.

Comparison of literature and calculated values for $\Delta H°$, C_p°, and $S°$ shows that for primary alcohols the agreement is reasonably good. However, initial agreement between literature and estimated values for secondary and tertiary alcohols was not as good as with primary alcohols. We found that significantly smaller residuals resulted for secondary and tertiary alcohols if a methyl repulsion correction was applied for tertiary or quaternary carbon atom attached to an oxygen atom.

Agreement between literature and calculated values for secondary aliphatic alcohols, diols, triols, and tetrols for $\Delta_f H°$, $C_p°$, and $S°$ are somewhat inconsistent. Large residuals occasionally appear but do not seem to show a consistent trend. The residuals for some phenolic compounds can be improved with the application of an *ortho* correction for OH–OH interactions. Some of the literature data are not recent and may be suspect.

We found that better agreement between literature and calculated values was obtained if separate C–(H)(C)2(O) and C–(C)3(O) groups were assigned to alcohols and peroxides, and another for ethers and esters, rather than having global groups for all of the organic oxygen families. Hence, this separation is indicated in the list of groups and group values in Table 2 and under each compound in Tables 4 through 54 in the structural group notation.

Literature and calculated values for $\Delta_f H°$, $C_p°$, and $S°$ for ethers and ketones show generally good agreement. This is possible because of a significant quantity of good quality data in the gas and condensed phases.

For aldehydes, agreement between literature and calculated values for $\Delta_f H°$,$C_p°$, and $S°$ in the gas phase are generally satisfactory. Although satisfactory agreement is found for $\Delta_f H°$(liq), agreement for $C_p°$ and $S°$ in the liquid phase is poor. The $C_p°$ and $S°$ data of 56PAR/KEN at 298.15 K for butanal and heptanal in the liquid phase reflect the expected linear relationship when n-alkanals increase by a CH_2 group. The recent data reported for ethanal by 88LEB/VAS, propanal by 77KOR/VAS, butanal by 89VAS/LEB, hexanal by 91VAS/BYK, and heptanal by 83DYA, 84VAS/PET indicate that the relationship for 1-alkanals in the liquid phase is neither linear nor smooth. These authors describe anomalies in the liquid phase which they have found to be due to association in 1-alkanals through hydrogen bonds. The group values we have chosen are based on linearity, hence, significant deviation are reflected in the large residuals which occur.

We have found some large differences between the literature and calculated values for $\Delta_f H°$ and $C_p°$ for dibasic acids in the gas and solid phases. It is not clear whether these residuals are due to hydrogen bonding in dibasic acids, odd-even carbon atom effects, the need for a group correction factor, poor experimental data, or most of the above. A significant amount of these data were reported in the 1920's. It may be possible that the odd-even relationship which is observed for the melting temperatures of dicarboxylic acids is similarly reflected in their thermodynamic properties. A large fraction of the residuals in $\Delta_f H°$'s for the dibasic acids are $> \pm 8$ kJ/mol.

The experimental $\Delta_f H°$ values for 1-naphthoic and 2-naphthoic acid differ from each other by 9.4 kJ/mol in the gas phase and 12.4 kJ/mol in the solid phase. Examination of the structures of these acids by 74COL/ROU indicates that 2-naphthoic acid is planar, but 1-naphthoic acid is twisted 11° out of the naphthalene plane due to overcrowding, hence, these structural differences account for the observed energy differences.

Corrections have been developed for *ortho* and *meta* interactions between two or more carboxylic acid groups in aromatic acids. Similar corrections were developed for interactions between methoxy and carboxylic acid groups. In some instances, a clear interaction correction was not developed because the nature of the interaction between adjacent or near-adjacent groups could not be interpreted clearly, and/or the quality of the experimental data did not allow an interpretation. In these cases, we applied the *ortho* and *meta* corrections developed for hydrocarbon compounds.

Difficulty in resolving the agreement between literature and calculated $\Delta_f H°$ values for benzoic anhydride with aliphatic anhydrides led to the development of separate groups for O–(CO)2 and corresponding attachments to aliphatic and aromatic substituents. They are listed in Table 2 as: O–(CO)2, *aliphatic* and O–(CO)2, *aromatic.*

Thermodynamic property data on peroxides, hydroperoxides, and peroxyacids are limited to enthalpies of formation. From time to time, agreement between $\Delta_f H°$ experimental and calculated values is poor. This situation is due to a lack of high quality data on these substances and is understandable because of their explosive and thermally sensitive character. The preparation of sufficient amounts of high purity samples of thermally sensitive substances places a very high demand upon any research effort.

The unusually large difference between the literature and calculated $\Delta_f H°$ for diacetyl peroxide (DAP) in the liquid phase (see Table 21, 38.66 kJ/mol) may be due to the instability of the compound. Because of its instability, bomb calorimetric experiments on diacetyl peroxide were performed on a toluene solution (37.53 wt% DAP, 62.47wt% toluene; 57JAF/PRO). Bomb calorimetric experiments were made at only one concentration of DAP in toluene, hence, dilution errors or analytical errors cannot be easily detected. Examination of the experimental and calculated values for dipropionyl and dibutyryl peroxides shows their residuals to be satisfactory.

The differences found between the literature and estimated values for peroxy acids are large. The groups developed for the family appears to be the best that can be assembled. If some re-determinations of the thermodynamic properties for peroxy acids can be made, smaller residuals may result.

2.3. Organic Nitrogen Compounds

Literature and estimated thermodynamic properties on organic nitrogen compounds have been divided in seven CHN families and nine CHNO familes. The families which comprise the CHN compounds are: amine, imines, nitriles, hydrazines, diazenes, azides, and cyclic CHN compounds and are found in Tables 26 through 32. A total of 137 CHN compounds are shown. Agreement between experimental and calculated values shows 84 percent of the residuals for $\Delta_f H^\circ$ to be $< \pm 4$ kJ/mol, 10 percent of the residuals for $\Delta_f H^\circ$ to be $< \pm 4$ kJ/mol, 10 percent are $> \pm 4$ but $< \pm 8$ kJ/mol, and 6 percent are $> \pm 8$ kJ/mol. For C_p°, 85 percent of the residuals are $< \pm 4$ J/mol·K, 7 percent are $> \pm 4$ but $< \pm 8$ J/mol·K, and 8 percent are $> \pm 8$ J/mol·K. With respect to S°, 77 percent of the residuals are $< \pm 4$ J/mol·K, 15 percent are $> \pm 4$ and $< \pm 8$ J/mol·K, and 4 percent are $> \pm 8$ J/mol·K.

The families which comprise the CHNO compounds are: amides, ureas, amino acids, nitroso, nitro, nitrites, nitrates, nitramines, and cyclic CHNO compounds. A total of 171 CHNO compounds are shown in Tables 33 through 41. Comparison of literature and calculated values show that for $\Delta_f H^\circ$ residuals, 68 percent are $< \pm 4$ kJ/mol, 11 percent are $> \pm 4$ but $< \pm 8$ kJ/mol, and 21 percent are $> \pm 8$ percent. For C_p°, 80 percent of the residuals are $< \pm 4$ J/mol·K, 6 percent are $< \pm 4$ but $> \pm 8$ J/mol·K, and 14 percent are $> \pm 8$ J/mol·K. For S°, 69 percent are $< \pm 4$ J/mol·K, 10 percent are $< \pm 4$ but $> \pm 8$ J/mol·K, and 21 percent are $> \pm 8$ J/mol·K.

From an initial examination of the differences between the literature and calculated values, the CHN family appears to be amenable to prediction. We have applied the $-CH_3$ quaternary correction for alkane branching to nitrogen atoms in tertiary amines, *N,N*-dimethylsubstituted amides, and *N,N*-dimethylsubstituted ureas because better agreement resulted between experimental and estimated values. A corresponding application of the $-CH_3$ tertiary correction to nitrogen atoms in secondary amines, *N*-methylsubstituted amides, or *N*-methyl substituted ureas was not used because it did not lead to significantly smaller differences between experimental and estimated values.

Comparison of the experimental $\Delta_f H^\circ$ for the solid phase of acetamide with the estimated value shows a difference of -10.41 kJ/mol. This difference is larger than one would like. However, anomalous behavior has been reported for crystalline acetamide due to its tendency to supercool (86EMO/NAU). Acetamide forms an unstable solid phase along with a stable form. The stable and unstable forms have melting temperatures of 353.5 K and 342.15 K, and enthalpies of melting of 15.6 and $12.5 - 12.9$ kJ/mol, respectively.

The estimation of the thermodynamic properties of amino acids and peptides in the solid phase is a particularly challenging task. Some amino acids have been the subject of a significant amount of calorimetric study; glycine and hippuric acid are examples. Other amino acids as well as peptides have received only limited calorimetric attention. There is a mixture of high quality, medium quality, and limited quality data on these compounds. Other challenges included accounting for the dipolar nature of amino acids, and identifying differences when possible between (DL) racemic and optically active (R or D, and S or L) isomers. Because the enthalpy of combustion and formation of glycine has been so frequently determined, we have used the experimental values for this amino acid and the corresponding data on glycylglycine as the basis for deriving the C–(H)2(CO)(N) group and group value and the energy correction for the dipolar nature or zwitterion character of aliphatic amino acids. Since the zwitterion nature of amino acids and peptides is a unique property and not prominent in the other organic nitrogen compounds treated in this paper, a separate identification and energy correction was warranted. The establishment of the zwitterion energy correction also allows the C–(H)2(CO)(N) group to have property values not seriously divergent from those groups such as C–(H)2(C)2, C–(H)2(C)(CO), and C–(H)2(C)(N). The zwitterion energy correction for solid aliphatic amino acids and peptides for $\Delta_f H^\circ$, C_p°, and S° are -55.10 kJ/mol, -44.50 J/mol·K, and -13.40 J/mol·K, respectively. Using similar reasoning, a zwitterion energy correction was developed for amino acids and peptides containing an aromatic ring, but required differentiation between situations in which a $-CH_2-$ group breaks the conjugative nature of the aromatic ring from its linkage to the α-carbon of an amino acid or peptide. For these cases, the zwitterion energy is designated as "aromatic I" and was derived from $\Delta_f H^\circ$(solid) data for phenylalanine and phenylalanine peptides; the zwitterion energy correction (for aromatic I) for $\Delta_f H^\circ$, C_p°, and S° are -32.00 kJ/mol, -20.50 J/mol·K, and -13.00 J/mol·K, respectively. For situations in which the aromatic ring of an amino acid or peptide is bonded directly to amino groups or to carboxylic acid groups where the influence to ring conjugation should be stronger than it is for phenylalanine derivatives, a second aromatic zwitterion energy correction was derived to accommodate the estimation of the aminobenzoic acids, hippuric acid, and hippurylglycine, and designated as "aromatic II"; the zwitterion energy correction (for aromatic II) for $\Delta_f H^\circ$, C_p°, S° are -11.00 kJ/mol, 5.00 J/mol·K, and -9.00 J/mol·K, respectively. These group values are also found in Table 2. Agreement between literature and estimated values is variable. Future reconciliation of the large residuals may result from more precise calorimetric determinations of certain amino acids and peptides as well as some re-adjustment of group values. Better agreement was obtained between literature and estimated values when N–(H)2(CO) and N–(H)(C)(CO) groups were developed separately for amides and ureas in comparison to amino acids and peptides. At this time, it is not clear whether the better agreement is a function of differences in the molecular structure of these organic families or whether more accurate experimental data will offer new changes to their estimation.

The residual value for $\Delta_f H^\circ$ (solid) for nitrosobenzene is large, -85.65 kJ/mol. The group, CB–(NO), and corresponding $\Delta_f H^\circ$ group values, were derived from experimental data on 4-nitroso-1-naphthol. The $\Delta_f H^\circ$ experimental data for 4-nitroso-1-naphthol (68HAM/FAG) are more reliable than those for nitrosobenzene (30DRU/FLA). The large residual for nitrosobenzene is probably due to either sample purity or to difficulties with experimental bomb calorimetric procedures, or both.

As the development of the second-order group additivity approach to the estimation of thermodynamic properties (57BEN/BUS, 69BEN/CRU) began, the enthalpy of formation of the benzene (C_6H_6) molecule was divided by six to derive the group value for $\Delta_fH°$ C_B–(H)(C_B)$_2$ group in the gas phase. In this division, the resonance or conjugation energy of benzene (~150 kJ·mol^{-1}) had also undergone a corresponding division. We have attempted to extend this concept to pyridine and have introduced the N_I–(C_B) group which not only includes the energy content for a property, but also the corresponding component of the conjugation energy which resides in the pyridine molecule. Reasonable success was achieved for pyridine and substituted pyridines in Table 32. The further extension of this concept to five-membered ring systems becomes a more difficult task when they possess an intrinsic and sizeable conjugation energy, but in addition, contain a significant amount of strain energy. This situation is true for five-membered systems such as furan, pyrrole, and thiophene. We have treated the carbon atoms in these five-membered ring systems as benzene carbon atoms, using the C_B–(H)(C_B)$_2$ group, because their conjugation energies are in the range from 65 to 120 kJ·mol^{-1}. As a result of this treatment, the $\Delta_fH°$ ring strain corrections (rsc) for furan, pyrrole, and thiophene appear as negative values. In contrast, the conjugation energy in 1,3-cyclopentadiene is small when compared with its ring strain energy and its structural description has been assembled using C_d–(H)(C_d) and C_d–(H)(C) groups rather the C_B–(H)(C_B)$_2$ group.

2.4. Organic Sulfur Compounds

The families which comprise the CHS and CHSO compounds are: thiols, sulfides, disulfides, sulfoxides, sulfones, sulfites, sulfates, and cyclic CHS compounds. A total of 138 CHS and CHSO compounds are shown in Tables 42 through 49. Agreement between literature and calculated values shows 80 percent of the residuals for $\Delta_fH°$ to be $< \pm 4$ kJ·mol^{-1}, 14 percent of the residuals to be $> \pm 4$ but $< \pm 8$ kJ·mol^{-1}, and 6 percent to be $> \pm 8$ kJ·mol^{-1}. For $C_p°$, 92 percent of the residuals are $< \pm 4$ J·mol^{-1}·K^{-1}, 7 percent are $> \pm 4$ but $< \pm 8$ J·mol^{-1}·K^{-1}, and 1 percent are $> \pm 8$ J·mol^{-1}·K^{-1}. For $S°$, 87 percent of the residuals are $< \pm 4$ J·mol^{-1}·K^{-1}, 7 percent are $> \pm 4$ but $< \pm 8$ J·mol^{-1}·K^{-1}, and 6 percent are $> \pm 8$ J·mol^{-1}·K^{-1}.

Excluding hydrocarbon compounds, organic sulfur compounds containing the elements C, H, and S stand out as offering an extremely high quality array of experimental thermodynamic values for $\Delta_fH°$, $C_p°$, and $S°$. The establishment of this high quality array of data on CHS compounds is due to the need of the petroleum industry to understand the thermochemistry of organic sulfur compounds because of their presence in petroleum and because of the need to understand their energetics and equilibrium properties in petroleum refining. Much of the effort to establish high quality thermodynamic data for this class of organic compounds resulted from an experimental effort which took place at the U.S. Bureau of Mines Thermodynamics Laboratory in Bartlesville, OK (now called the National Institute for Petroleum and Energy Research (NIPER)) and at the Thermochemical Laboratory at Lund University, Lund, Sweden. The development of a high precision rotating bomb calorimeter was a key accomplishment which has led to the determination and publication of extemely precise and accurate thermodynamic properties for CHS compounds. A rotating-bomb calorimeter is needed because the final state of sulfur as an aqueous sulfuric acid solution is not homogeneous in its dispersal throughout the interior of the static combustion bomb and is energetically uncertain. An important phase of the research effort focused on the establishment of the enthalpies of formation of aqueous sulfuric acid in various states of dilution. These $\Delta_fH°$'s were then applied toward the identification of the final state of sulfur in the bomb combustion process for organic sulfur compounds. This feature is important because the energetics of the final thermodynamic state of the combustion process must be clearly and precisely defined. Without a knowledge of the final state of sulfur in the form of an aqueous sulfuric acid solution for the combustion reaction, highly precise and accurate data would not be available. For additional information, the reader should examine 56ROS, 62SKI, and 79SUN/MAN.

The research effort in the two laboratories at Bartlesville and Lund was responsible for publication of high quality data available on organic sulfur compounds in the chemical literature and the subsequent good agreement found here between experimental and estimated values as presented in Tables 42 through 49.

Collectively, the residuals shown for thiols and sulfides are very small. Of the organic sulfur families, sulfones appear to be less well-behaved, but agreement here between experimental and estimated values is still reasonably good.

2.5. Organic Halogen Compounds

The families which comprise the CHX and CHXO compounds are: fluorides, chlorides, bromides, iodides, and mixed halogen compounds. A total of 258 halogen compounds are shown in Tables 50 through 54. Agreement between experimental and calculated values shows 54 percent of the residuals for $\Delta_fH°$ to be $< \pm 4$ kJ·mol^{-1}, 17 percent to be $> \pm 4$ and $< \pm 8$ kJ·mol^{-1}, and 29 percent to be $> \pm 8$ kJ·mol^{-1}. For $C_p°$, 76 percent of the residuals are $< \pm 4$ J·mol^{-1}·K^{-1}, 11 percent are $> \pm 4$ but $< \pm 8$ kJ·mol^{-1}, and 13 percent are $> \pm 8$ J·mol^{-1}·K^{-1}. With respect to $S°$, 70 percent are $< \pm 4$ J·mol^{-1}·K^{-1}, 17 percent are $> \pm 4$ but $< \pm 8$ J·mol^{-1}·K^{-1}, and 13 percent are $> \pm 8$ J·mol^{-1}·K^{-1}.

In contrast to hydrocarbons and organic sulfur compounds, the thermodynamic properties of organic halogen compounds are collectively not known as precisely. In addition, halogen-halogen interactions operate which require interpetation. When these interactions are overlooked, they tend to make the differences between literature and estimated values larger than they should be.

The use of a rotating bomb calorimeter for the determination of enthalpies of combustion and for the derivation of enthalpies of formation is needed for organic halogen compounds. The enthalpy of formation of the final state of the hydrohalogen acid in aqueous solution must be determined in order to have a defined thermodynamic final state for the combustion process. Additional problems prevail with organic chlorine compounds in that they form about 15–20% elemental gaseous chlorine, Cl_2, and about 80–85% HCl in aqueous solution during the bomb combustion. A reducing agent such as a solution of arsenious oxide must be added to the combustion bomb prior to its closure with the sample so that the Cl_2 is converted to Cl^- and enters the aqueous solution. Similarly, without a reducing agent, organic bromine compounds form about 80–85% bromine, Br_2, and 15–20% HBr in aqueous solution. Aqueous arsenious oxide reduces the Br_2 to aqueous HBr during the oxidation reaction when the reducing agent is added to the bomb prior to closure. The combustion process for organic fluorine compounds give aqueous HF as the only fluorine combustion product while organic iodine compounds yield crystalline elemental iodine as the singular iodine-containing product. For additional information, the reader should examine 56ROS, 62SKI, and 79SUN/MAN.

The large differences between the experimental and estimated values for $\Delta_f H°$(gas) and $\Delta_f H°$(solid) for decafluorobiphenyl (322.8 and 337.84 kJ·mol^{-1}, respectively) are not easily explained. The study reported by 79PRI/SAP2 for the combustion of $C_{12}F_{10}$ indicates that CO_2, CF_4, and F_2 are the only products of combustion in excess oxygen. Several reasons may explain the large differences. Possible explanations include: the energy corrections for the interactions between fluorine atoms in $C_{12}F_{10}$ may be different than those which are currently viewed; or, the quantitative determinations of the CF_4 and F_2 as combustion products may be in error.

We have attempted to correct for the interactions between halogen atoms in the various halogen families using *cis*-, *ortho*, or *meta* corrections, but success here is limited.

2.6. Comparison with an Extended Second-order Group Additivity Scheme

An extended multi-parameterized second-order group-additivity estimation scheme has been developed by J.B. Pedley and co-workers (86PED/NAY).

The Pedley scheme is limited to the estimation of enthalpies of formation of organic compounds at 298.15 K in the gas phase. The additional parameterization accounts more comprehensively for nearest- and next-to-nearest neighbor interactions than the estimation scheme developed by S.W. Benson and co-workers and used in this work.

The details of the Pedley scheme are discussed in a cursory manner in Appendix 3 and more fully in 86PED/NAY. A comparison of estimated values from the Pedley scheme and that used in this work has been made for 20 hydrocarbons and 20 organic oxygen compounds. The results indicate that differences between literature and estimated values are about the same for the two groups of compounds tested.

2.7. Summary and Conclusions

We have demonstrated the successful extension of the second-order group-additivity method for the estimation of $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K to liquid and solid organic compounds. A re-examination of group values for the gas phase was performed in order to maintain internal consistency with the condensed phase. This work has been carried out for 1512 organic compounds containing the elements carbon, hydrogen, oxygen, nitrogen, sulfur, and halogens. A total of over 3700 comparisons between literature and estimated values have been made for $\Delta_f H°$, $C_p°$, and $S°$ in the gas, liquid, and solid phases. Overall, for the compounds covered, the estimation of $\Delta_f H°$ showed that 67 percent of the residuals were $< \pm 4$ kJ·mol^{-1}, 16 percent were $> \pm 4$ but $< \pm 8$ kJ·mol^{-1}, and 17 percent were $> \pm 8$ kJ·mol^{-1}. Values for $C_p°$ showed that 80 percent of the residuals are $< \pm 4$ J·mol^{-1}·K^{-1}, 10 percent are $> \pm 4$ but $< \pm 8$ J·mol^{-1}·K^{-1}, and 10 percent are $> \pm 8$ J·mol^{-1}·K^{-1}. Values for $S°$ show that 76 percent of the residuals are $< \pm 4$ J·mol^{-1}·K^{-1}, 14 percent are $> \pm 4$ but $< \pm 8$ J·mol^{-1}·K^{-1}, and 10 percent are $> \pm 8$ J·mol^{-1}·K^{-1}.

The groups and group values developed in this work should be helpful to thermochemists and chemical engineers for the estimation of enthalpies of formation, heat capacities, and entropies at 298.15 K and 101,325 Pa when their needs for predicted values of these thermodynamic properties arise. This estimation technique can also be used to establish whether a new experimentally determined value for $\Delta_f H°$, $C_p°$, or $S°$ comes within the range of expectations of group additivity as dictated by the experience already shown with this method.

Comparisons in Appendix 2 between literature values for the enthalpy and entropy of fusion and the enthalpy of vaporization, corrected from either T_m or T_b to 298.15 K, with corresponding differences [$\Delta_f H°$(solid) − $\Delta_f H°$(liq)], [$S°$(solid) − $S°$(liq)], and [$\Delta_f H°$(liq) − $\Delta_f H°$(g)], respectively, show that internal consistency does exist for the compounds tested.

The limited comparison of hydrocarbon and oxygen-containing compounds in Appendix 3 suggest that the extra effort taken in the Pedley scheme to account for nearest- and next-to-nearest neighbor interactions may have either a very small or even negligible effect upon reducing the degree of differences between literature and estimated values for enthalpies of formation at 298.15 K in the gas phase.

3. Tables of C–H–N–O–S–Halogen Compounds

TABLE 1. Summary of tables of C–H–N–O–S Halogen Families

Table 1.	C–H–N–O–S–Halogen Families
Table 2.	Listing of Groups and Group Values
Table 3.	General Definitions and Examples of Notations for Molecular Groups

Hydrocarbon Compounds

Table	Name	Description	No. of Compounds
Table 4.	*n*-Alkanes	normal alkanes	25
Table 5.	*t*-alkanes	tertiary branched alkanes	35
Table 6.	*q*-Alkanes	quaternary branched alkanes	16
Table 7.	*n*-Alkenes	linear alkenes	32
Table 8.	s-Alkenes	branched alkenes	34
Table 9.	Alkynes	alkyne hydrocarbons	28
Table 10.	Aromatic CH–01	aromatic hydrocarbons	42
Table 11.	Aromatic CH–02	aromatic hydrocarbons	80
Table 12.	Cyclic CH–01	cyclic hydrocarbons	40
Table 13.	Cyclic CH–02	cyclic hydrocarbons	48
Table 14.	Cyclic CH–03	cyclic hydrocarbons	47
Total Hydrocarbon compounds			427

CHO Compounds

Table	Name	Description	No. of Compounds
Table 15.	Alcohols	alcohols, diols, triols, phenols	69
Table 16.	Ethers	linear, branched, and cyclic ethers	52
Table 17.	Aldehydes	aldehydes	16
Table 18.	Ketones	ketones	42
Table 19.	Acids	linear, branched, cyclic, and aromatic acids	89
Table 20.	Anhydrides	anhydrides	11
Table 21.	Esters	esters and lactones	74
Table 22.	Peroxides	peroxides	7
Table 23.	Hydroperoxides	hydroperoxides	9
Table 24.	Peroxyacids	peroxyacids	8
Table 25.	Carbonates	carbonates	3
Total CHO compounds			381

CHN Compounds

Table	Name	Description	No. of Compounds
Table 26.	Amines	Linear, branched, cyclic, aromatic	50
Table 27.	Imines	imines	2
Table 28.	Nitriles	linear, branched, cyclic, aromatic	27
Table 29.	Hydrazines	hydrazines	6
Table 30.	Diazenes	diazenes	14
Table 31.	Azides	azides	6
Table 32.	Cyclic CHN	heterocyclic nitrogen compounds	32
Total CHN compounds			137

TABLE 1. C–H–N–O–S–Halogen families (Continued)

CHNO Compounds

Table	Name	Description	No. of compounds
Table 33.	Amides	Linear, Branched, Cyclic, Aromatic	28
Table 34.	Ureas	Ureas	24
Table 35.	Amino acids	Amino acids and peptides	38
Table 36.	Nitroso compounds	Nitroso and cyanato compounds	9
Table 37.	Nitro compounds	Linear, branched, cyclic, aromatic	50
Table 38.	Nitrites	Nitrites	3
Table 39.	Nitrates	Nitrates	6
Table 40.	Nitramines	Nitramines	10
Table 41.	Cyclic CHNO	Cyclic amides	3
Total CHNO compounds			171

CHS and CHSO Compounds

Table	Name	Description	No. of compounds
Table 42.	Thiols	Linear, branched, cyclic, aromatic	31
Table 43.	Sulfides	Linear, branched, aromatic	33
Table 44.	Disulfides	Disulfides	8
Table 45.	Sulfoxides	Sulfoxides	6
Table 46.	Sulfones	Linear, branched, aromatic	38
Table 47.	Sulfites	Sulfites	5
Table 48.	Sulfates	Sulfates	4
Table 49.	Cyclic CHS	Heterocyclic sulfur compounds	13
Total CHS and CHSO compounds			138

Halogen Compounds

Table	Name	Description	No. of compounds
Table 50.	Fluorides	CHF and CHFO compounds	46
Table 51.	Chlorides	CHCl and CHClO compounds	116
Table 52.	Bromides	CHBr and CHBrO compounds	39
Table 53.	Iodides	CHI and CHIO compounds	39
Table 54.	Mixed Halogen compounds	CHClF, CHClBr, CHBrF, CHFI compounds	18
Total Halogen compounds			258
Total of all compounds			1512

TABLE 2. Listing of groups and group values

Group	$\Delta_f H^\circ$ (gas)	C_p° (gas)	S° (gas)	$\Delta_f H^\circ$ (liq)	C_p° (liq)	S° (liq)	$\Delta_f H^\circ$ (solid)	C_p° (solid)	S° (solid)
				CH Groups					
C–(H)$_3$(C)	−42.26	25.73	127.32	−47.61	36.48	83.30	−46.74	67.45	56.69
C–(H)$_2$(C)$_2$	−20.63	22.89	39.16	−25.73	30.42	32.38	−29.41	21.92	23.01
C–(H)(C)$_3$	−1.17	20.08	−53.60	−4.77	21.38	−23.89	−5.98	−48.81	−16.89
–CH$_3$ corr (tertiary)	−2.26	0.00	0.00	−2.18	0.00	0.00	−2.34	0.00	0.00
C–(C)$_4$	19.20	16.53	−149.49	17.99	10.24	−98.65	12.47	−83.63	−33.19
–CH$_3$ corr (quaternary)	−4.56	0.00	0.00	−4.39	0.00	0.00	−4.35	0.00	0.00
–CH$_3$ corr (tert/quat)	−1.80	0.00	0.00	−1.77	0.00	0.00	−2.70	0.00	0.00
–CH$_3$ corr (quat/quat)	−0.64	0.00	0.00	−0.64	0.00	0.00	−2.24	0.00	0.00
C$_d$–(H)$_2$	26.32	21.38	115.52	21.75	28.37	86.19	22.43		
C$_d$–(H)(C)	36.32	18.74	33.05	31.05	24.60	28.58	25.48		
C$_d$–(C)$_2$	44.14	15.10	−50.84	39.16	23.22	−29.83	32.97		
C$_d$–(H)(C$_d$)	28.28	18.54	27.74	22.18	31.67	13.30	17.53	35.65	21.75
C$_d$–(C)(C$_d$)	36.78	17.57	−61.33	30.42	26.19	−41.92	27.91		
C$_d$–(C$_d$)(C$_B$)							56.07		
C$_d$–(H)(C$_B$)	28.28	18.54	27.74	22.18	31.67	13.30	17.53	35.65	21.75
C$_d$–(C)(C$_B$)	37.95	15.90	−51.97	38.58					
C$_d$–(H)(C$_t$)	28.28	18.54	27.74	22.18	31.67	13.30	17.53	35.65	21.75
C–(H)$_4$, Methane	−74.48	35.73	206.92						
C$_d$–(C$_B$)$_2$	32.88			30.83	25.10		49.91	32.50	
C–(H)$_2$(C)(C$_d$)	−20.88	20.63	38.20	−25.73	29.29	31.67	−24.35		
C–(H)(C)$_2$(C$_d$)	−1.63	27.49	−50.38	−5.02	30.12	−28.07	−6.49		
–CH$_3$ corr (tertiary)	−2.26	0.00	0.00	−2.18	0.00	0.00	−2.34	0.00	0.00
C–(C)$_3$(C$_d$)	22.13	9.16	−150.23	20.79	28.74	−108.20	12.51		
–CH$_3$ corr (quaternary)	−4.56	0.00	0.00	−4.39	0.00	0.00	−4.35	0.00	0.00
C–(H)(C)(C$_d$)$_2$	−1.17	20.08	−53.60	−4.77	21.38	−23.89	−5.98	−48.81	−16.89
C–(H)$_2$(C$_d$)$_2$	−18.92	24.77	42.08	−24.43	40.88	19.32	−21.60		
C–(H)$_2$(C$_d$)(C$_B$)				−24.73					
C–(H)(C)(C$_d$)(C$_B$)				−6.90					
cis (unsat) corr	4.85	−8.03	5.06	5.27	0.00	0.00	5.73	0.00	0.00
tert-Butyl *cis* corr	17.24	0.00	0.00	17.48	0.00	0.00	17.57	0.00	0.00
C$_t$–(H)	113.50	22.55	101.96	104.47	39.96	67.57	110.34		
C$_t$–(C)	115.10	13.22	26.32	107.15	25.59	14.25	101.66		
C$_t$–(C$_d$)	121.42	10.71	39.92	114.77					
C$_t$–(C$_B$)	120.76	10.17	17.77	119.00			103.28	32.30	
C$_t$–(C$_t$)	120.76	14.27	25.94	104.80			103.28		
C–(H)$_2$(C)(C$_t$)	−19.70	20.97	42.80	−22.13	30.39	32.36	−29.41		
C–(H)(C)$_2$(C$_t$)	−3.16	17.45	−45.69						
–CH$_3$ corr (tertiary)	−2.26	0.00	0.00	−2.18	0.00	0.00	−2.34	0.00	0.00
C–(C)$_3$(C$_t$)				22.83			26.38		
–CH$_3$ corr (quaternary)	−4.56	0.00	0.00	−4.39	0.00	0.00	−4.35	0.00	0.00
C–(H)$_2$(C$_t$)$_2$	−41.14			−39.08					
C–(C)$_2$(C$_t$)$_2$				20.67					
C$_a$	142.67	15.86	26.28	134.68	30.04	14.39	131.08		
C$_B$–(H)(C$_B$)$_2$	13.81	13.61	48.31	8.16	22.68	28.87	6.53	20.13	22.75
C$_B$–(C)(C$_B$)$_2$	23.64	9.75	−35.61	19.16	10.10	−19.50	13.90	−23.26	−5.50
C$_B$–(C$_d$)(C$_B$)$_2$	24.17	14.12	−33.85	19.12	9.44	−9.04	20.27	−20.00	−10.00
C$_B$–(C$_t$)(C$_B$)$_2$	24.17	14.12	−33.85	19.12	9.44	−9.04	20.07	−20.00	−10.00
C$_B$–(C$_B$)$_3$	21.66	13.12	−36.57	17.21	17.07		17.03	−1.72	−6.00
C–(C)$_2$(C$_B$)$_2$							52.81		
C–(H)$_2$(C)(C$_B$)	−21.34	25.61	42.59	−24.81	22.90	47.40	−22.10	49.38	26.90
C–(H)(C)$_2$(C$_B$)	−4.52	22.45	−48.00	−5.82	17.50	−13.90	−3.50		
C–(C$_B$)(C)$_3$	18.28	18.28	−147.19	18.70	5.17	−96.10	21.57		
C–(H)$_2$(C$_B$)$_2$	−46.43			−26.50	32.91	51.97	−21.44	69.06	22.85
C–(H)(C)(C$_B$)$_2$				−21.47	11.50	28.12	16.40	43.55	
C–(H)(C$_B$)$_3$	−6.86						34.48	63.64	−12.62
C–(C$_B$)$_3$(C)							116.25	39.83	

TABLE 2. Listing of groups and group values

Group	$\Delta_f H°$ (gas)	C_p° (gas)	$S°$ (gas)	$\Delta_f H°$ (liq)	C_p° (liq)	$S°$ (liq)	$\Delta_f H°$ (solid)	C_p° (solid)	$S°$ (solid)
CH Groups									
$C-(C_B)_4$	27.04						64.89	58.74	
$C_{BF}-(C_{BF})(C_B)_2$	20.10	0.00	0.00	15.83	9.52	−5.54	14.10	2.30	−6.00
$C_{BF}-(C_B)(C_{BF})_2$	16.00			11.50			12.00	5.77	2.00
$C_{BF}-(C_{BF})_3$	3.59			−0.90			1.94	8.00	7.00
$C_B-(C_B)_2(C_{BF})$							−8.77		
$C_B-(C_B)(C_{BF})_2$	22.46						47.93		
ortho corr, hydrocarbons	1.26	6.40	−2.50	3.26	3.50	0.00	5.00	0.00	0.00
meta corr, hydrocarbons	−0.63	0.71	0.00	0.00	0.00	0.00	2.00	0.00	0.00
Cyclopropane rsc (unsub)	115.15	−12.73	134.86	111.58	−28.53				
Cyclobutane rsc	110.89	−19.34	126.04	106.64	−10.68	51.48	114.43		
Cyclopentane rsc (unsub)	26.75	−31.44	116.22	22.84	−23.32	42.24	34.00		
Cyclohexane rsc (unsub)	0.68	−31.07	78.18	−1.77	−26.21	10.07	10.94		
Cycloheptane rsc	26.34	−37.14	73.97	23.50	−32.19	15.89			
Cyclooctane rsc	40.65	−43.17	70.78	38.10	−27.88	2.96			
Cyclononane rsc	52.91			50.40					
Cyclodecane rsc	51.99			50.61					
Cycloundecane rsc	47.56			47.55					
Cyclododecane rsc	17.31						46.27		
Cyclotridecane rsc	21.84			24.83					
Cyclotetradecane rsc	49.37						37.48		
Cyclopentadecane rsc	8.03						65.09		
Cyclohexadecane rsc	8.41						67.14		
Cycloheptadecane rsc	−13.59						69.56		
Cyclopropene rsc	223.26								
Cyclobutene rsc	125.81	−11.67	126.77						
Cyclopentene rsc (unsub)	24.18	−26.53	113.76	21.45	−15.82	48.37			
Cyclohexene rsc	5.61	−19.50	95.69	2.04	−20.26	29.34			
Cycloheptene rsc	21.81								
Cyclooctene rsc	24.65			18.26					
1,3-Cyclopentadiene rsc	24.07			23.95					
1,3-Cyclohexadiene rsc	17.14			16.41	−26.56	50.18			
1,4-Cyclohexadiene rsc	−2.69			−5.64	−34.22	36.41			
1,3-Cycloheptadiene rsc	27.54								
1,5-Cyclooctadiene rsc	39.34			36.42	−7.45	23.35			
1,3,5-Cycloheptatriene rsc	16.84	−18.63	102.26	18.59	−54.00	84.96			
Cyclooctatetraene rsc	71.37	−26.31	116.38	77.07	−68.18	113.89			
Spiropentane rsc	248.50	−19.97	286.59	242.58	2.60	162.81			
Cyclopropane (sub) rsc	105.95			96.58					
Cyclopentane (sub) rsc	19.55	−27.87	118.39	23.59	−23.32	56.65	34.00		
Cyclohexane (sub) rsc	−0.39	−22.82	83.97	−2.06	−26.21	25.10	10.30		
Cyclopentene (sub) rsc	24.31	−24.50	117.11	19.82	−15.82	48.37			
Naphthalene (unsub)	0.00	11.83	−19.66	0.00	0.00	0.00	0.00	0.00	0.00
Naphthalene (1 sub)	0.00	14.39	−21.50	0.00	0.00	0.00	0.00	0.00	0.00
Naphthalene (2 sub)	0.00	16.48	−23.00	0.00	0.00	0.00	0.00	0.00	0.00
cis-Decalin rsc	127.00	−183.44		−4.02	−54.12	53.75			
trans-Decalin rsc	123.81	−183.24		−15.22	−57.63	53.67			
cis-Hexahydroindan rsc	19.51			16.39	−41.52	86.59			
trans-Hexahydroindan rsc	15.16			13.29	−46.00	79.98			
2,2-Metacyclophane rsc	52.08						55.06	−24.92	
2,2-Metaparacyclophane rsc	99.35						109.46	−4.02	
2,2-Paracyclophane rsc	125.09						127.26	−13.18	−1.92
3,3-Paracyclophane rsc	50.95						65.53	14.90	
Adamantane rsc	−6.14						3.18		
Fluoranthene rsc	63.21	62.47	59.66	−4.43	−5.92				

TABLE 2. Listing of groups and group values — Continued

Group	$\Delta_f H^\circ$ (gas)	C_p° (gas)	S° (gas)	$\Delta_f H^\circ$ (liq)	C_p° (liq)	S° (liq)	$\Delta_f H^\circ$ (solid)	C_p° (solid)	S° (solid)
CH Groups									
Bicyclo[2.2.2]octane rsc	27.12				−67.59	−63.45	41.52		
Bicyclo[3.3.3]undecane rsc	99.06						124.10		
cis-Bicyclo[6.1.0]nonane rsc	115.55			109.35					
Bicyclo[1.1.0]butane rsc	260.70			254.70					
Bicyclo[3.1.0]hexane rsc	123.16			117.56					
Bicyclo[2.2.1]hepta-2,5-diene rsc	125.29			124.87					
Tetracyclo-[3.2.02,7.04,6]heptane rsc	366.75			356.45					
Tricyclo[2.2.1.02,6]heptane rsc	148.67			139.67					
Bicyclo[2.2.1]hept-2-ene rsc	82.79			73.58			102.73		
Bicyclo[2.2.1]heptane rsc	43.49			45.39			57.01		
Bicyclo[4.1.0]heptane rsc	106.99			101.39					
Pentacyclo-[4.2.0.02,5.03,8.04,7]-octane rsc	674.60						632.84		
Bicyclo[2.2.2]oct-2-ene rsc	33.64						56.36		
Bicyclo[4.2.0]octane rsc	100.72			95.72					
Bicyclo[5.1.0]octane rsc	109.42			103.62					
trans-Bicyclo[6.1.0]nonane rsc	107.05			107.25					
Bicyclo[3.3.1]nonane rsc	19.25						39.63		
cis-Bicyclo[3.3.0]octane rsc	33.22			27.92					
trans-Bicyclo[3.3.0]octane rsc	59.52			54.72					
CHO Groups									
CO–(H)$_2$, Formaldehyde	−108.60	35.40	224.54						
CO–(C)(CO)	−121.29			−135.04			−140.75		
CO–(H)(CO)	−105.98								
CO–(CO)(C$_B$)	−112.30						−117.75		
CO–(O)(CO)	−123.75			−123.30	40.63		−120.81		
CO–(C$_d$)(O)	−136.73	24.56	62.59	−155.56	48.16		−134.10	43.75	32.90
CO–(C)(O)	−137.24	24.56	62.59	−149.37	44.98	32.72	−153.60	44.98	32.13
CO–(H)(O)	−124.39	29.00	147.03	−142.42	65.10	94.68			
CO–(O)$_2$	−111.88			−122.00	31.46		−123.00	4.25	−42.92
CO–(H)(C$_d$)	−126.96			−153.05					
CO–(C$_B$)$_2$	−110.00			−119.00			−116.00	109.33	
CO–(C)(C$_B$)	−148.82			−145.22	73.35		−143.70	71.38	23.72
CO–(H)(C$_B$)	−121.35			−138.12	54.22		−160.18		
CO–(O)(C$_B$)	−125.00			−140.00	48.16		−145.00	43.75	32.13
CO–(C)$_2$	−132.67	23.43	64.31	−152.76	52.97	33.81	−157.95		
CO–(H)(C)	−124.39	29.00	147.03	−142.42	65.10	93.55			
CO–(C)(C$_d$)					27.07				
O–(CO)$_2$, aliphatic	−214.50	−1.08	34.16	−230.50	5.28		−235.00		
O–(CO)$_2$, aromatic	−238.30			−220.90			−207.00		
O–(C$_d$)(CO)	−198.03			−201.42	19.58				
O–(C)(CO)	−188.87	11.80	36.03	−196.02	19.58	38.28	−210.60	−6.00	12.09
O–(H)(CO)	−254.30	16.23	101.71	−285.64	37.82	38.28	−282.15	44.60	21.78
O–(C$_B$)(CO)	−167.00			−165.50			−170.00	29.08	45.32
O–(C)(O)	−20.75			−23.50			−30.20		
O–(H)(O)	−72.26			−101.75			−105.30		
O–(C$_d$)$_2$	−139.29			−137.32					
O–(H)(C$_d$)					37.78				
O–(C)(C$_d$)	−129.33			−133.72	51.21				
O–(C$_B$)$_2$	−77.66			−85.27		23.31	−96.20	15.90	3.14
O–(C)(C$_B$)	−92.55			−104.85	8.10		−122.87		
O–(H)(C$_B$)	−160.30	18.16	121.50	−191.75	44.64	43.89	−199.25	29.25	28.62
O–(C)$_2$	−101.42	18.54	29.33	−110.83	24.27	26.78	−119.00		
O–(H)(C)	−159.33	18.16	121.50	−191.50	44.64	43.89	−199.66	29.25	28.62
C$_d$–(H)(CO)	32.30	15.61	35.19	26.61	28.12		7.82	−18.66	27.53
C$_d$–(C)(CO)					18.62				

TABLE 2. Listing of groups and group values — Continued

Group	$\Delta_f H°$ (gas)	$C_p°$ (gas)	$S°$ (gas)	$\Delta_f H°$ (liq)	$C_p°$ (liq)	$S°$ (liq)	$\Delta_f H°$ (solid)	$C_p°$ (solid)	$S°$ (solid)
CHO Groups									
C_d–(O)(C_d)	36.78	17.57	−61.34	30.42	26.19	−41.92	27.91		
C_d–(O)(C)	44.14	15.10	−50.84	39.08	23.22	−29.83	32.97		
C_d–(O)(H)	36.32	18.74	33.05	31.05	24.60	28.58	25.48		
C_t–(CO)							144.52		
C_B–(CO)$(C_B)_2$	15.50			10.50	4.39		8.15	−42.89	0.08
C_B–(O)$(C_B)_2$	−4.75	15.86	−43.72	−5.61	39.71	−10.59	1.00	−0.29	1.59
C–$(H)_2(CO)_2$	−30.74			−23.06	15.56		−19.10		
C–(CO)$(C)_3$	23.93			26.15	7.99	−85.98	24.02	−114.10	
C–(H)(CO)$(C)_2$	−0.25			−3.89	17.41	−24.52	−9.83	−80.51	
C–$(H)_2$(CO)(C)	−21.84	24.69	39.58	−24.14	29.29	39.87	−27.90	21.92	24.73
C–$(H)_3$(CO)	−42.26	25.73	127.32	−47.61	36.48	83.30	−46.74	67.45	56.69
C–$(H)_2$(CO)(C_d)	−16.95			−19.62					
C–$(H)_2$(CO)(C_t)	−25.48			−26.61					
C–$(H)_2$(CO)(C_B)	−16.20			−11.67					
C–(H)(CO)(C)(C_B)							14.81		
C–(H)(O)(CO)(C)	126.63			123.43	7.44	−46.71	−14.39	−58.45	8.08
C–$(O)_4$	−152.46			−133.34					
C–(H)$(O)_3$	−113.97			−107.74	21.71				
C–$(O)_3$(C)	−114.39			−99.54					
C–$(O)_2(C)_2$	−53.56			−41.30					
C–(H)$(O)_2$(C)	−57.78			−51.42	12.38				
C–$(H)_2(O)_2$	−62.22			−62.89	39.92	23.85			
C–$(H)_2$(O)(C_B)	−33.76			−29.17	46.48				
C–$(H)_2$(O)(C_d)	−27.49	17.74	37.49	−28.62	41.30				
C–(H)(CO)(C)(C_B)							−14.39		
C–(H)(CO)$(C_B)_2$							3.72		
C–(O)$(C_B)_3$							60.46	57.49	
C–(O)$(C)_3$ (ethers,esters)	9.50	14.60	−141.92	0.79	20.46	−94.68	−0.50		
C–(H)(O)$(C)_2$ (ethers,esters)	−19.46	17.78	−52.80	−21.00	25.56	−25.31	−20.08		
C–(O)$(C)_3$ (alcohols,peroxides)	−13.50	15.73	−144.60	−11.13	65.58	−122.48	−12.25	−85.48	−14.77
C–(H)(O)$(C)_2$ (alcohols,peroxides)	−26.10	19.96	−43.05	−27.60	49.83	−29.83	−29.08	4.77	6.95
C–$(H)_2$(O)(C)	−32.90	20.33	43.43	−35.80	33.64	32.59	−33.00	21.92	24.73
C–$(H)_3$(O)	−42.26	25.73	127.32	−47.61	36.48	83.30	−46.74	67.45	56.69
O–(CO)(O)	−88.00			−90.00			−80.50		
C–$(C)_2$(O)(C_B)	15.30			25.80			29.30		
C–(H)(C)$(O)_2$							−52.50		
Glutaric anhydride rsc	20.89						8.91		
Succinic anhydride rsc	4.76			−11.08			−10.60		
Phthalic anhydride rsc	30.66						−5.52		
Cyclopentanone rsc	22.85			15.10					
Cyclohexanone rsc	10.50	−31.82	66.98	5.60	−25.61	11.29			
Cycloheptanone rsc	10.76			6.31					
Cyclooctanone rsc	7.33			9.01			37.38		
Cyclononanone rsc	20.43			22.57			55.28		
Cyclodecanone rsc	15.70			17.73					
Cycloundecanone rsc	19.39			20.53					
Cyclododecanone rsc	12.91			18.02			47.11		
Cyclopentadecanone rsc	9.41						74.77		
Cycloheptadecanone rsc	4.87						89.49		
Cyclobutane-1,3-dione rsc	140.48						94.10		
Ethylene oxide rsc	114.62	−10.92	132.00	104.82	−23.90	80.50			
Trimethylene oxide rsc	107.35				−22.38				
Furan rsc	−12.18			−9.97					
Tetrahydrofuran rsc	24.28	−28.73	113.66	17.70	−28.49	47.18	14.60		
Tetrahydropyran rsc	5.71			1.32	−42.22		0.80		

TABLE 2. Listing of groups and group values — Continued

Group	$\Delta_f H^\circ$ (gas)	C_p° (gas)	S° (gas)	$\Delta_f H^\circ$ (liq)	C_p° (liq)	S° (liq)	$\Delta_f H^\circ$ (solid)	C_p° (solid)	S° (solid)
				CHO Groups					
1,3-Dioxolane rsc	29.06			18.75	−37.74				
1,3-Dioxane rsc	10.90			4.40	−42.26				
1,4-Dioxane rsc	19.15	−24.34	73.16	9.76	−29.50	86.28	−12.00		
1,3-Dioxepane rsc	25.52			20.01	−49.20				
Trioxane rsc	25.02								
Tetraoxane rsc	34.23								
β-Propiolactone rsc	97.95			75.43	−5.40	31.85			
τ-Butyrolactone rsc	34.98			10.16	−16.61	21.56			
τ-Valerolactone rsc	26.06			4.75					
δ-Valerolactone rsc	42.51			19.19	−16.74	10.77			
Caprolactone rsc					−21.92	−4.92			
Undecanolactone rsc					−28.12	−33.05			
Ethylene carbonate rsc							23.90		
Cyclobutane methyl carboxylate rsc	75.21			79.08					
Bicyclobutane methyl carboxylate rsc	222.27			219.98					
1,4-Dimethylcubane dicarboxylate rsc	595.80						590.73		
2-Deoxy-D-ribose rsc							0.25		
β-D-Ribose rsc							12.65		
α-D-Glucose rsc							6.30		
COOH–COOH (*ortho* corr)							34.14	15.00	8.96
COOH–COOH (*meta* corr)	−23.94						13.14	30.00	0.00
CH_3O–COOH (*ortho* corr)	15.00						23.00		
CH_3O–COOH (*meta* corr)	5.00						5.00		
OH–OH (*ortho* corr)	7.00						16.00		
OH–OH (*meta* corr)	0.00						2.00		
OH–COOH (*ortho* corr)	−20.00						0.00		
				CHN and CHNO Groups					
C–$(H)_3$(N)	−42.26	25.73	127.32	−47.61	36.48	83.30	−46.74	67.45	56.69
C–$(H)_2$(C)(N)	−28.30	22.68	42.26	−30.80	30.42	32.38	−34.00	21.92	23.01
C–(H)$(C)_2$(N)	−16.70	18.62	−63.55	−14.65	28.28	−20.00	−13.90		
–CH_3 corr (tertiary)	−2.26	0.00	0.00	−2.18	0.00	0.00	−2.34	0.00	0.00
C–$(C)_3$(N)	0.29	18.41	−152.59	5.10	19.66	−87.99	1.00	−84.14	
–CH_3 corr (quaternary)	−4.56	0.00	0.00	−4.39	0.00	0.00	−4.35	0.00	0.00
C–$(H)_2(N)_2$	−30.00						−26.00		
C–$(H)_2(C_B)$(N)	−24.14			−26.09	19.79		−33.31		
N–$(H)_2$(C) (first, amino acids)	19.25	24.35	124.40	0.33	62.59	71.71	−6.30	32.00	39.00
N–$(H)_2$(C) (second, amino acids)	19.25	24.35	126.90	0.33	62.59	71.71	−46.00	71.27	48.75
N–(H)$(C)_2$	67.55	12.28	33.96	51.50	59.37	32.09	47.80	−8.00	
N–$(C)_3$	116.50	15.10	−61.71	112.00	26.11	−38.62	101.00	−39.00	
N–$(H)_2$(N)	47.70	26.36	122.18	25.30	49.41	60.58	18.97		
N–(H)(C)(N)	89.16			75.00	49.04	22.05			
N–$(C)_2$(N)	120.71			119.00	41.67	−26.94			
N–$(C_B)_2$(N)							137.35		
N–(H)(C_B)(N)	87.50			73.40			66.90		
N–$(CO)_2$(N)							73.62		
N–(H)$(C_d)_2$	83.55			50.50			45.40		
N–(C)$(C_d)_2$	120.64			97.38			88.92		
N–$(H)_2(C_B)$	19.25	24.35	126.90	−11.00	62.59	71.71	−21.60	26.00	70.00
N–(H)(C)(C_B)	59.00			26.25	65.20		36.55	−50.00	
N–$(C)_2(C_B)$	126.40			109.40	10.75		96.50	−36.50	
N–(C)$(C_B)_2$	120.44			97.38	7.95		89.30		
N–(H)$(C_B)_2$	83.55			50.50			45.40	−3.00	

TABLE 2. Listing of groups and group values — Continued

Group	$\Delta_fH°$ (gas)	$C_p°$ (gas)	$S°$ (gas)	$\Delta_fH°$ (liq)	$C_p°$ (liq)	$S°$ (liq)	$\Delta_fH°$ (solid)	$C_p°$ (solid)	$S°$ (solid)
				CHN and CHNO Groups					
N–(C$_B$)$_3$	123.15			121.80			107.50	−39.00	
N$_I$–(C)	81.46			73.68					
N$_I$–(C$_B$)	69.00	10.07	47.01	54.50	19.75	36.40	57.00		
N$_A$–(C)	109.50			104.85			103.00		
N$_A$–(C$_B$)	109.50			104.85			103.00		
N$_A$–(oxide)(C)	40.80			22.65					
C–(H)$_2$(C)(N$_A$)	−20.70			−25.70			−29.41		
C–(H)(C)$_2$(N$_A$)	−2.66			−5.42					
C–(C)$_3$(N$_A$)	11.50			15.50			10.50		
C$_d$–(H)(N)	−16.00			−15.50			−13.00		
C$_d$–(C)(N)	−5.74			−5.62			−3.95		
C$_B$–(N)(C$_B$)$_2$	−1.30	16.07	−43.53	1.50	15.02	−24.43	9.75	13.00	−37.57
C$_B$–(NO)(C$_B$)$_2$	21.50						23.00		
C$_B$–(NO$_2$)(C$_B$)$_2$	−1.45			−28.30	73.30	79.95	−32.50	50.96	110.46
C$_B$–(CNO)(C$_B$)$_2$	−177.63						155.69		
C$_B$–(CN)(C$_B$)$_2$	151.00	41.09	85.25	122.38	51.80	64.75	121.20		50.45
C$_B$–(N$_A$)(C$_B$)$_2$	22.55			20.08			18.65		
C$_B$–(H)(N$_I$)$_2$	6.30						0.25		
CO–(H)(N)	−124.39	29.00	147.03	−188.00	65.10	93.55			
CO–(C)(N)	−133.26	22.50	56.70	−185.00	49.16		−194.60	39.00	40.00
CO–(C$_B$)(N) (amides)							−177.75	111.50	
CO–(C$_B$)(N) (amino acids)							−177.75	37.00	
CO–(C$_d$)(N)	−171.80								
CO–(N)$_2$	−111.00	32.40	96.00	−190.50			−203.10	124.00	69.00
N–(H)$_2$(CO) (amides, ureas)	−63.00	17.00	88.25	−63.90	43.01		−65.25	−15.50	18.00
N–(H)$_2$(CO) (amino acids)	−63.00			−63.90	43.01		−59.75	45.88	33.03
N–(H)(C)(CO) (amides, ureas)	−16.28			−17.10	23.51		−9.80	−36.00	
N–(H)(C)(CO) (amino acids)	−16.28			−17.10	23.51		5.50	3.30	
N–(C)$_2$(CO)	45.00			62.00	13.93		55.00		
N–(H)(C$_B$)(CO)	−20.84						−3.50	−41.00	
N–(H)(CO)$_2$	−91.00						−30.80	−157.02	
N–(C)(CO)$_2$	−11.64			56.20			64.00		
N–(C$_B$)(CO)$_2$	9.12								
N–(C$_B$)$_2$(CO)							60.85		
N–(C)(C$_B$)(CO)							72.00		
C–(H)$_3$(CN), Acetonitrile	74.04	52.22	252.60	40.56	91.46	149.62			
C–(H)$_2$(C)(CN)	94.52	47.86	167.25	66.07	83.01	106.02	69.85	72.80	96.15
C–(H)(C)$_2$(CN)	113.50	44.94	67.86	81.50	83.09		69.00		
C–(C)$_3$(CN)	137.96			116.20	69.91	−17.91	102.07		
C–(C)$_2$(CN)$_2$								44.60	74.57
C–(H)$_2$(C$_d$)(CN)	95.31			66.40					
C$_d$–(H)(CN)	146.65	42.38	158.41	117.28	80.42	92.72			
C$_t$–(CN)	264.60			250.20					
C–(H)$_3$(NO$_2$), Nitromethane	−74.86	57.32	284.14	−112.60	105.98	171.75			
C–(H)$_2$(NO$_2$)$_2$, Dinitromethane	−58.90			−104.90					
C–(H)(NO$_2$)$_3$, Trinitromethane	−0.30			−32.80			−48.00		
C–(NO$_2$)$_4$, Tetranitromethane	82.30			38.30					
C–(H)$_2$(C)(NO$_2$)	−60.50	53.14	203.60	−93.50	97.74		−99.00		
C–(H)(C)$_2$(NO$_2$)	−53.00	49.58	115.32	−82.50			−89.00		
C–(C)$_3$(NO$_2$)	−36.65			−61.20			−76.55		
C–(H)$_2$(C$_B$)(NO$_2$)	−62.00			−82.76			−81.00		
C–(H)(C)(NO$_2$)$_2$	−36.80			−88.80			−91.50		
C–(C)$_2$(NO$_2$)$_2$	−28.50			−77.20			−90.30	71.38	
C–(H)(C)(CO)(N)	−18.70						−11.65	−22.85	−4.00
C–(H)$_2$(CO)(N)	−3.10						−30.95	21.92	24.00
C–(H)(C$_B$)(CO)(N)								61.21	

TABLE 2. Listing of groups and group values – Continued

Group	$\Delta_fH°$ (gas)	$C_p°$ (gas)	$S°$ (gas)	$\Delta_fH°$ (liq)	$C_p°$ (liq)	$S°$ (liq)	$\Delta_fH°$ (solid)	$C_p°$ (solid)	$S°$ (solid)
CHN and CHNO Groups									
O–(C)(NO)	−24.23	37.49	166.11	−46.50					
O–(C)(NO_2)	−79.71	51.46	191.92	−108.96	96.40	127.50	−124.00		
N–(H)(C)(NO_2)							−16.50	65.73	
N–(H)(C_B)(NO_2)								−47.53	
N–(H)(CO)(NO_2)							−14.00		
N–(C)(NO_2)$_2$	100.30			53.50					
N–(C)(C_B)(NO_2)	183.00			167.00			150.50		
N–(C)$_2$(NO)	90.00			59.00			55.00		
N–(C)$_2$(NO_2)	88.00			50.00			40.00		
C–(H)$_2$(C)(N_3)				321.70					
C–(H)(C)$_2$(N_3)	274.00			255.00					
C–(H)$_2$(C_B)(N_3)	347.00			327.40					
C–(C_B)$_3$(N_3)	328.60						346.50		
C_B–(N_3)(C_B)$_2$	320.00			303.50					
Zwitterion energy, aliphatic	0.00	0.00	0.00	0.00	0.00	0.00	−55.10	−44.50	−13.40
Zwitterion energy, aromatic I	0.00	0.00	0.00	0.00	0.00	0.00	−32.00	−20.50	−13.00
Zwitterion energy, aromatic II	0.00	0.00	0.00	0.00	0.00	0.00	−11.00	5.00	−9.00
Ethyleneimine rsc	115.53	−5.13	137.90	101.98					
Pyrrolidine rsc	26.71	−22.29	118.45	20.36	−24.48	42.40			
Piperidine rsc	3.14			−1.09	−29.79	15.98			
Hexamethyleneimine rsc					−36.86				
Octahydroazocine rsc					−42.31				
Pyrrolizidine rsc	35.42			18.87					
3,5-Dimethylpyrrolizidine rsc	38.46			20.05					
Trimethyl cyanurate rsc	−95.00						−120.40		
Succinimide rsc	25.70						16.70		
Glutarimide rsc	28.23						17.57		
Azetidine rsc	116.00			102.00					
Pyrrole rsc	−30.48			−20.03			−17.84		
Cyclotetramethylenediazene rsc	12.86			−4.34					
Cyclotrimethylenediazene rsc	−10.47						−23.97		
Cyclopropanenitrile rsc	110.56			110.76	−28.53				
Cyclobutanenitrile rsc	91.39			98.69	−28.35				
Cyclopentanenitrile rsc	10.82			22.12	−37.27				
Cyclohexanenitrile rsc	−5.55			−0.05	−57.29				
N–Nitrosopiperidine rsc	45.20			48.70					
N–Nitropiperidine rsc	−13.91			−4.11			8.48		
R-salt rsc							195.30		
RDX rsc	32.00						30.00		
HMX rsc	17.00						32.00		
DINO-PMTA rsc							46.70		
cis-Azobenzene corr	48.40						49.10		
Azidocyclopentane rsc	29.42			27.02					
Azidocyclohexane rsc	−16.45			−17.95					
NO_2–NO_2 (*ortho* corr)	44.00			45.25			40.60	3.76	
NO_2–NO_2 (*meta* corr)	11.00			13.50			13.50	5.84	
NO_2–CH_3 (*ortho* corr)	2.00			2.00			4.00		
NO_2–CH_3 (*meta* corr)				−4.00					
NO_2–OH (*ortho* corr)	10.00			16.00			13.00		
NO_2–OH (*meta* corr)	6.00						0.00		
NO_2–NO_2 (aliphatic-adjacent corr)	20.00			20.00			20.00		
NO_2–COOH (*ortho* corr)	25.00			30.00			25.00	0.00	
NO_2–COOH (*meta* corr)	14.00			16.00			14.00	0.00	

TABLE 2. Listing of groups and group values — Continued

Group	$\Delta_f H^\circ$ (gas)	C_p° (gas)	S° (gas)	$\Delta_f H^\circ$ (liq)	C_p° (liq)	S° (liq)	$\Delta_f H^\circ$ (solid)	C_p° (solid)	S° (solid)
				CHN and CHNO Groups					
NO_2–OH(*ortho* corr)	10.00			16.00			13.00		
NO_2–OH(*meta* corr)	6.00			0.00			0.00		
NH_2–NO_2 (*ortho* corr)	−4.00			−4.00			−4.00	0.00	
NH_2–NO_2 (*meta* corr)	−10.00			−10.00			−10.00		
(ONO_2)–(ONO_2)(aliphatic-adjacent corr)	15.10			15.90			16.00		
N_I–(CH_3) (*ortho* corr)	−6.30			−4.00					
N_I–N_I (*ortho* corr)	85.06			83.16					
CH_3–CN (*cis*, unsat corr)	−6.00			−6.00					
NH_2–NH_2 (*ortho* corr)							−3.00		
NH_2–NH_2 (*meta* corr)							−10.00		
NH_2–COOH (*ortho* corr)				12.00			14.00	−4.71	
NH_2–COOH (*meta* corr)				2.00			4.00	−7.22	
				CHS and CHSO Groups					
C–$(H)_3$(S)	−42.26	25.73	127.32	−47.61	36.48	83.30	−46.74	67.45	56.69
C–$(H)_2$(C)(S)	−23.17	20.90	41.87	−26.77	24.18	41.09			
C–(H)$(C)_2$(S)	−5.88	20.29	−47.36	−6.07	17.78	−16.61			
–CH_3 corr (tertiary)	−2.26	0.00	0.00	−2.18	0.00	0.00	−2.34	0.00	0.00
C–$(C)_3$(S)	13.52	17.02	−145.38	16.69	8.88	−86.86			
–CH_3 corr (quaternary)	−4.56	0.00	0.00	−4.39	0.00	0.00	−4.35	0.00	0.00
–CH_3 corr (tert/quat)	−1.80	0.00	0.00	−1.77	0.00	0.00	−2.70	0.00	0.00
–CH_3 corr (quat/quat)	−0.64	0.00	0.00	−0.64	0.00	0.00	−2.24	0.00	0.00
C–$(H)_2$(C_B)(S)	−18.53			−23.82					
C–$(H)_2$(C_d)(S)	−25.93			−32.44					
C–$(H)_2$$(S)_2$	−25.10								
C_B–(S)$(C_B)_2$	−4.75	15.86	43.72	−5.61	39.71	−10.59	1.00	−0.29	1.59
C_d–(H)(S)	36.32	18.74	33.05	31.05	24.60	28.58	25.48		
C_d–(C)(S)	45.73	14.64	−51.92						
S–(C)(H)	18.64	25.76	137.67	0.06	51.34	85.95			
S–(C_B)(H)	48.10	20.98	57.34	28.51	20.11	89.04			
S–$(C)_2$	46.99	22.64	55.19	29.82	45.15	29.80			
S–(H)(C_d)	25.52								
S–(C)(C_d)	54.39								
S–$(C_d)_2$	102.60	20.04	68.59						
S–(C_B)(C)	76.21			58.20	16.43	35.44	42.00		
S–(C)(S)	27.62	23.25	50.50	14.36	40.71	30.84			
S–(C_B)(S)	57.45						40.60		
S–$(S)_2$	12.59	19.66	56.07						
S–$(C_B)_2$	102.60	20.04	68.59	93.02	−35.10				
S–(H)(S)	7.95								
S–(H)(CO)	−5.90	31.92	130.54						
CO–(C)(S)	−132.67	23.43	64.31	−152.76	52.97	33.81		33.89	
C–$(H)_3$(SO)	−42.26	25.73	127.32	−47.61	36.48	83.30	−46.74	67.45	56.69
C–$(H)_2$(C)(SO)	−29.16			−36.88					
C–(H)$(C)_2$(SO)									
–CH_3 corr (tertiary)	−2.26	0.00	0.00	−2.18	0.00	0.00	−2.34	0.00	0.00
C–$(C)_3$(SO)	4.56			0.97					
–CH_3 corr (quaternary)	−4.56	0.00	0.00	−4.39	0.00	0.00	−4.35	0.00	0.00
C–$(H)_2$(C_d)(SO)	−27.56			−32.63					
cis correction	4.11	−8.03	5.06	5.27	0.00	0.00	5.73	0.00	0.00
C_B–(SO)$(C_B)_2$	15.48			25.44	4.39		7.55	−42.89	0.08
O–(SO)(H)	−158.60								
O–(C)(SO)	−92.60								

TABLE 2. Listing of groups and group values — Continued

Group	$\Delta_f H°$ (gas)	$C_p°$ (gas)	$S°$ (gas)	$\Delta_f H°$ (liq)	$C_p°$ (liq)	$S°$ (liq)	$\Delta_f H°$ (solid)	$C_p°$ (solid)	$S°$ (solid)
				CHS and CHSO Groups					
$SO-(C)_2$	−66.78	37.15	75.73	−108.98	80.22	22.18			
$SO-(C_B)_2$	−62.26								
$SO-(O)_2$	−213.00								
$SO-(C)(C_B)$	−72.00								
$C-(H)_3(SO_2)$	−42.26	25.73	127.32	−47.61	36.48	83.30	−46.74	67.45	56.69
$C-(H)_2(C)(SO_2)$	−27.03			−33.76			−35.96		
$C-(H)(C)_2(SO_2)$	−14.00								
$-CH_3$ corr (tertiary)	−2.26	0.00	0.00	−2.18	0.00	0.00	−2.34	0.00	0.00
$C-(C)_3(SO_2)$	1.52			2.00			3.78		
$-CH_3$ corr (quaternary)	−4.56	0.00	0.00	−4.39	0.00	0.00	−4.35	0.00	0.00
$-CH_3$ corr (quat/quat)	−0.64			−0.64			−2.24		
$C-(H)_2(C_d)(SO_2)$	−29.49			−49.05					
$C-(H)(C)(C_d)(SO_2)$	−71.99								
$C-(H)_2(C_B)(SO_2)$	−29.80								
$C-(H)_2(C_t)(SO_2)$	16.36								
$C_B-(SO_2)(C_B)_2$	15.48			25.44	4.39		7.55	−42.89	0.08
$C_d-(H)(SO_2)$	51.58								
$C_d-(C)(SO_2)$	64.01								
$C_t-(SO_2)$	177.10								
$SO_2-(C_d)(C_B)$	−291.55								
$SO_2-(C_d)_2$	−306.70								
$SO_2-(C)_2$	−288.58	48.54	87.37	−341.14			−356.62	−9.55	32.10
$SO_2-(C)(C_B)$	−289.10								
$SO_2-(C_B)_2$	−287.76						−305.40		
$SO_2-(SO_2)(C_B)$	−325.18						−361.75		
$SO_2-(O)_2$	−417.30								
$SO_2-(C)(C_d)$	−316.80								
$SO_2-(C_t)(C_B)$	−296.30								
$O-(SO_2)(H)$	−158.60								
$O-(C)(SO_2)$	−91.40								
Thiacyclopropane rsc	81.57	−10.76	122.10	75.32					
Thiacyclobutane rsc	80.98	−18.00	112.89	74.55	−10.54	40.57			
Thiacyclopentane rsc	6.41	−19.34	97.87	2.08	−14.19	31.08			
Thiacyclohexane rsc	−2.02	−24.91	66.85	−5.09	−21.47	9.12			
Thiacycloheptane rsc	20.53	−31.40	66.35	13.84					
2,5-Dihydrothiophene rsc	19.13			19.96					
Thiophene rsc	−43.54	−1.59	22.79						
2,3-Dihydrothiophene rsc	7.72								
				CHX and CHXO Groups					
$C-(H)_3(F)$, Methyl fluoride	−247.00	37.49	231.93						
$C-(H)_3(Cl)$, Methyl chloride	−81.90	40.75	243.60						
$C-(H)_3(Br)$, Methyl bromide	−37.66	42.43	254.94	−61.10					
$C-(H)_3(I)$, Methyl iodide	14.30	44.14	263.14	−11.70	82.76				
$C-(C)(F)_3$	−673.81	52.99	178.22	−709.07	73.18	135.56			
$C-(H)_2(C)(F)$	−221.12	33.66	146.80						
$C-(H)(C)_2(F)$	−204.46	30.55	55.76						
$C-(C)_3(F)$	−202.92								
$C-(H)(C)(F)_2$	−454.74	42.22	164.32	−487.23	68.04				
$C-(C)_2(F)_2$	−411.39	41.42	74.48	−400.37			−428.77		
$C-(C)(Cl)(F)_2$	−462.70	57.32	169.45	−466.00	83.64	138.31			
$C-(H)(C)(Cl)(F)$	−271.14								
$C-(C)(Cl)_3$	−81.98	68.18	202.14	−112.93	102.20	145.91			
$C-(H)(C)(Cl)_2$	−79.10	50.69	183.28	−102.60	85.02	128.45			

TABLE 2. Listing of groups and group values — Continued

Group	$\Delta_f H°$ (gas)	$C_p°$ (gas)	$S°$ (gas)	$\Delta_f H°$ (liq)	$C_p°$ (liq)	$S°$ (liq)	$\Delta_f H°$ (solid)	$C_p°$ (solid)	$S°$ (solid)
				CHX and CHXO Groups					
C–(H)$_2$(C)(Cl)	−69.45	37.53	159.24	−86.90	63.76	104.27	−85.65		
C–(C)$_2$(Cl)$_2$	−79.56	54.40	95.41	−101.80	74.24				
C–(H)(C)$_2$(Cl)	−55.61	35.00	71.34	−71.17	66.02				
C–(C)$_3$(Cl)	−43.70	29.63	−24.26	−56.78					
C–(C)(Br)$_3$		69.87	233.05						
C–(H)(C)(Br)$_2$									
C–(H)$_2$(C)(Br)	−21.78	37.82	173.31	−42.65	66.00	113.00			
C–(C)$_2$(Br)$_2$									
C–(H)(C)$_2$(Br)	−10.75	36.77	84.69	−27.31	59.24				
C–(C)$_3$(Br)	7.26	39.33	−13.46	−7.40					
C–(C)(I)$_3$									
C–(H)(C)(I)$_2$	108.78	51.04	228.45						
C–(H)$_2$(C)(I)	33.54	40.94	177.78	4.14	65.36		3.65		
C–(C)$_2$(I)$_2$									
C–(H)(C)$_2$(I)	48.74	38.62	88.10	24.78					
C–(C)$_3$(I)	68.46	41.09	−3.21	48.60					
C–(H)(C)(Br)(Cl)	−18.45	51.88	191.21						
N–(C)(F)$_2$	−32.64								
C–(H)(C)(Cl)(O)	−90.37	37.66	66.53						
C–(H)$_2$(I)(O)	15.90		170.29						
C–(C)(Cl)$_2$(F)	−322.54			−343.87	89.29	141.71			
C–(C)(Br)(F)$_2$	−394.55				85.40	149.70			
C–(C)(Br)$_2$(F)									
C–(Br)(Cl)(F)									
C$_d$–(H)(F)	−165.12	28.45	137.24						
C$_d$–(H)(Cl)	4.37	32.75	147.85	−12.67	56.62				
C$_d$–(H)(Br)	50.94	34.10	159.91		79.13				
C$_d$–(H)(I)	102.36	36.82	169.45						
C$_d$–(C)(Cl)	−5.06		62.76	−2.23					
C$_d$–(F)$_2$	−329.90	39.43	155.63						
C$_d$–(Cl)$_2$	−11.51	46.86	175.41	−32.08	76.47	115.35			
C$_d$–(Br)$_2$		51.46	199.16						
C$_d$–(I)$_2$									
C$_d$–(Cl)(F)	−235.10	44.50	175.61						
C$_d$–(Br)(F)		45.19	177.82						
C$_d$–(Cl)(Br)		50.63	188.70						
C$_t$–(F)									
C$_t$–(Cl)		33.01	140.00						
C$_t$–(Br)		34.69	151.30						
C$_t$–(I)	35.53	158.41							
C$_B$–(F)(C$_B$)$_2$	−181.26	26.10	67.52	−191.20	37.09	54.19	−194.00	32.05	39.79
C$_B$–(Cl)(C$_B$)$_2$	−17.03	29.33	77.08	−32.20	35.27	55.47	−32.00	33.55	43.37
C$_B$–(Br)(C$_B$)$_2$	36.35	29.65	88.60	19.90	40.91	74.85	13.50		54.45
C$_B$–(I)(C$_B$)$_2$	94.50	32.70	98.26	73.70	45.17	61.08	70.40	40.08	
cis corr-(I)(I)	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C–(H)$_2$(CO)(Cl)	−44.26			−58.41			−74.75		
C–(H)(CO)(Cl)$_2$	−40.40			−55.11					
CO–(C)(F)	−379.84			−419.59					
C–(C$_B$)(F)$_3$	−691.79	52.30	179.08	−696.66					
C–(H)$_2$(C$_B$)(Br)	−29.49			−44.06					
C–(H)$_2$(C$_B$)(I)	7.31			−7.24					
C–(H)$_2$(C$_B$)(Cl)	−73.79			−92.56					
CO–(C)(Cl)	−200.54	42.09	176.66	−225.29	80.67				
CO–(C$_B$)(Cl)				−216.67	69.21		−212.99		
CO–(C)(Br)	−148.54			−175.49					
CO–(C)(I)	−83.94			−117.09					

TABLE 2. Listing of groups and group values — Continued

Group	$\Delta_f H^\circ$ (gas)	C_p° (gas)	S° (gas)	$\Delta_f H^\circ$ (liq)	C_p° (liq)	S° (liq)	$\Delta_f H^\circ$ (solid)	C_p° (solid)	S° (solid)
				CHX and CHXO Groups					
C–(H)(C)(CO)(Cl)	−39.88			−35.46	49.45				
C–(C)(CO)(Cl)$_2$					74.22				
ortho corr-(I)(I)	7.56	0.00	0.00	6.96	0.00	0.00	5.50	0.00	0.00
ortho corr-(F)(F)	20.90	0.00	0.00	25.00	0.00	0.00	25.50	0.00	0.00
ortho corr-(Cl)(Cl)	9.50	0.00	0.00	14.00	0.00	0.00	8.50	0.00	0.00
ortho corr-(alkyl)(X)	2.51	0.00	0.00	6.30	0.00	0.00	0.00	0.00	0.00
cis corr-(Cl)(Cl)	−4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
cis corr-(CH$_3$)(Br)	−4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ortho corr-(F)(Cl)	13.50	0.00	0.00	18.50	0.00	0.00	19.50	0.00	0.00
ortho corr-(F)(Br)	37.25	0.00	0.00	40.60	0.00	0.00	42.50	0.00	0.00
ortho corr-(F)(I)	85.40	0.00	0.00	83.55	0.00	0.00	85.20	0.00	0.00
meta corr-(I)(I)	0.00	0.00	0.00	0.00	0.00	0.00	20.08	0.00	0.00
meta corr-(COCl)(COCl)	0.00	0.00	0.00	0.00	0.00	0.00	16.06	0.00	0.00
ortho corr-(COCl)(COCl)	0.00	0.00	0.00	0.00	10.58	0.00		0.00	0.00
ortho corr-(F)(CF$_3$)	111.00	0.00	0.00	112.00	0.00	0.00	0.00	0.00	0.00
meta corr-(F)(CF$_3$)	2.00	0.00	0.00	6.00	0.00	0.00	0.00	0.00	0.00
ortho corr-(F)(CH$_3$)	−3.30	0.00	0.00	−6.00	0.00	0.00	0.00	0.00	0.00
ortho corr-(F)(F')	8.00	0.00	0.00	8.00	0.00	0.00	8.00	0.00	0.00
ortho corr-(Cl)(Cl')	8.00	0.00	0.00	8.00	0.00	0.00	8.00	0.00	0.00
meta corr-(F)(F)	0.00	0.00	0.00	6.00	0.00	0.00	8.50	0.00	0.00
meta corr-(Cl)(Cl)	−5.00	0.00	0.00	10.00	0.00	0.00	4.00	0.00	0.00
ortho corr-(Cl)(CHO)	−6.75	0.00	0.00	8.50	0.00	0.00	0.00	0.00	0.00
ortho corr-(F)(COOH)	20.00	0.00	0.00	0.00	0.00	0.00	20.00	0.00	0.00
ortho corr-(Cl)(COCl)	0.00	0.00	0.00	34.43	0.00	0.00	0.00	0.00	0.00
ortho corr-(F)(OH)	25.50	0.00	0.00	23.00	0.00	0.00	20.00	0.00	0.00
ortho corr-(Cl)(COOH)	0.00	0.00	0.00	0.00	0.00	0.00	20.00	0.00	0.00
ortho corr-(Br)(COOH)	0.00	0.00	0.00	0.00	0.00	0.00	20.00	0.00	0.00
ortho corr-(I)(COOH)	0.00	0.00	0.00	0.00	0.00	0.00	20.00	0.00	0.00
ortho corr-(NH$_2$)(NH$_2$)	−10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
meta corr-(NH$_2$)(NH$_2$)	0.00	0.00	0.00	0.00	0.00	0.00	14.00	0.00	0.00
ortho corr-(OH)(Cl)	7.50	0.00	0.00	0.00	0.00	0.00	11.00	0.00	0.00
cis corr-(CH$_3$)(I)	−4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Group identities

C–(H)$_3$(C)	= C–(H)$_3$(C$_d$) = C–(H)$_3$(C$_t$) = C–(H)$_3$C$_B$) = C–(H)$_3$(O)
	= C–(H)$_3$(CO) = C–(H)$_3$(N) = C–(H)$_3$(N$_A$) = C–(H)$_3$(N$_I$)
	= C–(H)$_3$(S) = C–(H)$_3$(S) = C–(H)$_3$(SO$_2$)
C–(H)(C$_3$)	= C–(H)(C)(C$_d$)$_2$
C$_d$–(H)	= C$_d$–(H)(O) = C$_d$–(H)(S)
C$_d$–(H)(C$_d$)	= C$_d$–(H)(C$_t$) = C$_d$–(H)(C$_B$) = C$_d$–(O)(C$_d$)
C$_B$–(H)(C$_B$)$_2$	= C$_B$–(H)(O)(C$_B$) = C$_B$–(H)(N)(C$_B$) = C$_B$–(H)(N$_I$)(C$_B$)
	= C$_B$–(H)(S)(C$_B$) = C$_B$–(C)(O)(C$_B$) = C$_B$–(C)(N)(C$_B$)
	= C$_B$–(C)(S)(C$_B$)
C$_B$–(C$_d$)(C$_B$)$_2$	= C$_B$–(C$_t$)(C$_B$)$_2$
C$_B$–(SO)(C$_B$)$_2$	= C$_B$–(SO$_2$)(C$_B$)$_2$
S–(C$_d$)$_2$	= S–(C$_B$)$_2$

TABLE 3. General definitions and examples of notations for organic groups

C–(H)$_3$(C)	A carbon atom with three bonds to hydrogen atoms and the fourth bond to a carbon atom. Example: Ethane.
C–(H)$_2$(C)$_2$	A carbon atom with two bonds to hydrogen atoms and two bonds to carbon atoms. Example: *n*-Hexane.
C–(H)(C)$_3$	A carbon atom with one bond to a hydrogen atom and three bonds to carbon atoms. Example: 2-Methylpropane.
C–(C)$_4$	A carbon atom with four bonds to carbon atoms. Example: 2,2-Dimethylpropane.
C$_d$–(H)$_2$	A doubly-bonded carbon atom attached to two hydrogen atoms. Example: Ethylene.
C$_d$–(C)$_2$	A doubly-bonded carbon atom attached to two carbon atoms. Example: Propene.
C$_t$–(H)	A triply-bonded carbon atom attached to a hydrogen atom. Example: Ethyne.
C$_t$–(C)	A triply-bonded carbon atom attached to a carbon atom. Example: Propyne.
C$_B$–(H)(C$_B$)$_2$	An aromatic ring (benzene) carbon atom bonded to a hydrogen atom and two other aromatic ring carbon atoms. Example: Benzene.
C$_B$–(C$_B$)$_3$	An aromatic ring (benzene) carbon atom bonded to three aromatic ring carbon atoms. Example: Biphenyl.
C$_{BF}$–(C$_{BF}$)(C$_B$)$_2$	A fused aromatic ring carbon atom (such as the two fused ring carbon atoms in naphthalene) bonded to one other fused aromatic ring carbon atom and aromatic ring carbon atoms. Example: Naphthalene.
C$_{BF}$–(C$_{BF}$)$_3$	A fused aromatic ring carbon atom bonded to three other fused aromatic ring carbon atoms. Example: Pyrene.
C$_a$	An allenic carbon atom. When allene is unsubstituted, the group values are equal to allene itself. Example: Allene.
–CH$_3$ corr (tertiary)	A correction for the attachment of each methyl group to a tertiary carbon atom. Example: 2-Methylpropane.
–CH$_3$ corr (quaternary)	A correction for the attachment of each methyl group to a quaternary carbon atom. Example: 2,2-Dimethylpropane.
–CH$_3$ corr (tert/quat)	A correction for the attachment of each methyl group when there is both a tertiary and a quaternary carbon atom present in the longest chain of a hydrocarbon. Example: 2,2,3-Trimethylpentane.
–CH$_3$ corr (quat/quat)	A correction for the attachment of each methyl group when there are two quaternary carbon atoms present in the longest chain of a hydrocarbon. Example: 2,2,4,4-Tetramethylpentane.
ortho corr, hydrocarbons	An aromatic ring correction for *ortho* substitution in hydrocarbon compounds. Example: *o*-Xylene.
meta corr, hydrocarbons	An aromatic ring correction for *meta* substitution in hydrocarbon compounds. Example: *m*-Xylene.
rsc	Ring strain correction, rsc, for a cyclic non-aromatic compound. Example: Cyclopropane.
rsc (unsub)	Ring strain correction, rsc, for a cyclic non-aromatic unsubstituted compound. Example: Cyclopentane.
rsc (sub)	Ring strain correction, rsc, for a cyclic non-aromatic substituted compound. Example: Methylcyclopentane.

TABLE 3. General definitions and examples of notations for organic groups — Continued

C–(H)$_2$(C)(O)	A carbon atom bonded to two hydrogen atoms, a carbon atom, and an oxygen atom. Example: Methanol.
O–(C)$_2$	An oxygen atom bonded to two carbon atoms. Example: Dimethyl ether.
C–(H)(O)(C)$_2$ (alcohols, peroxides)	Tertiary carbon atom group in alcohols and peroxides. Example: 2-Propanol, *n*-Heptyl-2-hydroperoxide.
C–(H)(O)(C)$_2$ (ethers, esters)	Tertiary carbon atom group in ethers and esters. Example: Methylisopropyl ether, Isopropyl acetate.
C–(O)(C)$_3$ (alcohols, peroxides)	Quaternary carbon atom group in alcohols and peroxides. Example: *tert*-Butyl alcohol, *Di-tert*-butyl peroxide.
C–(O)(C)$_3$ (ethers, esters)	Quaternary carbon atom group in ethers and esters. Example: *Di-tert*-butyl ether, *tert*-Butyl acetate.
C–(H)$_2$(C)(CN)	A carbon atom bonded to two hydrogen atoms, a carbon atom, and a nitrile (cyano) group. Example: Propanenitrile.
CB–(NO$_2$)(CB)$_2$	An aromatic ring carbon atom bonded to a nitro group and two other aromatic ring carbon atoms. Example: Nitrobenzene.
NO$_2$–NO$_2$ (*ortho* corr)	A correction for adjacent (*ortho*) substitution of NO$_2$ groups on an aromatic ring. Example: *o*-Dintrobenzene.
NO$_2$–COOH (*ortho* corr)	A correction for substitution of an NO$_2$ group adjacent to a COOH group on an aromatic ring. Example: *o*-Nitrobenzoic acid.
N–(H)$_2$(C) (first, amino acids)	The first (and only) NH$_2$ group bonded to a carbon atom in an amino acid. Example: Glycine
N–(H)$_2$(C) (second, amino acids)	The second NH$_2$ group bonded to a carbon atom in an amino acid. Example: Lysine
N–(H)$_2$(CO) (amides, ureas)	A NH$_2$ group bonded to a carbonyl group, CO, in amides and ureas. Example: Acetamide, Urea.
N–(H)$_2$(CO) (amino acids)	A NH$_2$ group bonded to a carbonyl group, CO, in amino acids. Example: Asparagine
N–(H)(C)(CO) (amides, ureas)	A NH group bonded to a hydrogen atom, carbon atom, and a carbonyl group in amides and ureas. Example: *N*-Methylformamide, Methylurea.
N–(H)(C)(CO) (amino acids)	A NH group bonded to a hydrogen atom, carbon atom, and a carbonyl group in amino acids. Example: Glycylglycine.
Zwitterion energy, aliphatic	A correction for the conversion of an amino acid or to a zwitterion in amino acids and peptides with aliphatic moieties. Example: Glycine, Glycylalanine.
Zwitterion energy, aromatic I	A correction for the conversion of an aromatic amino acid or peptide to a zwitterion containing an aromatic ring attached directly to a conjugation detering group (such as a –CH$_2$– group). Example: Phenylalanine, Glycylphenylalanine.
Zwitterion energy, aromatic II	A correction for the conversion of an aromatic amino acid or peptide to a zwitterion containing an aromatic ring attached directly to a conjugation enhancing group (such as a >C=O group). Example: Hippuric acid, Hippurylglycine.

TABLE 3. General definitions and examples of notations for organic groups — Continued

N_A–(C)	A doubly-bonded (azo) nitrogen atom bonded to a carbon atom. Example: Azomethane.
N_A–(C_B)	A doubly-bonded (azo) nitrogen atom bonded to an aromatic ring carbon atom. Example: *trans*-Azobenzene.
N_A–(oxide)(C)	A doubly-bonded (azoxy) nitrogen atom bonded to a carbon atom. Example: *Di-tert*-butyldiazene *N*-oxide
N_I–(C)	A doubly-bonded (imino) nitrogen atom bonded to a carbon atom. Example: *N*-Butylisobutyleneimine.
N_I–(C_B)	A doubly-bonded (pyridine-type) nitrogen atom bonded to an aromatic ring carbon atom. Example: Pyridine.
N_I–(CH_3) (*ortho* corr)	A doubly-bonded (pyridine-type) nitrogen atom in an aromatic ring adjacent to a substituted methyl group. Example: 2-Picoline
N_I–N_I (*ortho* corr)	A doubly-bonded (pyridine-type) nitrogen atom adjacent to an identical (pyridine-type) nitrogen atom in an aromatic ring. Example: Pyridazine
C–$(H)_2$(C)(S)	A carbon atom bonded to two hydrogen atoms, a carbon atom, and a sulfur atom. Example: Methanethiol.
S–(C)(S)	A sulfur atom bonded to a carbon atom and another sulfur atom. Example: Dimethyl disulfide.
C–$(H)_2$(C)(F)	A carbon atom bonded to two hydrogen atoms, a carbon atom, and a fluorine atom. Example: Fluoroethane.
ortho corr, (F)(F)	A correction for the adjacent (*ortho*) substitution of two fluorine atoms on an aromatic ring. Example: *o*-Difluorobenzene.
ortho corr, (I)(COOH)	A correction for the substitution of a iodine atom adjacent (*ortho*) to a COOH group on an aromatic ring. Example: 2-iodobenzoic acid.
ortho corr (Cl)(Cl′)	A correction for the substitution of a chlorine atom in an aromatic ring in the near proximity of another chlorine atom in a different aromatic ring which is bonded to the first ring. Example: 2,2′-Dichlorobiphenyl

TABLE 4. *n*-Alkanes (25)

Methane CH_4

$(1\times C\text{-}(H)_4)$, $\sigma = 12$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−74.48	−74.48	0.00	72PIT/PIL
C_p° =	35.71	35.73	−0.02	89FRI/ELY
S° =	186.27	186.26	0.01	89FRI/ELY
$\Delta_f S^\circ$ =		−80.62		
$\Delta_f G^\circ$ =		−50.44		
$\ln K_f$ =		20.35		

Ethane C_2H_6

$(1\times 2\times C\text{-}(H)_3(C))$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−83.85	−83.85	0.00	72PIT/PIL
C_p° =	52.47	52.63	−0.16	73CHA/WIL
S° =	229.12	229.49	−0.37	73CHA/WIL
$\Delta_f S^\circ$ =		−173.71		
$\Delta_f G^\circ$ =		−32.06		
$\ln K_f$ =		12.93		

Propane C_3H_8

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−104.68	−105.15	0.47	72PIT/PIL
C_p° =	73.60	74.35	−0.75	73CHA/WIL
S° =	270.20	269.77	0.43	73CHA/WIL
$\Delta_f S^\circ$ =		−269.74		
$\Delta_f G^\circ$ =		−24.73		
$\ln K_f$ =		9.98		

Butane C_4H_{10}

$(2\times C\text{-}(H)_3(C))+(2\times C\text{-}(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−125.65	−125.78	0.13	72PIT/PIL
C_p° =	98.49	97.24	1.25	75CHE/WIL
S° =	309.91	308.93	0.98	75CHE/WIL
$\Delta_f S^\circ$ =		−366.89		
$\Delta_f G^\circ$ =		−16.39		
$\ln K_f$ =		6.61		

TABLE 4. *n*-Alkanes (25) – Continued

Pentane C_5H_{12}

$(2\times C\text{-}(H)_3(C))+(3\times C\text{-}(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−146.82	−146.41	−0.41	70GOO
C_p° =	120.21	120.13	0.08	69STU/WES
S° =	348.95	348.09	0.86	69STU/WES
$\Delta_f S^\circ$ =		−464.04		
$\Delta_f G^\circ$ =		−8.06		
$\ln K_f$ =		3.25		
Liquid phase				
$\Delta_f H^\circ$ =	−173.51	−172.41	−1.10	70GOO
C_p° =	167.19	164.22	2.97	67MES/GUT
S° =	263.47	263.74	−0.27	67MES/GUT
$\Delta_f S^\circ$ =		−548.39		
$\Delta_f G^\circ$ =		−8.91		
$\ln K_f$ =		3.59		

Hexane C_6H_{14}

$(2\times C\text{-}(H)_3(C))+(4\times C\text{-}(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−167.28	−167.04	−0.24	47OSB/GIN
C_p° =	143.09	143.02	0.07	69STU/WES
S° =	388.40	387.25	1.15	69STU/WES
$\Delta_f S^\circ$ =		−561.19		
$\Delta_f G^\circ$ =		0.28		
$\ln K_f$ =		−0.11		
Liquid phase				
$\Delta_f H^\circ$ =	−198.66	−198.14	−0.52	69GOO/SMI
C_p° =	194.97	194.64	0.33	46DOU/HUF
S° =	296.06	296.12	−0.06	46DOU/HUF
$\Delta_f S^\circ$ =		−652.32		
$\Delta_f G^\circ$ =		−3.65		
$\ln K_f$ =		1.47		

Heptane C_7H_{16}

$(2\times C\text{-}(H)_3(C))+(5\times C\text{-}(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−187.48	−187.67	0.19	47OSB/GIN
C_p° =	165.98	165.91	0.07	69STU/WES
S° =	427.90	426.41	1.49	69STU/WES
$\Delta_f S^\circ$ =		−658.34		
$\Delta_f G^\circ$ =		8.61		
$\ln K_f$ =		−3.47		

TABLE 4. *n*-Alkanes (25) – Continued

Heptane (Continued) C_7H_{16}
$(2\times C-(H)_3(C))+(5\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−224.05	−223.87	−0.18	44PRO/ROS
$C_p°$ =	224.93	225.06	−0.13	61HUF/GRO
$S°$ =	328.57	328.50	0.07	61HUF/GRO
$\Delta_fS°$ =		−756.25		
$\Delta_fG°$ =		1.61		
$\ln K_f$ =		−0.65		

Octane C_8H_{18}
$(2\times C-(H)_3(C))+(6\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−208.27	−208.30	0.03	47OSB/GIN
$C_p°$ =	188.87	188.80	0.07	69STU/WES
$S°$ =	466.73	465.57	1.16	69STU/WES
$\Delta_fS°$ =		−755.49		
$\Delta_fG°$ =		16.95		
$\ln K_f$ =		−6.84		
Liquid phase				
$\Delta_fH°$ =	−249.78	−249.60	−0.18	44PRO/ROS
$C_p°$ =	254.14	255.48	−1.34	54FIN/GRO2
$S°$ =	361.20	360.88	0.32	54FIN/GRO2
$\Delta_fS°$ =		−860.18		
$\Delta_fG°$ =		6.86		
$\ln K_f$ =		−2.77		

Nonane C_9H_{20}
$(2\times C-(H)_3(C))+(7\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−228.24	−228.93	0.69	47OSB/GIN
$C_p°$ =	211.71	211.69	0.02	69STU/WES
$S°$ =	505.68	504.73	0.95	69STU/WES
$\Delta_fS°$ =		−852.64		
$\Delta_fG°$ =		25.29		
$\ln K_f$ =		−10.20		
Liquid phase				
$\Delta_fH°$ =	−274.68	−275.33	0.65	69GOO
$C_p°$ =	284.39	285.90	−1.51	54FIN/GRO2
$S°$ =	393.67	393.26	0.41	54FIN/GRO2
$\Delta_fS°$ =		−964.11		
$\Delta_fG°$ =		12.12		
$\ln K_f$ =		−4.89		

TABLE 4. *n*-Alkanes (25) – Continued

Decane $C_{10}H_{22}$
$(2\times C-(H)_3(C))+(8\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−249.66	−249.56	−0.10	47OSB/GIN
$C_p°$ =	234.60	234.58	0.02	69STU/WES
$S°$ =	544.63	543.89	0.74	69STU/WES
$\Delta_fS°$ =		−949.79		
$\Delta_fG°$ =		33.62		
$\ln K_f$ =		−13.56		
Liquid phase				
$\Delta_fH°$ =	−300.62	−301.06	0.44	44PRO/ROS
$C_p°$ =	314.47	316.32	−1.85	54FIN/GRO2
$S°$ =	425.89	425.64	0.25	54FIN/GRO2
$\Delta_fS°$ =		−1068.04		
$\Delta_fG°$ =		17.38		
$\ln K_f$ =		−7.01		

Undecane $C_{11}H_{24}$
$(2\times C-(H)_3(C))+(9\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−270.91	−270.19	−0.72	45PRO/ROS2
$C_p°$ =	257.44	257.47	−0.03	69STU/WES
$S°$ =	583.58	583.05	0.53	69STU/WES
$\Delta_fS°$ =		−1046.94		
$\Delta_fG°$ =		41.96		
$\ln K_f$ =		−16.92		
Liquid phase				
$\Delta_fH°$ =	−326.60	−326.79	0.19	45PRO/ROS2
$C_p°$ =	345.05	346.74	−1.69	54FIN/GRO2
$S°$ =	458.15	458.02	0.13	54FIN/GRO2
$\Delta_fS°$ =		−1171.97		
$\Delta_fG°$ =		22.63		
$\ln K_f$ =		−9.13		

Dodecane $C_{12}H_{26}$
$(2\times C-(H)_3(C))+(10\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−290.87	−290.82	−0.05	45PRO/ROS2
$C_p°$ =	280.33	280.36	−0.03	69STU/WES
$S°$ =	622.50	622.21	0.29	69STU/WES
$\Delta_fS°$ =		−1144.10		
$\Delta_fG°$ =		50.29		
$\ln K_f$ =		−20.29		

TABLE 4. *n*-Alkanes (25) — Continued

Dodecane (Continued) $C_{12}H_{26}$

$(2\times C-(H)_3(C))+(10\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−352.13	−352.52	0.39	45PRO/ROS2
$C_p°$ =	375.97	377.16	−1.19	54FIN/GRO2
$S°$ =	490.66	490.40	0.26	54FIN/GRO2
$\Delta_fS°$ =		−1275.90		
$\Delta_fG°$ =		27.89		
$\ln K_f$ =		−11.25		

Tridecane $C_{13}H_{28}$

$(2\times C-(H)_3(C))+(11\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−311.50	−311.45	−0.05	45PRO/ROS2
$C_p°$ =	303.21	303.25	−0.04	69STU/WES
$S°$ =	661.45	661.37	0.08	69STU/WES
$\Delta_fS°$ =		−1241.25		
$\Delta_fG°$ =		58.63		
$\ln K_f$ =		−23.65		
Liquid phase				
$\Delta_fH°$ =	−377.69	−378.25	0.56	45PRO/ROS2
$C_p°$ =	406.89	407.58	−0.69	54FIN/GRO2
$S°$ =	522.87	522.78	0.09	54FIN/GRO2
$\Delta_fS°$ =		−1379.83		
$\Delta_fG°$ =		33.15		
$\ln K_f$ =		−13.37		

Tetradecane $C_{14}H_{30}$

$(2\times C-(H)_3(C))+(12\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−332.13	−332.08	−0.05	45PRO/ROS2
$C_p°$ =	326.06	326.14	−0.08	69STU/WES
$S°$ =	700.40	700.53	−0.13	69STU/WES
$\Delta_fS°$ =		−1338.40		
$\Delta_fG°$ =		66.96		
$\ln K_f$ =		−27.01		
Liquid phase				
$\Delta_fH°$ =	−403.25	−403.98	0.73	45PRO/ROS2
$C_p°$ =	438.44	438.00	0.44	54FIN/GRO2
$S°$ =	555.43	555.16	0.27	54FIN/GRO2
$\Delta_fS°$ =		−1483.76		
$\Delta_fG°$ =		38.40		
$\ln K_f$ =		−15.49		

TABLE 4. *n*-Alkanes (25) — Continued

Pentadecane $C_{15}H_{32}$

$(2\times C-(H)_3(C))+(13\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−352.75	−352.71	−0.04	45PRO/ROS2
$C_p°$ =	348.95	349.03	−0.08	69STU/WES
$S°$ =	739.35	739.69	−0.34	69STU/WES
$\Delta_fS°$ =		−1435.55		
$\Delta_fG°$ =		75.30		
$\ln K_f$ =		−30.37		
Liquid phase				
$\Delta_fH°$ =	−428.82	−429.71	0.89	45PRO/ROS2
$C_p°$ =	469.95	468.42	1.53	54FIN/GRO2
$S°$ =	587.52	587.54	−0.02	54FIN/GRO2
$\Delta_fS°$ =		−1587.70		
$\Delta_fG°$ =		43.66		
$\ln K_f$ =		−17.61		

Hexadecane $C_{16}H_{34}$

$(2\times C-(H)_3(C))+(14\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−374.76	−373.34	−1.42	72MOR
$C_p°$ =	371.79	371.92	−0.13	69STU/WES
$S°$ =	778.31	778.85	−0.54	69STU/WES
$\Delta_fS°$ =		−1532.70		
$\Delta_fG°$ =		83.63		
$\ln K_f$ =		−33.74		
Liquid phase				
$\Delta_fH°$ =	−456.14	−455.44	−0.70	55FRA/PRO
$C_p°$ =	501.45	498.84	2.61	54FIN/GRO2
$S°$ =	619.65	619.92	−0.27	54FIN/GRO2
$\Delta_fS°$ =		−1691.63		
$\Delta_fG°$ =		48.92		
$\ln K_f$ =		−19.73		
Solid phase				
$\Delta_fH°$ =	−507.50	−505.22	−2.28	69STU/WES
$C_p°$ =	441.79	441.78	0.01	
$S°$ =	434.84	435.52	−0.68	
$\Delta_fS°$ =		−1876.03		
$\Delta_fG°$ =		54.12		
$\ln K_f$ =		−21.83		

TABLE 4. *n*-Alkanes (25) — Continued

Heptadecane $C_{17}H_{36}$
$(2\times C-(H)_3(C))+(15\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−393.92	−393.97	0.05	45PRO/ROS2
$C_p°$ =	394.68	394.81	−0.13	69STU/WES
$S°$ =	817.26	818.01	−0.75	69STU/WES
$\Delta_fS°$ =		−1629.85		
$\Delta_fG°$ =		91.97		
$\ln K_f$ =		−37.10		
Liquid phase				
$\Delta_fH°$ =	−479.86	−481.17	1.31	45PRO/ROS2
$C_p°$ =	534.34	529.26	5.08	67MES/GUT
$S°$ =	652.24	652.30	−0.06	67MES/GUT
$\Delta_fS°$ =		−1795.56		
$\Delta_fG°$ =		54.18		
$\ln K_f$ =		−21.85		
Solid phase				
$\Delta_fH°$ =	−530.97	−534.63	3.66	67MES/GUT
$C_p°$ =		463.70		
$S°$ =		458.53		
$\Delta_fS°$ =		−1989.33		
$\Delta_fG°$ =		58.49		
$\ln K_f$ =		−23.59		

Octadecane $C_{18}H_{38}$
$(2\times C-(H)_3(C))+(16\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−414.55	−414.60	0.05	45PRO/ROS2
$C_p°$ =	417.56	417.70	−0.14	69STU/WES
$S°$ =	856.21	857.17	−0.96	69STU/WES
$\Delta_fS°$ =		−1727.00		
$\Delta_fG°$ =		100.31		
$\ln K_f$ =		−40.46		
Liquid phase				
$\Delta_fH°$ =	−505.43	−506.90	1.47	45PRO/ROS2
$C_p°$ =		559.68		
$S°$ =		684.68		
$\Delta_fS°$ =		−1899.49		
$\Delta_fG°$ =		59.43		
$\ln K_f$ =		−23.97		
Solid phase				
$\Delta_fH°$ =	−567.14	−564.04	−3.10	67MES/GUT
$C_p°$ =	485.64	485.62	0.02	67MES/GUT
$S°$ =	480.20	481.54	−1.34	67MES/GUT
$\Delta_fS°$ =		−2102.63		
$\Delta_fG°$ =		62.86		
$\ln K_f$ =		−25.36		

TABLE 4. *n*-Alkanes (25) — Continued

Nonadecane $C_{19}H_{40}$
$(2\times C-(H)_3(C))+(17\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−435.14	−435.23	0.09	45PRO/ROS2
$C_p°$ =	440.41	440.59	−0.18	69STU/WES
$S°$ =	895.17	896.33	−1.16	69STU/WES
$\Delta_fS°$ =		−1824.15		
$\Delta_fG°$ =		108.64		
$\ln K_f$ =		−43.83		
Liquid phase				
$\Delta_fH°$ =	−530.95	−532.63	1.68	45PRO/ROS2
$C_p°$ =		590.10		
$S°$ =		717.06		
$\Delta_fS°$ =		−2003.42		
$\Delta_fG°$ =		64.69		
$\ln K_f$ =		−26.10		
Solid phase				
$\Delta_fH°$ =		−593.45		
$C_p°$ =		507.54		
$S°$ =		504.55		
$\Delta_fS°$ =		−2215.93		
$\Delta_fG°$ =		67.23		
$\ln K_f$ =		−27.12		

Eicosane $C_{20}H_{42}$
$(2\times C-(H)_3(C))+(18\times C-(H)_2(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−455.76	−455.86	0.10	45PRO/ROS2
$C_p°$ =	463.29	463.48	−0.19	69STU/WES
$S°$ =	934.12	935.49	−1.37	69STU/WES
$\Delta_fS°$ =		−1921.30		
$\Delta_fG°$ =		116.98		
$\ln K_f$ =		−47.19		
Liquid phase				
$\Delta_fH°$ =	−556.51	−558.36	1.85	45PRO/ROS2
$C_p°$ =		620.52		
$S°$ =		749.44		
$\Delta_fS°$ =		−2107.35		
$\Delta_fG°$ =		69.95		
$\ln K_f$ =		−28.22		
Solid phase				
$\Delta_fH°$ =		−622.86		
$C_p°$ =	479.90	529.46	−49.56	30PAR/HUF
$S°$ =	558.56	527.56	31.00	30PAR/HUF
$\Delta_fS°$ =		−2329.23		
$\Delta_fG°$ =		71.60		
$\ln K_f$ =		−28.88		

TABLE 4. *n*-Alkanes (25) — Continued

Tetracosane $C_{24}H_{50}$
$(2\times C-(H)_3(C))+(22\times C-(H)_2(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−538.38		
C_p° =		555.04		
Liquid phase				
$\Delta_f H^\circ$ =		−661.28		
C_p° =		742.20		
S° =		878.96		
$\Delta_f S^\circ$ =		−2523.07		
$\Delta_f G^\circ$ =		90.97		
$\ln K_f$ =		−36.70		
Solid phase				
$\Delta_f H^\circ$ =		−740.50		
C_p° =	730.94	617.14	113.80	49PAR/MOO
S° =	651.03	619.60	31.43	49PAR/MOO
$\Delta_f S^\circ$ =		−2782.44		
$\Delta_f G^\circ$ =		89.08		
$\ln K_f$ =		−35.94		

Pentacosane $C_{25}H_{52}$
$(2\times C-(H)_3(C))+(23\times C-(H)_2(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−559.01		
C_p° =		577.93		
Liquid phase				
$\Delta_f H^\circ$ =		−687.01		
C_p° =		772.62		
S° =		911.34		
$\Delta_f S^\circ$ =		−2627.01		
$\Delta_f G^\circ$ =		96.23		
$\ln K_f$ =		−38.82		
Solid phase				
$\Delta_f H^\circ$ =		−769.91		
C_p° =	769.02	639.06	129.96	30PAR/HUF
S° =	671.11	642.61	28.50	30PAR/HUF
$\Delta_f S^\circ$ =		−2895.74		
$\Delta_f G^\circ$ =		93.45		
$\ln K_f$ =		−37.70		

TABLE 4. *n*-Alkanes (25) — Continued

Hexacosane $C_{26}H_{54}$
$(2\times C-(H)_3(C))+(24\times C-(H)_2(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−579.64		
C_p° =		600.82		
Liquid phase				
$\Delta_f H^\circ$ =		−712.74		
C_p° =		803.04		
S° =		943.72		
$\Delta_f S^\circ$ =		−2730.94		
$\Delta_f G^\circ$ =		101.49		
$\ln K_f$ =		−40.94		
Solid phase				
$\Delta_f H^\circ$ =		−799.32		
C_p° =	661.20	660.98	0.22	76AND/MAR
S° =	667.01	665.62	1.39	76AND/MAR
$\Delta_f S^\circ$ =		−3009.04		
$\Delta_f G^\circ$ =		97.82		
$\ln K_f$ =		−39.46		

Dotriacontane $C_{32}H_{66}$
$(2\times C-(H)_3(C))+(30\times C-(H)_2(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−703.42		
C_p° =		738.16		
Liquid phase				
$\Delta_f H^\circ$ =		−867.12		
C_p° =		985.56		
S° =		1138.00		
$\Delta_f S^\circ$ =		−3354.52		
$\Delta_f G^\circ$ =		133.03		
$\ln K_f$ =		−53.66		
Solid phase				
$\Delta_f H^\circ$ =	−968.34	−975.78	7.44	31BEC
C_p° =	877.38	792.50	84.88	49PAR/MOO
S° =	851.44	803.68	47.76	49PAR/MOO
$\Delta_f S^\circ$ =		−3688.84		
$\Delta_f G^\circ$ =		124.05		
$\ln K_f$ =		−50.04		

TABLE 4. n-Alkanes (25) – Continued

Tritriacontane $C_{33}H_{68}$
$(2 \times C-(H)_3(C)) + (31 \times C-(H)_2(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−724.05		
C_p° =		761.05		
Liquid phase				
$\Delta_f H^\circ$ =		−892.85		
C_p° =		1015.98		
S° =		1170.38		
$\Delta_f S^\circ$ =		−3458.45		
$\Delta_f G^\circ$ =		138.29		
$\ln K_f$ =		−55.78		
Solid phase				
$\Delta_f H^\circ$ =		−1005.19		
C_p° =	900.82	814.42	86.40	30PAR/HUF
S° =	877.80	826.69	51.11	30PAR/HUF
$\Delta_f S^\circ$ =		−3802.14		
$\Delta_f G^\circ$ =		128.42		
$\ln K_f$ =		−51.80		

TABLE 5. t-Alkanes (35)

2-Methylpropane C_4H_{10}
$(3 \times C-(H)_3(C)) + (1 \times C-(H)(C)_3) + (3 \times -CH_3$ corr (tertiary)), $\sigma = 81$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H^\circ$ =	−134.18	−134.73	0.55	72PIT/PIL
C_p° =	96.65	97.27	−0.62	75CHE/WIL
S° =	295.39	291.82	3.57	75CHE/WIL
$\Delta_f S^\circ$ =		−383.99		
$\Delta_f G^\circ$ =		−20.24		
$\ln K_f$ =		8.17		

2-Methylbutane C_5H_{12}
$(3 \times C-(H)_3(C)) + (1 \times C-(H)_2(C)_2) + (1 \times C-(H)(C)_3) + (2 \times -CH_3$ corr (tertiary)), $\sigma = 27$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H^\circ$ =	−152.93	−153.10	0.17	70GOO
C_p° =	118.78	120.16	−1.38	69STU/WES
S° =	343.59	340.12	3.47	69STU/WES
$\Delta_f S^\circ$ =		−472.01		
$\Delta_f G^\circ$ =		−12.37		
$\ln K_f$ =		4.99		
Liquid Phase				
$\Delta_f H^\circ$ =	−178.91	−177.69	−1.22	70GOO
C_p° =	164.85	161.24	3.61	43GUT/HUF
S° =	260.41	258.39	2.02	43GUT/HUF
$\Delta_f S^\circ$ =		−553.74		
$\Delta_f G^\circ$ =		−12.59		
$\ln K_f$ =		5.08		

2-Methylpentane C_6H_{14}
$(3 \times C-(H)_3(C)) + (2 \times C-(H)_2(C)_2) + (1 \times C-(H)(C)_3) + (2 \times -CH_3$ corr (tertiary)), $\sigma = 27$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H^\circ$ =	−174.77	−173.73	−1.04	49WAD/SMI
C_p° =	144.18	143.05	1.13	69STU/WES
S° =	380.53	379.28	1.25	69STU/WES
$\Delta_f S^\circ$ =		−569.16		
$\Delta_f G^\circ$ =		−4.03		
$\ln K_f$ =		1.63		
Liquid Phase				
$\Delta_f H^\circ$ =	−204.64	−203.42	−1.22	41PRO/ROS
C_p° =	193.72	191.66	2.06	46DOU/HUF
S° =	290.58	290.77	−0.19	46DOU/HUF
$\Delta_f S^\circ$ =		−657.67		
$\Delta_f G^\circ$ =		−7.34		
$\ln K_f$ =		2.96		

TABLE 5. *t*-Alkanes (35) — Continued

2-Methylhexane C_7H_{16}

$(3\times C\text{-}(H)_3(C)) + (3\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)(C)_3) + (2\times\text{-}CH_3 \text{ corr (tertiary)}), \sigma = 27$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−194.64	−194.36	−0.28	86TRC
$C_p°$ =	165.98	165.94	0.04	69STU/WES
$S°$ =	419.99	418.44	1.55	69STU/WES
$\Delta_f S°$ =		−666.31		
$\Delta_f G°$ =		4.30		
$\ln K_f$ =		−1.73		
Liquid phase				
$\Delta_f H°$ =	−229.49	−229.15	−0.34	41PRO/PRS2
$C_p°$ =	222.92	222.08	0.84	61HUF/GRO
$S°$ =	323.34	323.15	0.19	61HUF/GRO
$\Delta_f S°$ =		−761.60		
$\Delta_f G°$ =		−2.08		
$\ln K_f$ =		0.84		

2-Methylheptane C_8H_{18}

$(3\times C\text{-}(H)_3(C)) + (4\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)(C)_3) + (2\times\text{-}CH_3 \text{ corr (tertiary)}), \sigma = 27$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−215.35	−214.99	−0.36	47OSB/GIN
$C_p°$ =	188.87	188.83	0.04	69STU/WES
$S°$ =	455.26	457.60	−2.34	69STU/WES
$\Delta_f S°$ =		−763.46		
$\Delta_f G°$ =		12.64		
$\ln K_f$ =		−5.10		
Liquid phase				
$\Delta_f H°$ =	−255.01	−254.88	−0.13	45PRO/ROS
$C_p°$ =	252.00	252.50	−0.50	71MES/FIN
$S°$ =	356.39	355.53	0.86	71MES/FIN
$\Delta_f S°$ =		−865.53		
$\Delta_f G°$ =		3.18		
$\ln K_f$ =		−1.28		

2-Methyloctane C_9H_{20}

$(3\times C\text{-}(H)_3(C)) + (5\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)(C)_3) + (2\times\text{-}CH_3 \text{ corr (tertiary)}), \sigma = 27$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−235.62		
$C_p°$ =	217.07	211.72	5.35	69STU/WES
$S°$ =	495.89	496.76	−0.87	69STU/WES
$\Delta_f S°$ =		−860.61		
$\Delta_f G°$ =		20.97		
$\ln K_f$ =		−8.46		

TABLE 5. t-Alkanes (35) — Continued

2-Methyloctane (Continued) C_9H_{20}

$(3\times C\text{-}(H)_3(C)) + (5\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)(C)_3) + (2\times\text{-}CH_3 \text{ corr (tertiary)}), \sigma = 27$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		−280.61		
$C_p°$ =		282.92		
$S°$ =		387.91		
$\Delta_f S°$ =		−969.46		
$\Delta_f G°$ =		8.43		
$\ln K_f$ =		−3.40		

2-Methylnonane $C_{10}H_{22}$

$(3\times C\text{-}(H)_3(C)) + (6\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)(C)_3) + (2\times\text{-}CH_3 \text{ corr (tertiary)}), \sigma = 27$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−256.25		
$C_p°$ =	242.09	234.61	7.48	69STU/WES
$S°$ =	534.46	535.92	−1.46	69STU/WES
$\Delta_f S°$ =		−957.76		
$\Delta_f G°$ =		29.31		
$\ln K_f$ =		−11.82		
Liquid phase				
$\Delta_f H°$ =		−306.34		
$C_p°$ =	313.30	313.34	−0.04	41PAR/WES
$S°$ =	420.07	420.29	−0.22	41PAR/WES
$\Delta_f S°$ =		−1073.39		
$\Delta_f G°$ =		13.69		
$\ln K_f$ =		−5.52		

2-Methyldecane $C_{11}H_{24}$

$(3\times C\text{-}(H)_3(C)) + (7\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)(C)_3) + (2\times\text{-}CH_3 \text{ corr (tertiary)})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−276.88		
$C_p°$ =		257.50		
Liquid phase				
$\Delta_f H°$ =		−332.07		
$C_p°$ =	341.21	343.76	−2.55	71MES/FIN
$S°$ =	453.80	452.67	1.13	71MES/FIN
$\Delta_f S°$ =		−1177.32		
$\Delta_f G°$ =		18.95		
$\ln K_f$ =		−7.64		

TABLE 5. t-Alkanes (35) – Continued

3-Methylpentane C_6H_{14}

$(3\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)(C)_3)+(1\times -CH_3$ corr (tertiary)), $\sigma = 54$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−172.09	−171.47	−0.62	49WAD/SMI
$C_p°$ =	143.09	143.05	0.04	69STU/WES
$S°$ =	379.78	373.51	6.27	69STU/WES
$\Delta_fS°$ =		−574.92		
$\Delta_fG°$ =		−0.06		
$\ln K_f$ =		0.02		
Liquid phase				
$\Delta_fH°$ =	−202.38	−201.24	−1.14	41PRO/ROS
$C_p°$ =	190.66	191.66	−1.00	73MES/FIN
$S°$ =	292.55	290.77	1.78	73MES/FIN
$\Delta_fS°$ =		−657.67		
$\Delta_fG°$ =		−5.16		
$\ln K_f$ =		2.08		

3-Methylhexane C_7H_{16}

$(3\times C-(H)_3(C))+(3\times C-(H)_2(C)_2)+(1\times C-(H)(C)_3)+(1\times -CH_3$ corr (tertiary)), $\sigma = 27$, $\eta = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−191.33	−192.10	0.77	86TRC
$C_p°$ =	165.98	165.94	0.04	69STU/WES
$S°$ =	424.13	424.20	−0.07	69STU/WES
$\Delta_fS°$ =		−660.55		
$\Delta_fG°$ =		4.84		
$\ln K_f$ =		−1.95		
Liquid phase				
$\Delta_fH°$ =	−226.44	−226.97	0.53	41PRO/ROS2
$C_p°$ =	218.00	222.08	−4.08	30HUF/PAR2
$S°$ =	309.60	323.15	−13.55	30HUF/PAR2
$\Delta_fS°$ =		−761.60		
$\Delta_fG°$ =		0.10		
$\ln K_f$ =		−0.04		

3-Methylheptane C_8H_{18}

$(3\times C-(H)_3(C))+(4\times C-(H)_2(C)_2)+(1\times C-(H)(C)_3)+(1\times -CH_3$ corr (tertiary)), $\sigma = 27$, $\eta = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−212.51	−212.73	0.22	47OSB/GIN
$C_p°$ =	188.87	188.83	0.04	69STU/WES
$S°$ =	461.58	463.36	−1.78	69STU/WES
$\Delta_fS°$ =		−757.70		
$\Delta_fG°$ =		13.18		
$\ln K_f$ =		−5.32		

TABLE 5. t-Alkanes (35) – Continued

3-Methylheptane (Continued) C_8H_{18}

$(3\times C-(H)_3(C))+(4\times C-(H)_2(C)_2)+(1\times C-(H)(C)_3)+(1\times -CH_3$ corr (tertiary)), $\sigma = 27$, $\eta = 2$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−252.34	−252.70	0.36	45PRO/ROS
$C_p°$ =	250.20	252.50	−2.30	73FIN/MES
$S°$ =	362.63	355.53	7.10	73FIN/MES
$\Delta_fS°$ =		−865.53		
$\Delta_fG°$ =		5.36		
$\ln K_f$ =		−2.16		

3-Methyloctane C_9H_{20}

$(3\times C-(H)_3(C))+(5\times C-(H)_2(C)_2)+(1\times C-(H)(C)_3)+(1\times -CH_3$ corr (tertiary)), $\sigma = 27$, $\eta = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−233.36		
$C_p°$ =	212.59	211.72	0.87	69STU/WES
$S°$ =	501.66	502.52	−0.86	69STU/WES
$\Delta_fS°$ =		−854.85		
$\Delta_fG°$ =		21.51		
$\ln K_f$ =		−8.68		
Liquid phase				
$\Delta_fH°$ =		−278.43		
$C_p°$ =		282.92		
$S°$ =		387.91		
$\Delta_fS°$ =		−969.46		
$\Delta_fG°$ =		10.61		
$\ln K_f$ =		−4.28		

3-Methylnonane $C_{10}H_{22}$

$(3\times C-(H)_3(C))+(6\times C-(H)_2(C)_2)+(1\times C-(H)(C)_3)+(1\times -CH_3$ corr (tertiary)), $\sigma = 27$, $\eta = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−253.99		
$C_p°$ =	237.61	234.61	3.00	69STU/WES
$S°$ =	540.24	541.68	−1.44	69STU/WES
$\Delta_fS°$ =		−952.00		
$\Delta_fG°$ =		29.85		
$\ln K_f$ =		−12.04		
Liquid phase				
$\Delta_fH°$ =		−304.16		
$C_p°$ =	308.99	313.34	−4.35	41PAR/WES
$S°$ =	427.19	420.29	6.90	41PAR/WES
$\Delta_fS°$ =		−1073.39		
$\Delta_fG°$ =		15.87		
$\ln K_f$ =		−6.40		

TABLE 5. *t*-Alkanes (35) — Continued

4-Methylheptane C_8H_{18}
(3 × C-(H)$_3$(C)) + (4 × C-(H)$_2$(C)$_2$) + (1 × C-(H)(C)$_3$) + (1 × -CH$_3$ corr (tertiary)), $\sigma = 54$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−211.96	−212.73	0.77	47OSB/GIN
$C_p°$ =	188.87	188.83	0.04	69STU/WES
$S°$ =	453.34	451.83	1.51	69STU/WES
$\Delta_fS°$ =		−769.23		
$\Delta_fG°$ =		16.61		
$\ln K_f$ =		−6.70		
Liquid phase				
$\Delta_fH°$ =	−251.63	−252.70	1.07	45PRO/ROS
$C_p°$ =	251.09	252.50	−1.41	47OSB/GIN
$S°$ =		355.53		
$\Delta_fS°$ =		−865.53		
$\Delta_fG°$ =		5.36		
$\ln K_f$ =		−2.16		

4-Methyloctane C_9H_{20}
(3 × C-(H)$_3$(C)) + (5 × C-(H)$_2$(C)$_2$) + (1 × C-(H)(C)$_3$) + (1 × -CH$_3$ corr (tertiary)), $\sigma = 27$, $\eta = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−233.36		
$C_p°$ =	212.59	211.72	0.87	69STU/WES
$S°$ =	501.66	502.52	−0.86	69STU/WES
$\Delta_fS°$ =		−854.85		
$\Delta_fG°$ =		21.51		
$\ln K_f$ =		−8.68		
Liquid phase				
$\Delta_fH°$ =		−278.43		
$C_p°$ =		282.92		
$S°$ =		387.91		
$\Delta_fS°$ =		−969.46		
$\Delta_fG°$ =		10.61		
$\ln K_f$ =		−4.28		

4-Methylnonane $C_{10}H_{22}$
(3 × C-(H)$_3$(C)) + (6 × C-(H)$_2$(C)$_2$) + (1 × C-(H)(C)$_3$) + (1 × -CH$_3$ corr (tertiary)), $\sigma = 27$, $\eta = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−253.99		
$C_p°$ =	237.61	234.61	3.00	69STU/WES
$S°$ =	540.24	541.68	−1.44	69STU/WES
$\Delta_fS°$ =		−952.00		
$\Delta_fG°$ =		29.85		
$\ln K_f$ =		−12.04		

TABLE 5. *t*-Alkanes (35) — Continued

4-Methylnonane (Continued) $C_{10}H_{22}$
(3 × C-(H)$_3$(C)) + (6 × C-(H)$_2$(C)$_2$) + (1 × C-(H)(C)$_3$) + (1 × -CH$_3$ corr (tertiary)), $\sigma = 27$, $\eta = 2$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−304.16		
$C_p°$ =	317.36	313.34	4.02	41PAR/WES
$S°$ =	425.51	420.29	5.22	41PAR/WES
$\Delta_fS°$ =		−1073.39		
$\Delta_fG°$ =		15.87		
$\ln K_f$ =		−6.40		

5-Methylnonane $C_{10}H_{22}$
(3 × C-(H)$_3$(C)) + (6 × C-(H)$_2$(C)$_2$) + (1 × C-(H)(C)$_3$) + (1 × -CH$_3$ corr (tertiary)), $\sigma = 54$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−253.99		
$C_p°$ =	237.61	234.61	3.00	69STU/WES
$S°$ =	534.46	530.15	4.31	69STU/WES
$\Delta_fS°$ =		−963.53		
$\Delta_fG°$ =		33.29		
$\ln K_f$ =		−13.43		
Liquid phase				
$\Delta_fH°$ =		−304.16		
$C_p°$ =	314.43	313.34	1.09	41PAR/WES
$S°$ =	423.84	420.29	3.55	41PAR/WES
$\Delta_fS°$ =		−1073.39		
$\Delta_fG°$ =		15.87		
$\ln K_f$ =		−6.40		

3-Ethylpentane C_7H_{16}
(3 × C-(H)$_3$(C)) + (3 × C-(H)$_2$(C)$_2$) + (1 × C-(H)(C)$_3$), $\sigma = 54$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−189.33	−189.84	0.51	47OSB/GIN
$C_p°$ =	165.98	165.94	0.04	69STU/WES
$S°$ =	411.50	412.67	−1.17	69STU/WES
$\Delta_fS°$ =		−672.07		
$\Delta_fG°$ =		10.54		
$\ln K_f$ =		−4.25		
Liquid phase				
$\Delta_fH°$ =	−224.56	−224.79	0.23	41PRO/ROS2
$C_p°$ =	219.58	222.08	−2.50	61HUF/GRO
$S°$ =	314.55	323.15	−8.60	61HUF/GRO
$\Delta_fS°$ =		−761.60		
$\Delta_fG°$ =		2.28		
$\ln K_f$ =		−0.92		

TABLE 5. *t*-Alkanes (35) – Continued

3-Ethylhexane C_8H_{18}

(3×C-(H)$_3$(C))+(4×C-(H)$_2$(C)$_2$)+(1×C-(H)(C)$_3$), σ = 27

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−210.71	−210.47	−0.24	47OSB/GIN
$C_p°$ =	188.87	188.83	0.04	69STU/WES
$S°$ =	458.19	457.60	0.59	69STU/WES
$\Delta_fS°$ =		−763.46		
$\Delta_fG°$ =		17.16		
$\ln K_f$ =		−6.92		
Liquid phase				
$\Delta_fH°$ =	−250.41	−250.52	0.11	45PRO/ROS
$C_p°$ =		252.50		
$S°$ =		355.53		
$\Delta_fS°$ =		−865.53		
$\Delta_fG°$ =		7.54		
$\ln K_f$ =		−3.04		

3-Ethylheptane C_9H_{20}

(3×C-(H)$_3$(C))+(5×C-(H)$_2$(C)$_2$)+(1×C-(H)(C)$_3$), σ = 27

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−231.10		
$C_p°$ =	208.11	211.72	−3.61	69STU/WES
$S°$ =	495.89	496.76	−0.87	69STU/WES
$\Delta_fS°$ =		−860.61		
$\Delta_fG°$ =		25.49		
$\ln K_f$ =		−10.28		
Liquid phase				
$\Delta_fH°$ =		−276.25		
$C_p°$ =		282.92		
$S°$ =		387.91		
$\Delta_fS°$ =		−969.46		
$\Delta_fG°$ =		12.79		
$\ln K_f$ =		−5.16		

3-Ethyloctane $C_{10}H_{22}$

(3×C-(H)$_3$(C))+(6×C-(H)$_2$(C)$_2$)+(1×C-(H)(C)$_3$), σ = 27

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−251.73		
$C_p°$ =	233.13	234.61	−1.48	69STU/WES
$S°$ =	534.46	535.92	−1.46	69STU/WES
$\Delta_fS°$ =		−957.76		
$\Delta_fG°$ =		33.83		
$\ln K_f$ =		−13.65		

TABLE 5. *t*-Alkanes (35) – Continued

3-Ethyloctane (Continued) $C_{10}H_{22}$

(3×C-(H)$_3$(C))+(6×C-(H)$_2$(C)$_2$)+(1×C-(H)(C)$_3$), σ = 27

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−301.98		
$C_p°$ =		313.34		
$S°$ =		420.29		
$\Delta_fS°$ =		−1073.39		
$\Delta_fG°$ =		18.05		
$\ln K_f$ =		−7.28		

4-Ethylheptane C_9H_{20}

(3×C-(H)$_3$(C))+(5×C-(H)$_2$(C)$_2$)+(1×C-(H)(C)$_3$), σ = 54

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−231.10		
$C_p°$ =	208.11	211.72	−3.61	69STU/WES
$S°$ =	495.89	490.99	4.90	69STU/WES
$\Delta_fS°$ =		−866.38		
$\Delta_fG°$ =		27.21		
$\ln K_f$ =		−10.98		
Liquid phase				
$\Delta_fH°$ =		−276.25		
$C_p°$ =		282.92		
$S°$ =		387.91		
$\Delta_fS°$ =		−969.46		
$\Delta_fG°$ =		12.79		
$\ln K_f$ =		−5.16		

4-Ethyloctane $C_{10}H_{22}$

(3×C-(H)$_3$(C))+(6×C-(H)$_2$(C)$_2$)+(1×C-(H)(C)$_3$), σ = 27, η = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−251.73		
$C_p°$ =	233.13	234.61	−1.48	69STU/WES
$S°$ =	534.46	541.68	−7.22	69STU/WES
$\Delta_fS°$ =		−952.00		
$\Delta_fG°$ =		32.11		
$\ln K_f$ =		−12.95		
Liquid phase				
$\Delta_fH°$ =		−301.98		
$C_p°$ =		313.34		
$S°$ =		420.29		
$\Delta_fS°$ =		−1073.39		
$\Delta_fG°$ =		18.05		
$\ln K_f$ =		−7.28		

TABLE 5. t-Alkanes (35) — Continued

4-Propylheptane $C_{10}H_{22}$

$(3\times C-(H)_3(C))+(6\times C-(H)_2(C)_2)+(1\times C-(H)(C)_3)$, $\sigma = 54$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−251.73		
$C_p°$ =	233.13	234.61	−1.48	69STU/WES
$S°$ =	525.34	530.15	−4.81	69STU/WES
$\Delta_fS°$ =		−963.53		
$\Delta_fG°$ =		35.55		
$\ln K_f$ =		−14.34		
Liquid phase				
$\Delta_fH°$ =		−301.98		
$C_p°$ =		313.34		
$S°$ =		420.29		
$\Delta_fS°$ =		−1073.39		
$\Delta_fG°$ =		18.05		
$\ln K_f$ =		−7.28		

4-Isopropylheptane $C_{10}H_{22}$

$(4\times C-(H)_3(C))+(4\times C-(H)_2(C)_2)+(2\times C-(H)(C)_3)+(2\times -CH_3$ corr (tertiary)), $\sigma = 54$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−258.42		
$C_p°$ =	231.00	234.64	−3.64	69STU/WES
$S°$ =	521.45	525.55	−4.10	69STU/WES
$\Delta_fS°$ =		−968.13		
$\Delta_fG°$ =		30.23		
$\ln K_f$ =		−12.19		
Liquid phase				
$\Delta_fH°$ =		−307.26		
$C_p°$ =		310.36		
$S°$ =		414.94		
$\Delta_fS°$ =		−1078.74		
$\Delta_fG°$ =		14.37		
$\ln K_f$ =		−5.80		

2,4-Dimethylpentane C_7H_{16}

$(4\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(2\times C-(H)(C)_3)+(4\times -CH_3$ corr (tertiary)), $\sigma = 162$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−201.71	−201.05	−0.66	47OSB/GIN
$C_p°$ =	165.98	165.97	0.01	69STU/WES
$S°$ =	396.64	398.94	−2.30	69STU/WES
$\Delta_fS°$ =		−685.81		
$\Delta_fG°$ =		3.42		
$\ln K_f$ =		−1.38		

TABLE 5. t-Alkanes (35) — Continued

2,4-Dimethylpentane (Continued) C_7H_{16}

$(4\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(2\times C-(H)(C)_3)+(4\times -CH_3$ corr (tertiary)), $\sigma = 162$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−234.60	−234.43	−0.17	41PRO/ROS2
$C_p°$ =	224.22	219.10	5.12	61HUF/GRO
$S°$ =	303.17	317.80	−14.63	61HUF/GRO
$\Delta_fS°$ =		−766.95		
$\Delta_fG°$ =		−5.76		
$\ln K_f$ =		2.33		

2,4-Dimethylhexane C_8H_{18}

$(4\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(2\times C-(H)(C)_3)+(3\times -CH_3$ corr (tertiary)), $\sigma = 81$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−219.24	−219.42	0.18	47OSB/GIN
$C_p°$ =	188.87	188.86	0.01	69STU/WES
$S°$ =	445.64	449.63	−3.99	69STU/WES
$\Delta_fS°$ =		−771.43		
$\Delta_fG°$ =		10.58		
$\ln K_f$ =		−4.27		
Liquid phase				
$\Delta_fH°$ =	−257.02	−257.98	0.96	45PRO/ROS
$C_p°$ =		249.52		
$S°$ =		350.18		
$\Delta_fS°$ =		−870.88		
$\Delta_fG°$ =		1.67		
$\ln K_f$ =		−0.67		

2,5-Dimethylhexane C_8H_{18}

$(4\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(2\times C-(H)(C)_3)+(4\times -CH_3$ corr (tertiary)), $\sigma = 162$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−222.51	−221.68	−0.83	47OSB/GIN
$C_p°$ =	188.87	188.86	0.01	69STU/WES
$S°$ =	439.03	438.10	0.93	69STU/WES
$\Delta_fS°$ =		−782.96		
$\Delta_fG°$ =		11.76		
$\ln K_f$ =		−4.74		
Liquid phase				
$\Delta_fH°$ =	−260.37	−260.16	−0.21	45PRO/ROS
$C_p°$ =	249.20	249.52	−0.32	47OSB/GIN
$S°$ =		350.18		
$\Delta_fS°$ =		−870.88		
$\Delta_fG°$ =		−0.51		
$\ln K_f$ =		0.20		

TABLE 5. *t*-Alkanes (35) — Continued

2,3-Dimethylbutane C_6H_{14}

(4×C–(H)$_3$(C)) + (2×C–(H)(C)$_3$) + (4×–CH_3 corr (tertiary)), σ = 162

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−178.28	−180.42	2.14	47OSB/GIN
$C_p°$ =	140.54	143.08	−2.54	69STU/WES
$S°$ =	365.77	359.78	5.99	69STU/WES
$\Delta_fS°$ =		−588.66		
$\Delta_fG°$ =		−4.91		
lnK_f =		1.98		
Liquid phase				
$\Delta_fH°$ =	−207.40	−208.70	1.30	41PRO/ROS
$C_p°$ =		188.68		
$S°$ =		285.42		
$\Delta_fS°$ =		−663.02		
$\Delta_fG°$ =		−11.02		
lnK_f =		4.45		

2,3-Dimethylpentane C_7H_{16}

(4×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (2×C–(H)(C)$_3$) + (3×–CH_3 corr (tertiary)), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−198.87	−198.79	−0.08	47OSB/GIN
$C_p°$ =	165.98	165.97	0.01	69STU/WES
$S°$ =	414.05	410.47	3.58	69STU/WES
$\Delta_fS°$ =		−674.28		
$\Delta_fG°$ =		2.25		
lnK_f =		−0.91		
Liquid phase				
$\Delta_fH°$ =	−233.09	−232.25	−0.84	41PRO/ROS2
$C_p°$ =	218.30	219.10	−0.80	76FIN/GRO
$S°$ =	297.10	317.80	−20.70	76FIN/GRO
$\Delta_fS°$ =		−766.95		
$\Delta_fG°$ =		−3.58		
lnK_f =		1.45		

2,3-Dimethylhexane C_8H_{18}

(4×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)(C)$_3$) + (3×–CH_3 corr (tertiary)), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−213.80	−219.42	5.62	47OSB/GIN
$C_p°$ =	188.87	188.86	0.01	69STU/WES
$S°$ =	443.96	443.86	0.10	69STU/WES
$\Delta_fS°$ =		−777.20		
$\Delta_fG°$ =		12.30		
lnK_f =		−4.96		

TABLE 5. *t*-Alkanes (35) — Continued

2,3-Dimethylhexane (Continued) C_8H_{18}

(4×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)(C)$_3$) + (3×–CH_3 corr (tertiary)), σ = 81

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−252.59	−257.98	5.39	45PRO/ROS
$C_p°$ =		249.52		
$S°$ =		350.18		
$\Delta_fS°$ =		−870.88		
$\Delta_fG°$ =		1.67		
lnK_f =		−0.67		

3,4-Dimethylhexane C_8H_{18}

(4×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)(C)$_3$) + (2×–CH_3 corr (tertiary)), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−212.84	−217.16	4.32	47OSB/GIN
$C_p°$ =	188.87	188.86	0.01	69STU/WES
$S°$ =	448.32	449.63	−1.31	69STU/WES
$\Delta_fS°$ =		−771.43		
$\Delta_fG°$ =		12.84		
lnK_f =		−5.18		
Liquid phase				
$\Delta_fH°$ =	−251.83	−255.80	3.97	45PRO/ROS
$C_p°$ =		249.52		
$S°$ =		350.18		
$\Delta_fS°$ =		−870.88		
$\Delta_fG°$ =		3.85		
lnK_f =		−1.55		

3-Ethyl-2-methylpentane C_8H_{18}

(4×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)(C)$_3$) + (2×–CH_3 corr (tertiary)), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−211.04	−217.16	6.12	47OSB/GIN
$C_p°$ =	188.87	188.86	0.01	69STU/WES
$S°$ =	441.12	443.86	−2.74	69STU/WES
$\Delta_fS°$ =		−777.20		
$\Delta_fG°$ =		14.56		
lnK_f =		−5.87		
Liquid phase				
$\Delta_fH°$ =	−249.58	−255.80	6.22	45PRO/ROS
$C_p°$ =		249.52		
$S°$ =		350.18		
$\Delta_fS°$ =		−870.88		
$\Delta_fG°$ =		3.85		
lnK_f =		−1.55		

TABLE 5. *t*-Alkanes (35) – Continued

2,3,4-Trimethylpentane C_8H_{18}

(5×C–(H)$_3$(C))+(3×C–(H)(C)$_3$)+ (5×–CH$_3$ corr (tertiary)), σ = 243

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−217.32	−226.11	8.79	47OSB/GIN
$C_p^°$ =	188.87	188.89	−0.02	69STU/WES
$S°$ =	428.07	430.13	−2.06	69STU/WES
$\Delta_f S°$ =		−790.93		
$\Delta_f G°$ =		9.71		
$\ln K_f$ =		−3.92		
Liquid phase				
$\Delta_f H°$ =	−255.01	−263.26	8.25	45PRO/ROS
$C_p^°$ =	246.23	246.54	−0.31	41PIT/SCO
$S°$ =	329.32	344.83	−15.51	41PIT/SCO
$\Delta_f S°$ =		−876.23		
$\Delta_f G°$ =		−2.01		
$\ln K_f$ =		0.81		

2,7-Dimethyloctane $C_{10}H_{22}$

(4×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(2×C–(H)(C)$_3$)+ (4×–CH$_3$ corr (tertiary)), σ = 162

	Literature	Calculated	Residual	Reference
Gas phase				
$H°$ =	−264.01	−262.94	−1.07	69STU/WES
$C_p^°$ =	235.56	234.64	0.92	69STU/WES
$S°$ =	515.68	516.42	−0.74	69STU/WES
$\Delta_f S°$ =		−977.26		
$\Delta_f G°$ =		28.43		
$\ln K_f$ =		−11.47		
Liquid phase				
$\Delta_f H°$ =		−311.62		
$C_p^°$ =	301.67	310.36	−8.69	30PAR/HUF
$S°$ =		414.94		
$\Delta_f S°$ =		−1078.74		
$\Delta_f G°$ =		10.01		
$\ln K_f$ =		−4.04		

TABLE 6. *q*-Alkanes (16)

2,2-Dimethylpropane C_5H_{12}

(4×C–(H)$_3$(C))+(1×C–(C)$_4$)+ (4×–CH$_3$ corr (quaternary)), σ = 972

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−167.94	−168.08	0.14	70GOO
$C_p^°$ =	121.63	119.45	2.18	69STU/WES
$S°$ =	306.39	302.59	3.80	69STU/WES
$\Delta_f S°$ =		−509.53		
$\Delta_f G°$ =		−16.16		
$\ln K_f$ =		6.52		
Liquid phase				
$\Delta_f H°$ =	−190.33	−190.01	−0.32	70GOO
$C_p^°$ =	153.09	156.16	−3.07	69STU/WES
$S°$ =	216.81	234.55	−17.74	69STU/WES
$\Delta_f S°$ =		−577.58		
$\Delta_f G°$ =		−17.81		
$\ln K_f$ =		7.18		

2,2-Dimethylbutane C_6H_{14}

(4×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(C)$_4$)+ (3×–CH$_3$ corr (quaternary)), σ = 243

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−186.10	−184.15	−1.95	47OSB/GIN
$C_p^°$ =	141.88	142.34	−0.46	69STU/WES
$S°$ =	358.23	353.28	4.95	69STU/WES
$\Delta_f S°$ =		−595.16		
$\Delta_f G°$ =		−6.70		
$\ln K_f$ =		2.70		
Liquid phase				
$\Delta_f H°$ =	−213.80	−211.35	−2.45	41PRO/ROS
$C_p^°$ =	188.74	186.58	2.16	46DOU/HUF
$S°$ =	272.00	266.93	5.07	46DOU/HUF
$\Delta_f S°$ =		−681.51		
$\Delta_f G°$ =		−8.16		
$\ln K_f$ =		3.29		

2,2-Dimethylpentane C_7H_{16}

(4×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(C)$_4$)+ (3×–CH$_3$ corr (quaternary)), σ = 243

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−205.85	−204.78	−1.07	47OSB/GIN
$C_p^°$ =	165.98	165.23	0.75	69STU/WES
$S°$ =	392.88	392.44	0.44	69STU/WES
$\Delta_f S°$ =		−692.31		
$\Delta_f G°$ =		1.63		
$\ln K_f$ =		−0.66		

TABLE 6. q-Alkanes (16) — Continued

2,2-Dimethylpentane C_7H_{16}

$(4\times C\text{-}(H)_3(C)) + (2\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(C)_4) + (3\times\text{-}CH_3 \text{ corr (quaternary)})$, $\sigma = 243$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH° =$	−238.28	−237.08	−1.20	41PRO/ROS2
$C_p° =$	221.12	217.00	4.12	61HUF/GRO
$S° =$	300.29	299.31	0.98	61HUF/GRO
$\Delta_fS° =$		−785.44		
$\Delta_fG° =$		−2.90		
$\ln K_f =$		1.17		

2,2-Dimethylhexane C_8H_{18}

$(4\times C\text{-}(H)_3(C)) + (3\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(C)_4) + (3\times\text{-}CH_3 \text{ corr (quaternary)})$, $\sigma = 243$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH° =$	−224.60	−225.41	0.81	47OSB/GIN
$C_p° =$	188.87	188.12	0.75	69STU/WES
$S° =$	431.20	431.60	−0.40	69STU/WES
$\Delta_fS° =$		−789.46		
$\Delta_fG° =$		9.97		
$\ln K_f =$		−4.02		
Liquid phase				
$\Delta_fH° =$	−261.88	−262.81	0.93	45PRO/ROS
$C_p° =$		247.42		
$S° =$		331.69		
$\Delta_fS° =$		−889.37		
$\Delta_fG° =$		2.36		
$\ln K_f =$		−0.95		

3,3-Dimethylpentane C_7H_{16}

$(4\times C\text{-}(H)_3(C)) + (2\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(C)_4) + (2\times\text{-}CH_3 \text{ corr (quaternary)})$, $\sigma = 162$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH° =$	−201.17	−200.22	−0.95	47OSB/GIN
$C_p° =$	165.98	165.23	0.75	69STU/WES
$S° =$	399.70	395.81	3.89	69STU/WES
$\Delta_fS° =$		−688.94		
$\Delta_fG° =$		5.19		
$\ln K_f =$		−2.09		
Liquid phase				
$\Delta_fH° =$	−234.18	−232.69	−1.49	45PRO/ROS
$C_p° =$	214.80	217.00	−2.20	76FIN/GRO
$S° =$	305.60	299.31	6.29	76FIN/GRO
$\Delta_fS° =$		−785.44		
$\Delta_fG° =$		1.49		
$\ln K_f =$		−0.60		

TABLE 6. q-Alkanes (16) — Continued

3,3-Dimethylhexane C_8H_{18}

$(4\times C\text{-}(H)_3(C)) + (3\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(C)_4) + (2\times\text{-}CH_3 \text{ corr (quaternary)})$, $\sigma = 81$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH° =$	−219.99	−220.85	0.86	47OSB/GIN
$C_p° =$	188.87	188.12	0.75	69STU/WES
$S° =$	438.06	440.73	−2.67	69STU/WES
$\Delta_fS° =$		−780.33		
$\Delta_fG° =$		11.80		
$\ln K_f =$		−4.76		
Liquid phase				
$\Delta_fH° =$	−257.53	−258.42	0.89	45PRO/ROS
$C_p° =$	246.60	247.42	−0.82	47OSB/GIN
$S° =$		331.69		
$\Delta_fS° =$		−889.37		
$\Delta_fG° =$		6.75		
$\ln K_f =$		−2.72		

2,2,3-Trimethylbutane C_7H_{16}

$(5\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)(C)_3) + (1\times C\text{-}(C)_4) + (5\times\text{-}CH_3 \text{ corr } (tert/quat))$, $\sigma = 729$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH° =$	−204.47	−202.27	−2.20	47OSB/GIN
$C_p° =$	164.56	165.26	−0.70	69STU/WES
$S° =$	383.60	378.70	4.90	69STU/WES
$\Delta_fS° =$		−706.04		
$\Delta_fG° =$		8.24		
$\ln K_f =$		−3.32		
Liquid phase				
$\Delta_fH° =$	−236.52	−233.68	−2.84	41PRO/ROS2
$C_p° =$	213.51	214.02	−0.51	61HUF/GRO
$S° =$	292.25	293.96	−1.71	61HUF/GRO
$\Delta_fS° =$		−790.79		
$\Delta_fG° =$		2.09		
$\ln K_f =$		−0.84		

2,2,3-Trimethylpentane C_8H_{18}

$(5\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)(C)_3) + (1\times C\text{-}(C)_4) + (4\times\text{-}CH_3 \text{ corr } (tert/quat))$, $\sigma = 729$, $\eta = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH° =$	−219.99	−221.10	1.11	47OSB/GIN
$C_p° =$	188.87	188.15	0.72	69STU/WES
$S° =$	425.18	423.63	1.55	69STU/WES
$\Delta_fS° =$		−797.43		
$\Delta_fG° =$		16.65		
$\ln K_f =$		−6.72		

TABLE 6. q-Alkanes (16) — Continued

2,2,3-Trimethylpentane (Continued) C_8H_{18}

$(5\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)(C)_3)+(1\times C\text{-}(C)_4)+(4\times\text{-}CH_3$ corr $(tert/quat))$, $\sigma = 729$, $\eta = 2$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−256.90	−257.64	0.74	45PRO/ROS
$C_p°$ =		244.44		
$S°$ =		326.34		
$\Delta_fS°$ =		−894.72		
$\Delta_fG°$ =		9.12		
$\ln K_f$ =		−3.68		

2,2,4-Trimethylpentane C_8H_{18}

$(5\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)(C)_3)+(1\times C\text{-}(C)_4)+(5\times\text{-}CH_3$ corr $(tert/quat))$, $\sigma = 729$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−224.01	−222.90	−1.11	47OSB/GIN
$C_p°$ =	188.87	188.15	0.72	69STU/WES
$S°$ =	423.21	417.86	5.35	69STU/WES
$\Delta_fS°$ =		−803.20		
$\Delta_fG°$ =		16.57		
$\ln K_f$ =		−6.69		
Liquid phase				
$\Delta_fH°$ =	−259.16	−259.41	0.25	45PRO/ROS
$C_p°$ =	238.57	244.44	−5.87	47OSB/GIN
$S°$ =	328.03	326.34	1.69	40PIT
$\Delta_fS°$ =		−894.72		
$\Delta_fG°$ =		7.35		
$\ln K_f$ =		−2.97		

2,3,3-Trimethylpentane C_8H_{18}

$(5\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)(C)_3)+(1\times C\text{-}(C)_4)+(4\times\text{-}CH_3$ corr $(tert/quat))$, $\sigma = 243$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−216.27	−221.10	4.83	47OSB/GIN
$C_p°$ =	188.87	188.15	0.72	69STU/WES
$S°$ =	431.54	427.00	4.54	69STU/WES
$\Delta_fS°$ =		−794.06		
$\Delta_fG°$ =		15.65		
$\ln K_f$ =		−6.31		

TABLE 6. q-Alkanes (16) — Continued

2,3,3-Trimethylpentane (Continued) C_8H_{18}

$(5\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)(C)_3)+(1\times C\text{-}(C)_4)+(4\times\text{-}CH_3$ corr $(tert/quat))$, $\sigma = 243$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−253.51	−257.64	4.13	45PRO/ROS
$C_p°$ =	245.56	244.44	1.12	47OSB/GIN
$S°$ =		326.34		
$\Delta_fS°$ =		−894.72		
$\Delta_fG°$ =		9.12		
$\ln K_f$ =		−3.68		

2,2,3,3-Tetramethylbutane C_8H_{18}

$(6\times C\text{-}(H)_3(C))+(2\times C\text{-}(C)_4)+(6\times\text{-}CH_3$ corr $(quat/quat))$, $\sigma = 13122$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−225.22	−219.00	−6.22	47OSB/GIN
$C_p°$ =	192.59	187.44	5.15	69STU/WES
$S°$ =	389.36	386.10	3.26	69STU/WES
$\Delta_fS°$ =		−834.96		
$\Delta_fG°$ =		29.94		
$\ln K_f$ =		−12.08		
Liquid phase				
$\Delta_fH°$ =		−253.52		
$C_p°$ =		239.36		
$S°$ =		302.50		
$\Delta_fS°$ =		−918.56		
$\Delta_fG°$ =		20.35		
$\ln K_f$ =		−8.21		
Solid phase				
$\Delta_fH°$ =	−268.61	−268.94	0.33	45PRO/ROS
$C_p°$ =	237.44	237.44	0.00	52SCO/DOU
$S°$ =	273.76	273.76	0.00	52SCO/DOU
$\Delta_fS°$ =		−947.30		
$\Delta_fG°$ =		13.50		
$\ln K_f$ =		−5.44		

2,2,3,3-Tetramethylpentane C_9H_{20}

$(6\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(2\times C\text{-}(C)_4)+(5\times\text{-}CH_3$ corr $(quat/quat))$, $\sigma = 2187$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−237.11	−238.99	1.88	61LAB/GRE
$C_p°$ =	212.09	210.33	1.76	69STU/WES
$S°$ =	446.39	440.16	6.23	69STU/WES
$\Delta_fS°$ =		−917.21		
$\Delta_fG°$ =		34.48		
$\ln K_f$ =		−13.91		

TABLE 6. q-Alkanes (16) — Continued

2,2,3,3-Tetramethylpentane (Continued) C_9H_{20}
(6 × C–(H)$_3$(C)) + (1 × C–(H)$_2$(C)$_2$) + (2 × C–(C)$_4$) + (5 × –CH$_3$ corr (*quat/quat*)), σ = 2187

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−278.28	−278.61	0.33	47JOH/PRO
$C_p°$ =		269.78		
$S°$ =		334.88		
$\Delta_f S°$ =		−1022.49		
$\Delta_f G°$ =		26.25		
$\ln K_f$ =		−10.59		

2,2,4,4-Tetramethylpentane C_9H_{20}
(6 × C–(H)$_3$(C)) + (1 × C–(H)$_2$(C)$_2$) + (2 × C–(C)$_4$) + (6 × –CH$_3$ corr (*quat/quat*)), σ = 13122

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−241.84	−239.63	−2.21	61LAB/GRE
$C_p°$ =	211.63	210.33	1.30	69STU/WES
$S°$ =	431.50	425.26	6.24	69STU/WES
$\Delta_f S°$ =		−932.11		
$\Delta_f G°$ =		38.28		
$\ln K_f$ =		−15.44		
Liquid phase				
$\Delta_f H°$ =	−279.99	−279.25	−0.74	47JOH/PRO
$C_p°$ =		269.78		
$S°$ =		334.88		
$\Delta_f S°$ =		−1022.49		
$\Delta_f G°$ =		25.61		
$\ln K_f$ =		−10.33		

2,2,3,4,4-Pentmethylpentane $C_{10}H_{22}$
(7 × C–(H)$_3$(C)) + (1 × C–(H)(C)$_3$) + (2 × C–(C)$_4$) + (7 × –CH$_3$ corr (*quat/quat*)), σ = 19683

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−263.07		
$C_p°$ =	234.43	233.25	1.18	69STU/WES
$S°$ =	462.83	456.45	6.38	69STU/WES
$\Delta_f S°$ =		−1037.23		
$\Delta_f G°$ =		46.18		
$\ln K_f$ =		−18.63		
Liquid phase				
$\Delta_f H°$ =		−306.54		
$C_p°$ =		297.22		
$S°$ =		361.91		
$\Delta_f S°$ =		−1131.77		
$\Delta_f G°$ =		30.90		
$\ln K_f$ =		−12.46		

TABLE 6. q-Alkanes (16) — Continued

3-Ethyl-3-methylpentane C_8H_{18}
(4 × C–(H)$_3$(C)) + (3 × C–(H)$_2$(C)$_2$) + (1 × C–(C)$_4$) + (1 × –CH$_3$ corr (quaternary)), σ = 243

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−214.85	−216.29	1.44	47OSB/GIN
$C_p°$ =	188.87	188.12	0.75	69STU/WES
$S°$ =	432.96	431.60	1.36	69STU/WES
$\Delta_f S°$ =		−789.46		
$\Delta_f G°$ =		19.09		
$\ln K_f$ =		−7.70		
Liquid phase				
$\Delta_f H°$ =	−252.84	−254.03	1.19	45PRO/ROS
$C_p°$ =		247.42		
$S°$ =		331.69		
$\Delta_f S°$ =		−889.37		
$\Delta_f G°$ =		11.14		
$\ln K_f$ =		−4.49		

3,3-Diethylpentane C_9H_{20}
(4 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(C)$_4$), σ = 972

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−232.34	−232.36	0.02	61LAB/GRE
$C_p°$ =	204.18	211.01	−6.83	69STU/WES
$S°$ =	461.54	459.23	2.31	69STU/WES
$\Delta_f S°$ =		−898.14		
$\Delta_f G°$ =		35.42		
$\ln K_f$ =		−14.29		
Liquid phase				
$\Delta_f H°$ =	−275.39	−275.37	−0.02	47JOH/PRO
$C_p°$ =	278.80	277.84	0.96	76FIN/MES
$S°$ =	333.40	364.07	−30.67	76FIN/MES
$\Delta_f S°$ =		−993.30		
$\Delta_f G°$ =		20.78		
$\ln K_f$ =		−8.38		

TABLE 7. *n*-Alkenes (32)

Ethylene C_2H_4

($2\times C_d$–(H)$_2$), $\sigma = 4$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	52.50	52.64	−0.14	37ROS/KNO
$C_p°$ =	42.84	42.76	0.08	75CHA/ZWO
$S°$ =	219.20	219.51	−0.31	75CHA/ZWO
$\Delta_fS°$ =		−53.11		
$\Delta_fG°$ =		68.47		
$\ln K_f$ =		−27.62		

Propylene C_3H_6

($1\times C$–(H)$_3$(C)) + ($1\times C_d$–(H)$_2$) + ($1\times C_d$–(H)(C)), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	19.76	20.38	−0.62	37ROS/KNO
$C_p°$ =	64.31	65.85	−1.54	75CHA/ZWO
$S°$ =	266.60	266.76	−0.16	75CHA/ZWO
$\Delta_fS°$ =		−142.18		
$\Delta_fG°$ =		62.77		
$\ln K_f$ =		−25.32		

1-Butene C_4H_8

($1\times C$–(H)$_3$(C)) + ($1\times C_d$–(H)$_2$) + ($1\times C_d$–(H)(C)) + ($1\times C$–(H)$_2$(C)(C_d)), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−0.54	−0.50	−0.04	51PRO/MAR
$C_p°$ =	85.65	86.48	−0.83	69STU/WES
$S°$ =	305.60	304.96	0.64	69STU/WES
$\Delta_fS°$ =		−240.29		
$\Delta_fG°$ =		71.14		
$\ln K_f$ =		−28.70		

1-Pentene C_5H_{10}

($1\times C$–(H)$_3$(C)) + ($1\times C$–(H)$_2$(C)$_2$) + ($1\times C$–(H)$_2$(C)(C_d)) + ($1\times C_d$–(H)(C)) + ($1\times C_d$–(H)$_2$), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−21.50	−21.13	−0.37	86TRC
$C_p°$ =	109.58	109.37	0.21	69STU/WES
$S°$ =	345.81	344.12	1.69	69STU/WES
$\Delta_fS°$ =		−337.44		
$\Delta_fG°$ =		79.48		
$\ln K_f$ =		−32.06		

TABLE 7. *n*-Alkenes (32) – Continued

1-Pentene (Continued) C_5H_{10}

($1\times C$–(H)$_3$(C)) + ($1\times C$–(H)$_2$(C)$_2$) + ($1\times C$–(H)$_2$(C)(C_d)) + ($1\times C_d$–(H)(C)) + ($1\times C_d$–(H)$_2$), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−46.97	−46.27	−0.70	79GOO/SMI
$C_p°$ =	154.87	149.16	5.71	90MES/TOD
$S°$ =	262.60	262.12	0.48	90MES/TOD
$\Delta_fS°$ =		−419.43		
$\Delta_fG°$ =		78.78		
$\ln K_f$ =		−31.78		

1-Hexene C_6H_{12}

($1\times C$–(H)$_3$(C)) + ($2\times C$–(H)$_2$(C)$_2$) + ($1\times C$–(H)$_2$(C)(C_d)) + ($1\times C_d$–(H)$_2$) + ($1\times C_d$–(H)(C)), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−41.51	−41.76	0.25	56CAM/ROS
$C_p°$ =	132.34	132.26	0.08	69STU/WES
$S°$ =	384.64	383.28	1.36	69STU/WES
$\Delta_fS°$ =		−434.59		
$\Delta_fG°$ =		87.81		
$\ln K_f$ =		−35.42		
Liquid phase				
$\Delta_fH°$ =	−72.22	−72.00	−0.22	59SKE/SNE
$C_p°$ =	183.30	179.58	3.72	57MCC/FIN2
$S°$ =	295.18	294.50	0.68	57MCC/FIN2
$\Delta_fS°$ =		−523.37		
$\Delta_fG°$ =		84.04		
$\ln K_f$ =		−33.90		

1-Heptene C_7H_{14}

($1\times C$–(H)$_3$(C)) + ($3\times C$–(H)$_2$(C)$_2$) + ($1\times C$–(H)$_2$(C)(C_d)) + ($1\times C_d$–(H)$_2$) + ($1\times C_d$–(H)(C)), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−62.72	−62.39	−0.33	50FOR/CAM
$C_p°$ =	155.23	155.15	0.08	69STU/WES
$S°$ =	423.59	422.44	1.15	69STU/WES
$\Delta_fS°$ =		−531.74		
$\Delta_fG°$ =		96.15		
$\ln K_f$ =		−38.79		
Liquid phase				
$\Delta_fH°$ =	−98.37	−97.73	−0.64	76GOO
$C_p°$ =	211.79	210.00	1.79	57MCC/FIN2
$S°$ =	327.65	326.88	0.77	57MCC/FIN2
$\Delta_fS°$ =		−627.30		
$\Delta_fG°$ =		89.30		
$\ln K_f$ =		−36.02		

TABLE 7. *q*-Alkanes (16) – Continued

1-Octene C_8H_{16}

(1 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(C)(C$_d$)) + (1 × C$_d$–(H)$_2$) + (1 × C$_d$–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−82.93	−83.02	0.09	50FOR/CAM
$C_p°$ =	178.07	178.04	0.03	69STU/WES
$S°$ =	462.54	461.60	0.94	69STU/WES
$\Delta_fS°$ =		−628.89		
$\Delta_fG°$ =		104.48		
lnK_f =		−42.15		
Liquid phase				
$\Delta_fH°$ =	−123.80	−123.46	−0.34	61ROC/ROS
$C_p°$ =	241.21	240.42	0.79	57MCC/FIN2
$S°$ =	360.45	359.26	1.19	57MCC/FIN2
$\Delta_fS°$ =		−731.23		
$\Delta_fG°$ =		94.56		
lnK_f =		−38.14		

1-Nonene C_9H_{18}

(1 × C–(H)$_3$(C)) + (5 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(C)(C$_d$)) + (1 × C$_d$–(H)(C)) + (1 × C$_d$–(H)$_2$), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−103.51	−103.65	0.14	69STU/WES
$C_p°$ =	200.96	200.93	0.03	69STU/WES
$S°$ =	501.49	500.76	0.73	69STU/WES
$\Delta_fS°$ =		−726.04		
$\Delta_fG°$ =		112.82		
lnK_f =		−45.51		
Liquid phase				
$\Delta_fH°$ =	−149.03	−149.19	0.16	86TRC
$C_p°$ =	270.36	270.84	−0.48	90MES/TOD
$S°$ =	392.54	391.64	0.90	90MES/TOD
$\Delta_fS°$ =		−835.16		
$\Delta_fG°$ =		99.81		
lnK_f =		−40.26		

1-Decene $C_{10}H_{20}$

(1 × C–(H)$_3$(C)) + (6 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(C)(C$_d$)) + (1 × C$_d$–(H)(C)) + (1 × C$_d$–(H)$_2$), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−123.34	−124.28	0.94	50FOR/CAM
$C_p°$ =	223.80	223.82	−0.02	69STU/WES
$S°$ =	540.45	539.92	0.53	69STU/WES
$\Delta_fS°$ =		−823.19		
$\Delta_fG°$ =		121.16		
lnK_f =		−48.87		

TABLE 7. *q*-Alkanes (16) – Continued

1-Decene (Continued) $C_{10}H_{20}$

(1 × C–(H)$_3$(C)) + (6 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(C)(C$_d$)) + (1 × C$_d$–(H)(C)) + (1 × C$_d$–(H)$_2$), σ = 3

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−173.80	−174.92	1.12	61ROC/ROS
$C_p°$ =	300.83	301.26	−0.43	57MCC/FIN2
$S°$ =	425.01	424.02	0.99	57MCC/FIN2
$\Delta_fS°$ =		−939.09		
$\Delta_fG°$ =		105.07		
lnK_f =		−42.38		

1-Hexadecene $C_{16}H_{32}$

(1 × C–(H)$_3$(C)) + (12 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(C)(C$_d$)) + (1 × C$_d$–(H)(C)) + (1 × C$_d$–(H)$_2$), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−249.16	−248.06	−1.10	70ZWO/WIL
$C_p°$ =	361.04	361.16	−0.12	69STU/WES
$S°$ =	774.12	774.88	−0.76	69STU/WES
$\Delta_fS°$ =		−1406.10		
$\Delta_fG°$ =		171.17		
lnK_f =		−69.05		
Liquid phase				
$\Delta_fH°$ =	−329.24	−329.30	0.06	55FRA/PRO
$C_p°$ =	483.34	483.78	−0.44	90MES/TOD
$S°$ =	613.88	618.30	−4.42	90MES/TOD
$\Delta_fS°$ =		−1562.68		
$\Delta_fG°$ =		136.61		
lnK_f =		−55.11		

***cis*-2-Butene** C_4H_8

(2 × C–(H)$_3$(C)) + (2 × C$_d$–(H)(C)) + (1 × *cis*(unsat) corr), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−7.57	−7.03	−0.54	51PRO/MAR
$C_p°$ =	78.91	80.91	−2.00	69STU/WES
$S°$ =	300.83	301.77	−0.94	69STU/WES
$\Delta_fS°$ =		−243.48		
$\Delta_fG°$ =		65.56		
lnK_f =		−26.45		

TABLE 7. *n*-Alkenes (32) — Continued

***trans*-2-Butene** C_4H_8

$(2\times C\text{-}(H)_3(C))+(2\times C_d\text{-}(H)(C))$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−10.97	−11.88	0.91	51PRO/MAR
C_p° =	87.82	88.94	−1.12	69STU/WES
S° =	296.48	296.71	−0.23	69STU/WES
Δ_fS° =		−248.54		
Δ_fG° =		62.22		
$\ln K_f$ =		−25.10		

***cis*-2-Pentene** C_5H_{10}

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)(C_d))+(2\times C_d\text{-}(H)(C))+(1\times cis\,(\text{unsat})\ \text{corr})$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−26.67	−27.91	1.24	86TRC
C_p° =	101.75	101.54	0.21	69STU/WES
S° =	346.27	345.73	0.54	69STU/WES
Δ_fS° =		−335.82		
Δ_fG° =		72.22		
$\ln K_f$ =		−29.13		
Liquid phase				
Δ_fH° =	−53.49	−53.58	0.09	79GOO/SMI
C_p° =	151.71	151.45	0.26	47TOD/OLI
S° =	258.61	255.43	3.18	47TOD/OLI
Δ_fS° =		−426.13		
Δ_fG° =		73.47		
$\ln K_f$ =		−29.64		

***trans*-2-Pentene** C_5H_{10}

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)(C_d))+(2\times C_d\text{-}(H)(C))$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−31.29	−32.76	1.47	86TRC
C_p° =	108.45	109.57	−1.12	69STU/WES
S° =	340.41	340.67	−0.26	69STU/WES
Δ_fS° =		−340.88		
Δ_fG° =		68.87		
$\ln K_f$ =		−27.78		
Liquid phase				
Δ_fH° =	−57.98	−58.85	0.87	79GOO/SMI
C_p° =	156.98	151.45	5.53	47TOD/OLI
S° =	256.52	255.43	1.09	47TOD/OLI
Δ_fS° =		−426.13		
Δ_fG° =		68.20		
$\ln K_f$ =		−27.51		

TABLE 7. *n*-Alkenes (32) — Continued

***cis*-2-Hexene** C_6H_{12}

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_2(C)(C_d))+(2\times C_d\text{-}(H)(C))+(1\times cis\,(\text{unsat})\ \text{corr})$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−52.34	−48.54	−3.80	56CAM/ROS
C_p° =	125.69	124.43	1.26	69STU/WES
S° =	386.48	384.89	1.59	69STU/WES
Δ_fS° =		−432.97		
Δ_fG° =		80.55		
$\ln K_f$ =		−32.49		
Liquid phase				
Δ_fH° =	−83.89	−79.31	−4.58	60BAR/ROS
C_p° =	178.36	181.87	−3.51	90MES/TOD
S° =	291.86	287.81	4.05	90MES/TOD
Δ_fS° =		−530.06		
Δ_fG° =		78.73		
$\ln K_f$ =		−31.76		

***trans*-2-Hexene** C_6H_{12}

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_2(C)(C_d))+(2\times C_d\text{-}(H)(C))$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−53.89	−53.39	−0.50	56CAM/ROS
C_p° =	132.38	132.46	−0.08	69STU/WES
S° =	380.62	379.83	0.79	69STU/WES
Δ_fS° =		−438.03		
Δ_fG° =		77.21		
$\ln K_f$ =		−31.15		
Liquid phase				
Δ_fH° =	−85.52	−84.58	−0.94	60BAR/ROS
C_p° =		181.87		
S° =		287.81		
Δ_fS° =		−530.06		
Δ_fG° =		73.46		
$\ln K_f$ =		−29.63		

***cis*-3-Hexene** C_6H_{12}

$(2\times C\text{-}(H)_3(C))+(2\times C\text{-}(H)_2(C)(C_d))+(2\times C_d\text{-}(H)(C))+(1\times cis\,(\text{unsat})\ \text{corr})$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−47.61	−48.79	1.18	56CAM/ROS
C_p° =	123.64	122.17	1.47	69STU/WES
S° =	379.61	378.17	1.44	69STU/WES
Δ_fS° =		−439.70		
Δ_fG° =		82.31		
$\ln K_f$ =		−33.20		

TABLE 7. *n*-Alkenes (16) — Continued

***cis*-3-Hexene** C_6H_{12}
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)(C$_d$)) + (2×C$_d$–(H)(C)) + (1×*cis*(unsat) corr), σ = 18

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−78.95	−79.31	0.36	60BAR/ROS
$C_p°$ =		180.74		
$S°$ =		287.10		
$\Delta_fS°$ =		−530.77		
$\Delta_fG°$ =		78.94		
lnK_f =		−31.84		

***trans*-3-Hexene** C_6H_{12}
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)(C$_d$)) + (2×C$_d$–(H)(C)), σ = 18

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	−54.43	−53.64	−0.79	56CAM/ROS
$C_p°$ =	132.84	130.20	2.64	69STU/WES
$S°$ =	374.84	373.11	1.73	69STU/WES
$\Delta_fS°$ =		−444.76		
$\Delta_fG°$ =		78.96		
lnK_f =		−31.85		
Liquid phase				
$\Delta_fH°$ =	−86.06	−84.58	−1.48	60BAR/ROS
$C_p°$ =		180.74		
$S°$ =		287.10		
$\Delta_fS°$ =		−530.77		
$\Delta_fG°$ =		73.67		
lnK_f =		−29.72		

***cis*-2-Heptene** C_7H_{14}
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(C$_d$)) + (2×C$_d$–(H)(C)) + (1×*cis*(unsat) corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	−69.14	−69.17	0.03	86TRC
$C_p°$ =		147.32		
Liquid phase				
$\Delta_fH°$ =	−105.14	−105.04	−0.10	76GOO
$C_p°$ =		212.29		
$S°$ =		320.19		
$\Delta_fS°$ =		−633.99		
$\Delta_fG°$ =		83.98		
lnK_f =		−33.88		

TABLE 7. *n*-Alkenes (32) — Continued

***trans*-2-Heptene** C_7H_{14}
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(C$_d$)) + (2×C$_d$–(H)(C))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	−73.54	−74.02	0.48	86TRC
$C_p°$ =		155.35		
Liquid phase				
$\Delta_fH°$ =	−109.54	−110.31	0.77	76GOO
$C_p°$ =		212.29		
$S°$ =		320.19		
$\Delta_fS°$ =		−633.99		
$\Delta_fG°$ =		78.71		
lnK_f =		−31.75		

***cis*-2-Octene** C_8H_{16}
(2×C–(H)$_3$(C)) + (3×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(C$_d$)) + (2×C$_d$–(H)(C)) + (1×*cis*(unsat) corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		−89.80		
$C_p°$ =		170.21		
Liquid phase				
$\Delta_fH°$ =	−135.69	−130.77	−4.92	86PED/NAY
$C_p°$ =		242.71		
$S°$ =		352.57		
$\Delta_fS°$ =		−737.92		
$\Delta_fG°$ =		89.24		
lnK_f =		−36.00		

***trans*-2-Octene** C_8H_{16}
(2×C–(H)$_3$(C)) + (3×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(C$_d$)) + (2×C$_d$–(H)(C))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		−94.65		
$C_p°$ =		178.24		
Liquid phase				
$\Delta_fH°$ =	−135.69	−136.04	0.35	86PED/NAY
$C_p°$ =		242.71		
$S°$ =		352.57		
$\Delta_fS°$ =		−737.92		
$\Delta_fG°$ =		83.97		
lnK_f =		−33.87		

TABLE 7. *n*-Alkenes (32) — Continued

cis-3-Heptene C_7H_{14}

(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(C)(C$_d$)) + (2×C$_d$–(H)(C)) + (1×*cis*(unsat) corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−68.75	−69.42	0.67	86TRC
$C_p°$ =		145.06		
Liquid phase				
$\Delta_f H°$ =	−104.35	−105.04	0.69	76GOO
$C_p°$ =		211.16		
$S°$ =		319.48		
$\Delta_f S°$ =		−634.70		
$\Delta_f G°$ =		84.19		
$\ln K_f$ =		−33.96		

trans-3-Heptene C_7H_{14}

(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(C)(C$_d$)) + (2×C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−73.73	−74.27	0.54	86TRC
$C_p°$ =		153.09		
Liquid phase				
$\Delta_f H°$ =	−109.33	−110.31	0.98	76GOO
$C_p°$ =		211.16		
$S°$ =		319.48		
$\Delta_f S°$ =		−634.70		
$\Delta_f G°$ =		78.92		
$\ln K_f$ =		−31.84		

1,2-Butadiene C_4H_6

(1×C–(H)$_3$(C)) + (1×C$_d$–(H)(C)) + (1×C$_a$) + (1×C$_d$–(H)$_2$), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	162.26	163.05	−0.79	49PRO/MAR
$C_p°$ =	80.12	81.71	−1.59	69STU/WES
$S°$ =	293.01	293.04	−0.03	69STU/WES
$\Delta_f S°$ =		−121.64		
$\Delta_f G°$ =		199.32		
$\ln K_f$ =		−80.40		

TABLE 7. *n*-Alkenes (32) — Continued

1,2-Pentadiene C_5H_8

(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)(C$_d$)) + (1×C$_d$–(H)(C)) + (1×C$_a$) + (1×C$_d$–(H)$_2$), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	140.67	142.17	−1.50	55FRA/PRO
$C_p°$ =	105.44	102.34	3.10	69STU/WES
$S°$ =	333.46	331.24	2.22	69STU/WES
$\Delta_f S°$ =		−219.75		
$\Delta_f G°$ =		207.69		
$\ln K_f$ =		−83.78		
Liquid phase				
$\Delta_f H°$ =		114.14		
$C_p°$ =	150.83	148.78	2.05	70TOD/MES
$S°$ =	244.97	244.13	0.84	70TOD/MES
$\Delta_f S°$ =		−306.85		
$\Delta_f G°$ =		205.63		
$\ln K_f$ =		−82.95		

1,3-Butadiene C_4H_6

(2×C$_d$–(H)$_2$) + (2×C$_d$–(H)(C$_d$)), $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	108.82	109.20	−0.38	49PRO/MAR
$C_p°$ =	79.54	79.84	−0.30	69STU/WES
$S°$ =	278.74	280.76	−2.02	69STU/WES
$\Delta_f S°$ =		−133.92		
$\Delta_f G°$ =		149.13		
$\ln K_f$ =		−60.16		

cis-1,3-Pentadiene C_5H_8

(1×C–(H)$_3$(C)) + (1×C$_d$–(H)(C)) + (2×C$_d$–(H)(C$_d$)) + (1×C$_d$–(H)$_2$) + (1×*cis*(unsat) corr), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	82.76	81.79	0.97	55FRA/PRO
$C_p°$ =	94.56	94.90	−0.34	69STU/WES
$S°$ =	324.26	327.30	−3.04	69STU/WES
$\Delta_f S°$ =		−223.69		
$\Delta_f G°$ =		148.48		
$\ln K_f$ =		−59.90		
Liquid phase				
$\Delta_f H°$ =		54.82		
$C_p°$ =		152.79		
$S°$ =		224.67		
$\Delta_f S°$ =		−326.31		
$\Delta_f G°$ =		152.11		
$\ln K_f$ =		−61.36		

TABLE 7. *n*-Alkenes (16) – Continued

trans-1,3-Pentadiene C_5H_8

$(1\times C-(H)_3(C)) + (1\times C_d-(H)(C)) + (2\times C_d-(H)(C_d)) + (1\times C_d-(H)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	75.81	76.94	−1.13	55FRA/PRO
$C_p°$ =	103.34	102.93	0.41	69STU/WES
$S°$ =	319.66	322.24	−2.58	69STU/WES
$\Delta_f S°$ =		−228.75		
$\Delta_f G°$ =		145.14		
$\ln K_f$ =		−58.55		
Liquid phase				
$\Delta_f H°$ =		49.55		
$C_p°$ =		152.79		
$S°$ =		224.67		
$\Delta_f S°$ =		−326.31		
$\Delta_f G°$ =		146.84		
$\ln K_f$ =		−59.23		

1,4-Pentadiene C_5H_8

$(2\times C_d-(H)_2) + (2\times C_d-(H)(C)) + (1\times C-(H)_2(C_d)_2)$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	106.36	106.36	0.00	55FRA/PRO
$C_p°$ =	105.02	105.01	0.01	69STU/WES
$S°$ =	333.46	333.46	0.00	69STU/WES
$\Delta_f S°$ =		−217.53		
$\Delta_f G°$ =		171.22		
$\ln K_f$ =		−69.07		
Liquid phase				
$\Delta_f H°$ =	81.17	81.17	0.00	86TRC
$C_p°$ =	146.82	146.82	0.00	70MES/TOD
$S°$ =	248.86	248.86	0.00	70MES/TOD
$\Delta_f S°$ =		−302.12		
$\Delta_f G°$ =		171.25		
$\ln K_f$ =		−69.08		

2,3-Pentadiene C_5H_8

$(2\times C-(H)_3(C)) + (2\times C_d-(H)(C)) + (1\times C_a)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	133.05	130.79	2.26	55FRA/PRO
$C_p°$ =	101.25	104.80	−3.55	69STU/WES
$S°$ =	324.68	322.99	1.69	69STU/WES
$\Delta_f S°$ =		−228.00		
$\Delta_f G°$ =		198.77		
$\ln K_f$ =		−80.18		

TABLE 7. *n*-Alkenes (32) – Continued

2,3-Pentadiene (Continued) C_5H_8

$(2\times C-(H)_3(C)) + (2\times C_d-(H)(C)) + (1\times C_a)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	103.55	101.56	1.99	70MES/TOD
$C_p°$ =	152.34	152.20	0.14	70MES/TOD
$S°$ =	237.32	238.15	−0.83	70MES/TOD
$\Delta_f S°$ =		−312.83		
$\Delta_f G°$ =		194.83		
$\ln K_f$ =		−78.59		

Allene C_3H_4

$(1\times C_a) + (2\times C_d-(H)_2)$, $\sigma = 4$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	191.25	195.31	−4.06	36KIS/RUH2
$C_p°$ =	58.99	58.62	0.37	69STU/WES
$S°$ =	243.93	245.79	−1.86	69STU/WES
$\Delta_f S°$ =		−32.57		
$\Delta_f G°$ =		205.02		
$\ln K_f$ =		−82.70		

TABLE 8. *s*-Alkenes (34)

2-Methylpropene C_4H_8

$(2\times C\text{-}(H)_3(C)) + (1\times C_d\text{-}(H)_2) + (1\times C_d\text{-}(C)_2) + (2\times\text{-}CH_3 \text{ corr (tertiary)}), \sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−17.87	−18.58	0.71	51PRO/MAR
$C_p°$ =	89.12	87.94	1.18	69STU/WES
$S°$ =	293.59	295.29	−1.70	69STU/WES
$\Delta_f S°$ =		−249.96		
$\Delta_f G°$ =		55.94		
$\ln K_f$ =		−22.57		

2-Methyl-1-butene C_5H_{10}

$(2\times C\text{-}(H)_3(C)) + (1\times C_d\text{-}(H)_2) + (1\times C_d\text{-}(C)_2) + (1\times C\text{-}(H)_2(C)(C_d)) + (1\times\text{-}CH_3 \text{ corr (tertiary)}), \sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−35.10	−37.20	2.10	86TRC
$C_p°$ =	111.63	108.57	3.06	69STU/WES
$S°$ =	339.53	339.25	0.28	69STU/WES
$\Delta_f S°$ =		−342.30		
$\Delta_f G°$ =		64.86		
$\ln K_f$ =		−26.16		
Liquid phase				
$\Delta_f H°$ =	−60.96	−62.22	1.26	79GOO/SMI
$C_p°$ =	157.19	153.84	3.35	47TOD/OLI
$S°$ =	253.97	254.63	−0.66	47TOD/OLI
$\Delta_f S°$ =		−426.92		
$\Delta_f G°$ =		65.07		
$\ln K_f$ =		−26.25		

2-Methyl-1-pentene C_6H_{12}

$(2\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(C_d)) + (1\times C_d\text{-}(C)_2) + (1\times C_d\text{-}(H)_2) + (1\times\text{-}CH_3 \text{ corr (tertiary)}), \sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−59.37	−57.83	−1.54	56CAM/ROS
$C_p°$ =	135.60	131.46	4.14	69STU/WES
$S°$ =	382.17	378.41	3.76	69STU/WES
$\Delta_f S°$ =		439.45		
$\Delta_f G°$ =		73.19		
$\ln K_f$ =		−29.53		
Liquid phase				
$\Delta_f H°$ =	−89.96	−87.95	−2.01	60BAR/ROS
$C_p°$ =		184.26		
$S°$ =		287.01		
$\Delta_f S°$ =		−530.86		
$\Delta_f G°$ =		70.32		
$\ln K_f$ =		−28.37		

TABLE 8. *s*-Alkenes (34) — Continued

2-Methyl-2-butene C_5H_{10}

$(3\times C\text{-}(H)_3(C)) + (1\times C_d\text{-}(H)(C)) + (1\times C_d\text{-}(C)_2) + (2\times\text{-}CH_3 \text{ corr (tertiary)}), \sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−41.00	−50.84	9.84	49SCO/WAD
$C_p°$ =	105.02	111.03	−6.01	69STU/WES
$S°$ =	338.57	345.90	−7.33	69STU/WES
$\Delta_f S°$ =		−335.65		
$\Delta_f G°$ =		49.24		
$\ln K_f$ =		−19.86		
Liquid phase				
$\Delta_f H°$ =	−68.07	−76.98	8.91	79GOO/SMI
$C_p°$ =	152.80	157.26	−4.46	47TOD/OLI
$S°$ =	251.04	248.65	2.39	47TOD/OLI
$\Delta_f S°$ =		−432.90		
$\Delta_f G°$ =		52.09		
$\ln K_f$ =		−21.01		

2-Methyl-2-pentene C_6H_{12}

$(3\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)_2(C)(C_d)) + (1\times C_d\text{-}(H)(C)) + (1\times C_d\text{-}(C)_2) + (2\times\text{-}CH_3 \text{ corr (tertiary)}), \sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−66.86	−71.72	4.86	56CAM/ROS
$C_p°$ =	126.61	131.66	−5.05	69STU/WES
$S°$ =	378.44	384.10	−5.66	69STU/WES
$\Delta_f S°$ =		−433.76		
$\Delta_f G°$ =		57.61		
$\ln K_f$ =		−23.24		
Liquid phase				
$\Delta_f H°$ =	−98.53	−102.71	4.18	60BAR/ROS
$C_p°$ =		186.55		
$S°$ =		280.32		
$\Delta_f S°$ =		−537.55		
$\Delta_f G°$ =		57.56		
$\ln K_f$ =		−23.22		

2-Ethyl-1-butene C_6H_{12}

$(2\times C\text{-}(H)_3(C)) + (2\times C\text{-}(H)_2(C)(C_d)) + (1\times C_d\text{-}(C)_2) + (1\times C_d\text{-}(H)_2), \sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−56.02	−55.82	−0.20	56CAM/ROS
$C_p°$ =	133.55	129.20	4.35	69STU/WES
$S°$ =	376.60	371.69	4.91	69STU/WES
$\Delta_f S°$ =		−446.18		
$\Delta_f G°$ =		77.21		
$\ln K_f$ =		−31.15		

TABLE 8. s-Alkenes (34) — Continued

2-Ethyl-1-butene (Continued) C_6H_{12}

$(2\times C\text{-}(H)_3(C))+(2\times C\text{-}(H)_2(C)(C_d))+(1\times C_d\text{-}(C)_2)+(1\times C_d\text{-}(H)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−87.11	−85.77	−1.34	60BAR/ROS
$C_p°$ =		183.13		
$S°$ =		286.30		
$\Delta_fS°$ =		−531.57		
$\Delta_fG°$ =		72.72		
$\ln K_f$ =		−29.33		

3-Methyl-1-butene C_5H_{10}

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)(C)_2(C_d))+(2\times\text{-}CH_3\text{ corr (tertiary)})+(1\times C_d\text{-}(H)(C))+(1\times C_d\text{-}(H)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−27.75	−28.03	0.28	86TRC
$C_p°$ =	118.62	119.07	−0.45	69STU/WES
$S°$ =	333.46	334.56	−1.10	69STU/WES
$\Delta_fS°$ =		−346.99		
$\Delta_fG°$ =		75.43		
$\ln K_f$ =		−30.43		
Liquid phase				
$\Delta_fH°$ =	−51.60	−51.80	0.20	79GOO/SMI
$C_p°$ =	156.06	156.05	0.01	47TOD/OLI
$S°$ =	253.30	253.30	0.00	47TOD/OLI
$\Delta_fS°$ =		−428.26		
$\Delta_fG°$ =		75.88		
$\ln K_f$ =		−30.61		

3-Methyl-1-pentene C_6H_{12}

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)(C)_2(C_d))+(1\times\text{-}CH_3\text{ corr (tertiary)})+(1\times C_d\text{-}(H)(C))+(1\times C_d\text{-}(H)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−49.50	−46.40	−3.10	56CAM/ROS
$C_p°$ =	142.42	141.96	0.46	69STU/WES
$S°$ =	376.81	373.72	3.09	69STU/WES
$\Delta_fS°$ =		−444.14		
$\Delta_fG°$ =		86.02		
$\ln K_f$ =		−34.70		
Liquid phase				
$\Delta_fH°$ =	−78.16	−75.35	−2.81	60BAR/ROS
$C_p°$ =		186.47		
$S°$ =		285.68		
$\Delta_fS°$ =		−532.19		
$\Delta_fG°$ =		83.32		
$\ln K_f$ =		−33.61		

TABLE 8. s-Alkenes (34) — Continued

***cis*-3-Methyl-2-pentene** C_6H_{12}

$(3\times C\text{-}(H)_3(C))+(1\times\text{-}CH_3\text{ corr (tertiary)})+(1\times C\text{-}(H)_2(C)(C_d))+(1\times C_d\text{-}(C)_2)+(1\times cis\text{(unsat) corr})+(1\times C_d\text{-}(H)(C))$, $\sigma = 27$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−62.30	−64.61	2.31	56CAM/ROS
$C_p°$ =	126.61	123.63	2.98	69STU/WES
$S°$ =	378.44	380.03	−1.59	69STU/WES
$\Delta_fS°$ =		−437.84		
$\Delta_fG°$ =		65.93		
$\ln K_f$ =		−26.60		
Liquid phase				
$\Delta_fH°$ =	−94.47	−95.26	0.79	60BAR/ROS
$C_p°$ =		186.55		
$S°$ =		280.32		
$\Delta_fS°$ =		−537.55		
$\Delta_fG°$ =		65.01		
$\ln K_f$ =		−26.22		

***trans*-3-Methyl-2-pentene** C_6H_{12}

$(3\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)(C_d))+(1\times\text{-}CH_3\text{ corr (tertiary)})+(1\times C_d\text{-}(C)_2)+(1\times C_d\text{-}(H)(C))$, $\sigma = 27$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−63.14	−69.46	6.32	56CAM/ROS
$C_p°$ =	126.61	131.66	−5.05	69STU/WES
$S°$ =	381.83	374.97	6.86	69STU/WES
$\Delta_fS°$ =		−442.90		
$\Delta_fG°$ =		62.59		
$\ln K_f$ =		−25.25		
Liquid phase				
$\Delta_fH°$ =	−94.56	−100.53	5.97	60BAR/ROS
$C_p°$ =		186.55		
$S°$ =		280.32		
$\Delta_fS°$ =		−537.55		
$\Delta_fG°$ =		59.74		
$\ln K_f$ =		−24.10		

3-Methyl-*cis*-3-hexene C_7H_{14}

$(3\times C\text{-}(H)_3(C))+(1\times\text{-}CH_3\text{ corr (tertiary)})+(2\times C\text{-}(H)_2(C)(C_d))+(1\times C_d\text{-}(H)(C))+(1\times cis\text{(unsat) corr})+(1\times C_d\text{-}(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−79.41	−85.49	6.08	60CAM/ROS
$C_p°$ =		144.26		

TABLE 8. s-Alkenes (34) — Continued

3-Methyl-*cis*-3-hexene (Continued) C_7H_{14}

(3×C–(H)$_3$(C))+(1×–CH$_3$ corr (tertiary))+(2×C–(H)$_2$(C)(C$_d$))+(1×C$_d$–(H)(C))+(1×*cis*(unsat) corr)+(1×C$_d$–(C)$_2$)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−115.94	−120.99	5.05	61ROC/ROS
$C_p°$ =		215.84		
$S°$ =		311.99		
$\Delta_f S°$ =		−642.19		
$\Delta_f G°$ =		70.48		
$\ln K_f$ =		−28.43		

3-Methyl-*trans*-3-hexene C_7H_{14}

(3×C–(H)$_3$(C))+(1×–CH$_3$ corr (tertiary))+(2×C–(H)$_2$(C)(C$_d$))+(1×C$_d$–(H)(C))+(1×C$_d$–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−76.82	−90.34	13.52	60CAM/ROS
$C_p°$ =		152.29		
Liquid phase				
$\Delta_f H°$ =	−112.72	−126.26	13.54	61ROC/ROS
$C_p°$ =		215.84		
$S°$ =		311.99		
$\Delta_f S°$ =		−642.19		
$\Delta_f G°$ =		65.21		
$\ln K_f$ =		−26.30		

4-Methyl-1-pentene C_6H_{12}

(2×C–(H)$_3$(C))+(1×C–(H)(C)$_3$)+(2×–CH$_3$ corr (tertiary))+(1×C–(H)$_2$(C)(C$_d$))+(1×C$_d$–(H)$_2$)+(1×C$_d$–(H)(C)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−51.25	−48.45	−2.80	56CAM/ROS
$C_p°$ =	126.48	132.29	−5.81	69STU/WES
$S°$ =	367.73	369.54	−1.81	69STU/WES
$\Delta_f S°$ =		−448.32		
$\Delta_f G°$ =		85.22		
$\ln K_f$ =		−34.38		
Liquid phase				
$\Delta_f H°$ =	−80.04	−77.28	−2.76	60BAR/ROS
$C_p°$ =		176.60		
$S°$ =		289.15		
$\Delta_f S°$ =		−528.72		
$\Delta_f G°$ =		80.36		
$\ln K_f$ =		−32.42		

TABLE 8. s-Alkenes (34) — Continued

***cis*-4-Methyl-2-pentene** C_6H_{12}

(3×C–(H)$_3$(C))+(2×C$_d$–(H)(C))+(1×C–(H)(C)$_2$(C$_d$))+(2×–CH$_3$ corr (tertiary))+(1×*cis*(unsat) corr), σ = 27

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−57.49	−55.44	−2.05	56CAM/ROS
$C_p°$ =	133.55	134.13	−0.58	69STU/WES
$S°$ =	373.34	375.34	−2.00	69STU/WES
$\Delta_f S°$ =		−442.53		
$\Delta_f G°$ =		76.50		
$\ln K_f$ =		−30.86		
Liquid phase				
$\Delta_f H°$ =	−87.03	−84.84	−2.19	60BAR/ROS
$C_p°$ =		188.76		
$S°$ =		278.99		
$\Delta_f S°$ =		−538.88		
$\Delta_f G°$ =		75.83		
$\ln K_f$ =		−30.59		

***trans*-4-Methyl-2-pentene** C_6H_{12}

(3×C–(H)$_3$(C))+(2×–CH$_3$ corr (tertiary))+(1×C–(H)(C)$_2$(C$_d$))+(2×C$_d$–(H)(C)), σ = 27

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−61.50	−60.29	−1.21	56CAM/ROS
$C_p°$ =	141.42	142.16	−0.74	69STU/WES
$S°$ =	368.28	370.28	−2.00	69STU/WES
$\Delta_f S°$ =		−447.59		
$\Delta_f G°$ =		73.16		
$\ln K_f$ =		−29.51		
Liquid phase				
$\Delta_f H°$ =	−91.55	−90.11	−1.44	60BAR/ROS
$C_p°$ =		188.76		
$S°$ =		278.99		
$\Delta_f S°$ =		−538.88		
$\Delta_f G°$ =		70.56		
$\ln K_f$ =		−28.46		

***cis*-2,2-Dimethyl-3-hexene** C_8H_{16}

(4×C–(H)$_3$(C))+(1×C–(C)$_3$(C$_d$))+(3×–CH$_3$ corr (quaternary))+(1×C–(H)$_2$(C)(C$_d$))+(2×C$_d$–(H)(C))+(1×t-butyl *cis* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−89.29	−91.59	2.30	60CAM/ROS
$C_p°$ =		170.19		

TABLE 8. s-Alkenes (34) – Continued

cis-2,2-Dimethyl-3-hexene (Continued) C_8H_{16}

(4 × C–(H)₃(C)) + (1 × C–(C)₃(C_d)) + (3 × –CH₃ corr (quaternary)) + (1 × C–(H)₂(C)(C_d)) + (2 × C_d–(H)(C)) + (1 × t-butyl *cis* corr)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−126.44	−128.97	2.53	61ROC/ROS
$C_p°$ =		253.15		
$S°$ =		313.83		
$\Delta_f S°$ =		−776.66		
$\Delta_f G°$ =		102.59		
$\ln K_f$ =		−41.38		

trans-2,2-Dimethyl-3-hexene C_8H_{16}

(4 × C–(H)₃(C)) + (1 × C–(C)₃(C_d)) + (3 × –CH₃ corr (quaternary)) + (2 × C_d–(H)(C)) + (1 × C–(H)₂(C)(C_d))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−107.65	−108.83	1.18	60CAM/ROS
$C_p°$ =		170.19		
Liquid phase				
$\Delta_f H°$ =	−144.93	−146.45	1.52	61ROC/ROS
$C_p°$ =		253.15		
$S°$ =		313.83		
$\Delta_f S°$ =		−776.66		
$\Delta_f G°$ =		85.11		
$\ln K_f$ =		−34.33		

2,3-Dimethyl-1-butene C_6H_{12}

(3 × C–(H)₃(C)) + (1 × C–(H)(C)₂(C_d)) + (1 × C_d–(C)₂) + (1 × C_d–(H)₂) + (3 × –CH₃ corr (tertiary)), σ = 27

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−66.36	−64.73	−1.63	56CAM/ROS
$C_p°$ =	143.47	141.16	2.31	69STU/WES
$S°$ =	365.64	368.86	−3.22	69STU/WES
$\Delta_f S°$ =		−449.01		
$\Delta_f G°$ =		69.14		
$\ln K_f$ =		−27.89		
Liquid phase				
$\Delta_f H°$ =	−95.60	−93.48	−2.12	60BAR/ROS
$C_p°$ =		191.15		
$S°$ =		278.19		
$\Delta_f S°$ =		−539.68		
$\Delta_f G°$ =		67.42		
$\ln K_f$ =		−27.20		

TABLE 8. s-Alkenes (34) – Continued

2,3-Dimethyl-2-butene C_6H_{12}

(4 × C–(H)₃(C)) + (2 × C_d–(C)₂) + (4 × –CH₃ corr (tertiary)), σ = 162

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−69.79	−89.80	20.01	56CAN/ROS
$C_p°$ =	123.60	133.12	−9.52	69STU/WES
$S°$ =	364.64	365.30	−0.66	69STU/WES
$\Delta_f S°$ =		−452.57		
$\Delta_f G°$ =		45.13		
$\ln K_f$ =		−18.21		
Liquid phase				
$\Delta_f H°$ =	−102.42	−120.84	18.42	60BAR/ROS
$C_p°$ =	174.68	192.36	−17.68	55SCO/FIN
$S°$ =	270.20	273.54	−3.34	55SCO/FIN
$\Delta_f S°$ =		−544.33		
$\Delta_f G°$ =		41.45		
$\ln K_f$ =		−16.72		

2,4-Dimethyl-1-pentene C_7H_{14}

(3 × C–(H)₃(C)) + (1 × C–(H)(C)₃) + (1 × C–(H)₂(C)(C_d)) + (1 × C_d–(C)₂) + (1 × C_d–(H)₂) + (3 × –CH₃ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−83.81	−85.15	1.34	60CAM/ROS
$C_p°$ =		154.38		
Liquid phase				
$\Delta_f H°$ =	−116.98	−118.96	1.98	61ROC/ROS
$C_p°$ =		211.70		
$S°$ =		314.04		
$\Delta_f S°$ =		−640.14		
$\Delta_f G°$ =		71.90		
$\ln K_f$ =		−29.00		

2,4-Dimethyl-2-pentene C_7H_{14}

(4 × C–(H)₃(C)) + (1 × C–(H)(C)₂(C_d)) + (4 × –CH₃ corr (tertiary)) + (1 × C_d–(H)(C)) + (1 × C_d–(C)₂)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−88.70	−99.25	10.55	60CAM/ROS
$C_p°$ =		164.25		
Liquid phase				
$\Delta_f H°$ =	−123.09	−133.97	10.88	61ROC/ROS
$C_p°$ =		223.86		
$S°$ =		303.88		
$\Delta_f S°$ =		−650.30		
$\Delta_f G°$ =		59.92		
$\ln K_f$ =		−24.17		

TABLE 8. *s*-Alkenes (34) — Continued

3,3-Dimethyl-1-butene C_6H_{12}

(3 × C–(H)$_3$(C)) + (1 × C–(C)$_3$(C$_d$)) + (3 × –CH$_3$ corr (quaternary)) + (1 × C$_d$–(H)(C)) + (1 × C$_d$–(H)$_2$), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−61.59	−55.69	−5.90	56CAM/ROS
$C_p°$ =	126.48	126.47	0.01	69STU/WES
$S°$ =	343.76	343.76	0.00	69STU/WES
$\Delta_f S°$ =		−474.10		
$\Delta_f G°$ =		85.66		
$\ln K_f$ =		−34.56		
Liquid phase				
$\Delta_f H°$ =	−88.28	−82.41	−5.87	60BAR/ROS
$C_p°$ =	191.17	191.15	0.02	38KEN/SHO
$S°$ =	256.50	256.47	0.03	38KEN/SHO
$\Delta_f S°$ =		−561.40		
$\Delta_f G°$ =		84.97		
$\ln K_f$ =		−34.28		

***cis*-4,4-Dimethyl-2-pentene** C_7H_{14}

(4 × C–(H)$_3$(C)) + (1 × C–(C)$_3$(C$_d$)) + (3 × –CH$_3$ corr (quaternary)) + (2 × C$_d$–(H)(C)) + (1 × t-butyl *cis* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−72.63	−70.71	−1.92	60CAM/ROS
$C_p°$ =		149.56		
Liquid phase				
$\Delta_f H°$ =	−105.31	−103.24	−2.07	61ROC/ROS
$C_p°$ =		223.86		
$S°$ =		282.16		
$\Delta_f S°$ =		−672.02		
$\Delta_f G°$ =		97.12		
$\ln K_f$ =		−39.18		

***trans*-4,4-Dimethyl-2-pentene** C_7H_{14}

(4 × C–(H)$_3$(C)) + (1 × C–(C)$_3$(C$_d$)) + (3 × –CH$_3$ corr (quaternary)) + (2 × C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−88.78	−87.95	−0.83	60CAM/ROS
$C_p°$ =		149.56		

TABLE 8. *s*-Alkenes (34) — Continued

***trans*-4,4-Dimethyl-2-pentene (Continued)** C_7H_{14}

(4 × C–(H)$_3$(C)) + (1 × C–(C)$_3$(C$_d$)) + (3 × –CH$_3$ corr (quaternary)) + (2 × C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−121.71	−120.72	−0.99	61ROC/ROS
$C_p°$ =		223.86		
$S°$ =		282.16		
$\Delta_f S°$ =		−672.02		
$\Delta_f G°$ =		79.64		
$\ln K_f$ =		−32.13		

2,3,3-Trimethyl-1-butene C_7H_{14}

(4 × C–(H)$_3$(C)) + (1 × C–(C)$_3$(C$_d$)) + (3 × –CH$_3$ corr (quaternary)) + (1 × C$_d$–(C)$_2$) + (1 × –CH$_3$ corr (tertiary)) + (1 × C$_d$–(H)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−85.48	−92.39	6.91	60CAM/ROS
$C_p°$ =		148.56		
Liquid phase				
$\Delta_f H°$ =	−117.70	−124.09	6.39	61ROC/ROS
$C_p°$ =		226.25		
$S°$ =		281.36		
$\Delta_f S°$ =		−672.82		
$\Delta_f G°$ =		76.51		
$\ln K_f$ =		−30.86		

***cis*-2,5-Dimethyl-3-hexene** C_8H_{16}

(4 × C–(H)$_3$(C)) + (2 × C–(H)(C)$_2$(C$_d$)) + (4 × –CH$_3$ corr (tertiary)) + (2 × C$_d$–(H)(C)) + (1 × *cis*(unsat) corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−103.85		
$C_p°$ =		187.35		
Liquid phase				
$\Delta_f H°$ =	−151.08	−141.83	−9.25	73YAT/MCD
$C_p°$ =		255.36		
$S°$ =		334.22		
$\Delta_f S°$ =		−756.27		
$\Delta_f G°$ =		83.65		
$\ln K_f$ =		−33.74		

TABLE 8. *s*-Alkenes (34) — Continued

trans-2,5-Dimethyl-3-hexene C_8H_{16}
(4×C–(H)$_3$(C)) + (2×C–(H)(C)$_2$(C$_d$)) + (4×–CH$_3$ corr (tertiary)) + (2×C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−108.70		
$C_p°$ =		195.38		
Liquid phase				
$\Delta_f H°$ =	−159.28	−147.10	−12.18	73YAT/MCD
$C_p°$ =		255.36		
$S°$ =		334.22		
$\Delta_f S°$ =		−756.27		
$\Delta_f G°$ =		78.38		
$\ln K_f$ =		−31.62		

2,4,4-Trimethyl-1-pentene C_8H_{16}
(4×C–(H)$_3$(C)) + (1×C–(C)$_4$) + (3×–CH$_3$ corr (quaternary)) + (1×C–(H)$_2$(C)(C$_d$)) + (1×C$_d$–(C)$_2$) + (1×C$_d$–(H)$_2$) + (1×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−110.37	−116.20	5.83	60CAM/ROS
$C_p°$ =		176.56		
Liquid phase				
$\Delta_f H°$ =	−146.15	−152.62	6.47	61ROC/ROS
$C_p°$ =	240.20	237.04	3.16	36PAR/TOD2
$S°$ =	311.71	322.58	−10.87	36PAR/TOD2
$\Delta_f S°$ =		−767.91		
$\Delta_f G°$ =		76.33		
$\ln K_f$ =		−30.79		

2,4,4-Trimethyl-2-pentene C_8H_{16}
(5×C–(H)$_3$(C)) + (1×C–(C)$_3$(C$_d$)) + (3×–CH$_3$ corr (quaternary)) + (1×C$_d$–(H)(C)) + (1×C$_d$–(C)$_2$) + (2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−104.89	−126.91	22.02	60CAM/ROS
$C_p°$ =		171.65		
Liquid phase				
$\Delta_f H°$ =	−142.42	−164.58	22.16	61ROC/ROS
$C_p°$ =		258.96		
$S°$ =		307.05		
$\Delta_f S°$ =		−783.44		
$\Delta_f G°$ =		69.00		
$\ln K_f$ =		−27.83		

TABLE 8. *s*-Alkenes (34) — Continued

2-Methyl-3-ethyl-1-pentene C_8H_{16}
(3×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(C$_d$)) + (1×C$_d$–(C)$_2$) + (1×C$_d$–(H)$_2$) + (1×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−100.29	−101.47	1.18	60CAM/ROS
$C_p°$ =		186.94		
Liquid phase				
$\Delta_f H°$ =	−136.36	−140.58	4.22	61ROC/ROS
$C_p°$ =		251.99		
$S°$ =		342.95		
$\Delta_f S°$ =		−747.54		
$\Delta_f G°$ =		82.30		
$\ln K_f$ =		−33.20		

3-Methyl-2-ethyl-1-butene C_7H_{14}
(3×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(C$_d$)) + (2×–CH$_3$ corr (tertiary)) + (1×C–(H)$_2$(C)(C$_d$)) + (1×C$_d$–(C)$_2$) + (1×C$_d$–(H)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−79.54	−83.35	3.81	60CAM/ROS
$C_p°$ =		161.79		
Liquid phase				
$\Delta_f H°$ =	−114.06	−117.03	2.97	61ROC/ROS
$C_p°$ =		220.44		
$S°$ =		309.86		
$\Delta_f S°$ =		−644.32		
$\Delta_f G°$ =		75.07		
$\ln K_f$ =		−30.28		

2-Methyl-1,3-butadiene C_5H_8
(1×C–(H)$_3$(C)) + (2×C$_d$–(H)$_2$) + (1×C$_d$–(H)(C$_d$)) + (1×C$_d$–(C)(C$_d$)) + (1×–CH$_3$ corr (tertiary)), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	75.73	73.18	2.55	55FRA/PRO
$C_p°$ =	104.60	104.60	0.00	69STU/WES
$S°$ =	315.64	315.64	0.00	69STU/WES
$\Delta_f S°$ =		−235.35		
$\Delta_f G°$ =		143.35		
$\ln K_f$ =		−57.83		
Liquid phase				
$\Delta_f H°$ =	48.95	46.31	2.64	36BEK/WOO
$C_p°$ =	151.08	151.08	0.00	70MES/TOD
$S°$ =	228.28	227.06	1.22	70MES/TOD
$\Delta_f S°$ =		−323.92		
$\Delta_f G°$ =		142.89		
$\ln K_f$ =		−57.64		

TABLE 8. *s*-Alkenes (34) – Continued

3-Methyl-1,2-butadiene C_5H_8

$(2\times C\text{-}(H)_3(C))+(1\times C_d\text{-}(C)_2)+(2\times\text{-}CH_3 \text{ corr (tertiary)})+(1\times C_d\text{-}(H)_2)+(1\times C_a)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	129.08	124.09	4.99	86TRC
$C_p°$ =	105.44	103.80	1.64	69STU/WES
$S°$ =	319.66	321.57	−1.91	69STU/WES
$\Delta_fS°$ =		−229.42		
$\Delta_fG°$ =		192.49		
$\ln K_f$ =		−77.65		
Liquid phase				
$\Delta_fH°$ =	101.17	96.01	5.16	69GOO2
$C_p°$ =	152.42	154.59	−2.17	70MES/TOD
$S°$ =	231.79	237.35	−5.56	70MES/TOD
$\Delta_fS°$ =		−313.63		
$\Delta_fG°$ =		189.52		
$\ln K_f$ =		−76.45		

2,3-Dimethyl-1,3-butadiene C_6H_{10}

$(2\times C\text{-}(H)_3(C))+(2\times C_d\text{-}(H)_2)+(2\times C_d\text{-}(C)(C_d))+(2\times\text{-}CH_3 \text{ corr (tertiary)})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	45.10	37.16	7.94	37DOL/GRE
$C_p°$ =		129.36		
Liquid phase				
$\Delta_fH°$ =	14.14	4.76	9.38	55CUM/MCL
$C_p°$ =		182.08		
$S°$ =		255.14		
$\Delta_fS°$ =		−432.15		
$\Delta_fG°$ =		133.61		
$\ln K_f$ =		−53.90		

TABLE 9. Alkynes (28)

Acetylene C_2H_2

$(2\times C_t\text{-}(H))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	228.19	227.00	1.19	39CON/KIS
$C_p°$ =	43.93	45.10	−1.17	69STU/WES
$S°$ =	200.83	198.16	2.67	69STU/WES
$\Delta_fS°$ =		56.11		
$\Delta_fG°$ =		210.27		
$\ln K_f$ =		−84.82		

Propyne C_3H_4

$(1\times C\text{-}(H)_3(C))+(1\times C_t\text{-}(C))+(1\times C_t\text{-}(H))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	184.93	186.34	−1.41	39CON/KIS
$C_p°$ =	60.67	61.50	−0.83	69STU/WES
$S°$ =	248.11	246.47	1.64	69STU/WES
$\Delta_fS°$ =		−31.90		
$\Delta_fG°$ =		195.85		
$\ln K_f$ =		−79.00		

1-Butyne C_4H_6

$(1\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)(C_t))+(1\times C_t\text{-}(C))+(1\times C_t\text{-}(H))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	165.23	166.64	−1.41	51PRO/MAR
$C_p°$ =	81.42	82.47	−1.05	69STU/WES
$S°$ =	290.83	289.27	1.56	69STU/WES
$\Delta_fS°$ =		−125.41		
$\Delta_fG°$ =		204.03		
$\ln K_f$ =		−82.30		

1-Pentyne C_5H_8

$(1\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_2(C)(C_t))+(1\times C_t\text{-}(C))+(1\times C_t\text{-}(H))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		146.01		
$C_p°$ =	106.69	105.36	1.33	69STU/WES
$S°$ =	329.78	328.43	1.35	69STU/WES
$\Delta_fS°$ =		−222.56		
$\Delta_fG°$ =		212.37		
$\ln K_f$ =		−85.67		

TABLE 9. Alkynes (28) – Continued

1-Pentyne (Continued) C_5H_8

$(1 \times C\text{-}(H)_3(C)) + (1 \times C\text{-}(H)_2(C)_2) + (1 \times C\text{-}(H)_2(C)(C_t)) + (1 \times C_t\text{-}(C)) + (1 \times C_t\text{-}(H))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_f H^\circ =$		116.15		
$C_p^\circ =$		162.84		
$S^\circ =$		229.86		
$\Delta_f S^\circ =$		−321.12		
$\Delta_f G^\circ =$		211.89		
$\ln K_f =$		−85.48		

1-Hexyne C_6H_{10}

$(1 \times C\text{-}(H)_3(C)) + (2 \times C\text{-}(H)_2(C)_2) + (1 \times C\text{-}(H)_2(C)(C_t)) + (1 \times C_t\text{-}(C)) + (1 \times C_t\text{-}(H))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H^\circ =$	122.30	125.38	−3.08	79ROG/DAG
$C_p^\circ =$	128.24	128.25	−0.01	69STU/WES
$S^\circ =$	368.74	367.59	1.15	69STU/WES
$\Delta_f S^\circ =$		−319.71		
$\Delta_f G^\circ =$		220.70		
$\ln K_f =$		−89.03		
Liquid Phase				
$\Delta_f H^\circ =$		90.42		
$C_p^\circ =$		193.26		
$S^\circ =$		262.24		
$\Delta_f S^\circ =$		−425.05		
$\Delta_f G^\circ =$		217.15		
$\ln K_f =$		−87.60		

1-Heptyne C_7H_{12}

$(1 \times C\text{-}(H)_3(C)) + (3 \times C\text{-}(H)_2(C)_2) + (1 \times C\text{-}(H)_2(C)(C_t)) + (1 \times C_t\text{-}(C)) + (1 \times C_t\text{-}(H))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H^\circ =$	103.76	104.75	−0.99	79ROG/DAG
$C_p^\circ =$	151.08	151.14	−0.06	69STU/WES
$S^\circ =$	407.69	406.75	0.94	69STU/WES
$\Delta_f S^\circ =$		−416.86		
$\Delta_f G^\circ =$		229.04		
$\ln K_f =$		−92.39		
Liquid Phase				
$\Delta_f H^\circ =$		64.69		
$C_p^\circ =$		223.68		
$S^\circ =$		294.62		
$\Delta_f S^\circ =$		−528.99		
$\Delta_f G^\circ =$		222.41		
$\ln K_f =$		−89.72		

TABLE 9. Alkynes (28) – Continued

1-Octyne C_8H_{14}

$(1 \times C\text{-}(H)_3(C)) + (4 \times C\text{-}(H)_2(C)_2) + (1 \times C\text{-}(H)_2(C)(C_t)) + (1 \times C_t\text{-}(C)) + (1 \times C_t\text{-}(H))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H^\circ =$	80.71	84.12	−3.41	79ROG/DAG
$C_p^\circ =$	173.97	174.03	−0.06	69STU/WES
$S^\circ =$	446.64	445.91	0.73	69STU/WES
$\Delta_f S^\circ =$		−514.01		
$\Delta_f G^\circ =$		237.37		
$\ln K_f =$		−95.75		
Liquid Phase				
$\Delta_f H^\circ =$		38.96		
$C_p^\circ =$		254.10		
$S^\circ =$		327.00		
$\Delta_f S^\circ =$		−632.92		
$\Delta_f G^\circ =$		227.66		
$\ln K_f =$		−91.84		

1-Nonyne C_9H_{16}

$(1 \times C\text{-}(H)_3(C)) + (5 \times C\text{-}(H)_2(C)_2) + (1 \times C\text{-}(H)_2(C)(C_t)) + (1 \times C_t\text{-}(C)) + (1 \times C_t\text{-}(H))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H^\circ =$	62.25	63.49	−1.24	79ROG/DAG
$C_p^\circ =$	196.82	196.92	−0.10	69STU/WES
$S^\circ =$	485.60	485.07	0.53	69STU/WES
$\Delta_f S^\circ =$		−611.16		
$\Delta_f G^\circ =$		245.71		
$\ln K_f =$		−99.12		
Liquid Phase				
$\Delta_f H^\circ =$		13.23		
$C_p^\circ =$		284.52		
$S^\circ =$		359.38		
$\Delta_f S^\circ =$		−736.85		
$\Delta_f G^\circ =$		232.92		
$\ln K_f =$		−93.96		

1-Decyne $C_{10}H_{18}$

$(1 \times C\text{-}(H)_3(C)) + (6 \times C\text{-}(H)_2(C)_2) + (1 \times C\text{-}(H)_2(C)(C_t)) + (1 \times C_t\text{-}(C)) + (1 \times C_t\text{-}(H))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H^\circ =$	41.88	42.86	−0.98	79ROG/DAG
$C_p^\circ =$	219.70	219.81	−0.11	69STU/WES
$S^\circ =$	524.51	524.23	0.28	69STU/WES
$\Delta_f S^\circ =$		−708.31		
$\Delta_f G^\circ =$		254.04		
$\ln K_f =$		−102.48		

TABLE 9. Alkynes (28) — Continued

1-Decyne $C_{10}H_{18}$
(1×C–(H)$_3$(C))+(6×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(C$_t$))+(1×C$_t$–(C))+(1×C$_t$–(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	41.88	42.86	−0.98	79ROG/DAG
$C_p°$ =	219.70	219.81	−0.11	69STU/WES
$S°$ =	524.51	524.23	0.28	69STU/WES
$\Delta_fS°$ =		−708.31		
$\Delta_fG°$ =		254.04		
$\ln K_f$ =		−102.48		
Liquid Phase				
$\Delta_fH°$ =		−12.50		
$C_p°$ =		314.94		
$S°$ =		391.76		
$\Delta_fS°$ =		−840.78		
$\Delta_fG°$ =		238.18		
$\ln K_f$ =		−96.08		

1-Hexadecyne $C_{16}H_{30}$
(1×C–(H)$_3$(C))+(12×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(C$_t$))+(1×C$_t$–(C))+(1×C$_t$–(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−80.92		
$C_p°$ =	356.94	357.15	−0.21	69STU/WES
$S°$ =	758.22	759.19	−0.97	69STU/WES
$\Delta_fS°$ =		−1291.22		
$\Delta_fG°$ =		304.06		
$\ln K_f$ =		−122.65		
Liquid Phase				
$\Delta_fH°$ =		−166.88		
$C_p°$ =		497.46		
$S°$ =		586.04		
$\Delta_fS°$ =		−1464.36		
$\Delta_fG°$ =		269.72		
$\ln K_f$ =		−108.80		

2-Butyne C_4H_6
(2×C–(H)$_3$(C))+(2×C$_t$–(C)), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	145.14	145.68	−0.54	51PRO/MAR
$C_p°$ =	77.95	77.90	0.05	69STU/WES
$S°$ =	283.30	283.25	0.05	69STU/WES
$\Delta_fS°$ =		−131.43		
$\Delta_fG°$ =		184.86		
$\ln K_f$ =		−74.57		

2-Butyne (Continued) C_4H
(2×C–(H)$_3$(C))+(2×C$_t$–(C)), σ = 18

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	118.53	119.08	−0.55	50AST/MAS
$C_p°$ =	124.14	124.14	0.00	50AST/MAS
$S°$ =	195.10	195.10	0.00	50AST/MAS
$\Delta_fS°$ =		−219.57		
$\Delta_fG°$ =		184.55		
$\ln K_f$ =		−74.44		

2-Pentyne C_5H
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)(C$_t$))+(2×C$_t$–(C)), σ = 9

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	128.87	125.98	2.89	69STU/WES
$C_p°$ =	98.70	98.87	−0.17	69STU/WES
$S°$ =	331.79	331.81	−0.02	69STU/WES
$\Delta_fS°$ =		−219.17		
$\Delta_fG°$ =		191.33		
$\ln K_f$ =		−77.18		
Liquid Phase				
$\Delta_fH°$ =		96.95		
$C_p°$ =		154.53		
$S°$ =		227.46		
$\Delta_fS°$ =		−323.52		
$\Delta_fG°$ =		193.41		
$\ln K_f$ =		−78.02		

3-Methyl-1-butyne C_5H_8
(2×C–(H)$_3$(C))+(1×C–(H)(C)$_2$(C$_t$))+(2×–CH$_3$ corr (tertiary))+(1×C$_t$–(C))+(1×C$_t$–(H)), σ = 9

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	136.40	136.40	0.00	69STU/WES
$C_p°$ =	104.68	104.68	0.00	69STU/WES
$S°$ =	318.95	318.96	−0.01	69STU/WES
$\Delta_fS°$ =		−232.02		
$\Delta_fG°$ =		205.58		
$\ln K_f$ =		−82.93		

TABLE 9. Alkynes (28) – Continued

1-Buten-3-yne C_4H_4

$(1\times C_t-(H))+(1\times C_t-(C_d))+(1\times C_d-(H)(C_t))+(1\times C_d-(H)_2)$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		289.52		
$C_p°$ =	73.18	73.18	0.00	69STU/WES
$S°$ =	279.37	279.38	−0.01	69STU/WES
$\Delta_f S°$ =		−4.73		
$\Delta_f G°$ =		290.93		
$\ln K_f$ =		−117.36		

***cis*-3-Penten-1-yne** C_5H_6

$(1\times C-(H)_3(C))+(1\times C_d-(H)(C))+(1\times C_d-(H)(C_t))+(1\times C_t-(C_d)) + (1\times C_t-(H))+(1\times cis\text{(unsat) corr})$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		262.11		
$C_p°$ =		88.24		
Liquid Phase				
$\Delta_f H°$ =	226.35	230.13	−3.78	59SKI/SNE

***trans*-3-Penten-1-yne** C_5H_6

$(1\times C-(H)_3(C))+(1\times C_d-(H)(C))+(1\times C_d-(H)(C_t))+(1\times C_t-(C_d)) + (1\times C_t-(H))$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		257.26		
$C_p°$ =		96.27		
Liquid Phase				
$\Delta_f H°$ =	228.02	224.86	3.16	59SKI/SNE

***cis*-3-Decen-1-yne** $C_{10}H_{16}$

$(1\times C-(H)_3(C))+(4\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_d))+(1\times C_d-(H)(C))+(1\times cis\text{(unsat) corr})+(1\times C_d-(H)(C_t))+(1\times C_t-(C_d))+(1\times C_t-(H))$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		158.71		
$C_p°$ =		200.43		
Liquid Phase				
$\Delta_f H°$ =	99.50	101.48	−1.98	59SKI/SNE

***trans*-3-Decen-1-yne** $C_{10}H_{16}$

$(1\times C-(H)_3(C))+(4\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_d))+(1\times C_d-(H)(C))+(1\times C_d-(H)(C_t))+(1\times C_t-(C_d))+(1\times C_t-(H))$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		153.86		
$C_p°$ =		208.46		
Liquid Phase				
$\Delta_f H°$ =	100.75	96.21	4.54	59SKI/SNE

1-Octen-3-yne C_8H_{12}

$(1\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_t))+(1\times C_t-(C))+(1\times C_t-(C_d))+(1\times C_d-(H)(C_t))+(1\times C_d-(H)_2)$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		187.90		
$C_p°$ =		156.33		
Liquid Phase				
$\Delta_f H°$ =	140.71	144.65	−3.94	57FLI/SKI

Butadiyne C_4H_2

$(2\times C_t-(H))+(2\times C_t-(C_t))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	472.79	468.52	4.27	69STU/WES
$C_p°$ =	73.64	73.64	0.00	69STU/WES
$S°$ =	250.04	250.04	0.00	69STU/WES
$\Delta_f S°$ =		96.51		
$\Delta_f G°$ =		439.75		
$\ln K_f$ =		−177.39		

1,5-Hexadiyne C_6H_6

$(2\times C_t-(H))+(2\times C_t-(C))+(1\times C-(H)_2(C_t)_2)$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		416.06		
Liquid Phase				
$\Delta_f H°$ =	384.09	384.16	−0.07	59SKI/SNE

TABLE 9. Alkynes (28) — Continued

1,7-Octadiyne C_8H_{10}

$(2\times C_t-(H))+(2\times C_t-(C))+(2\times C-(H)_2(C)(C_t))+(2\times C-(H)_2(C)_2)$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =		376.54		
C_p° =		159.26		
Liquid Phase				
Δ_fH° =	334.72	327.52	7.20	57FLI/SKI
C_p° =		252.72		
S° =		293.12		
Δ_fS° =		−405.65		
Δ_fG° =		448.47		
$\ln K_f$ =		−180.91		

3,9-Dodecadiyne $C_{12}H_{18}$

$(2\times C-(H)_3(C))+(4\times C-(H)_2(C)(C_t))+(4\times C_t-(C))+(2\times C-(H)_2(C)_2)$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =		255.82		
C_p° =		234.00		
Liquid Phase				
Δ_fH° =	196.61	193.40	3.21	57FLI/SKI
C_p° =		357.72		
S° =		417.80		
Δ_fS° =		−826.22		
Δ_fG° =		439.74		
$\ln K_f$ =		−177.39		

5,7-Dodecadiyne $C_{12}H_{18}$

$(2\times C-(H)_3(C))+(4\times C-(H)_2(C)_2)+(2\times C-(H)_2(C)(C_t))+(2\times C_t-(C))+(2\times C_t-(C_t))$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =		265.28		
C_p° =		239.94		
Liquid Phase				
Δ_fH° =	180.29	181.50	−1.21	57FLI/SKI

TABLE 9. Alkynes (28) — Continued

3,3-Dimethyl-1-butyne C_6H_{10}

$(3\times C-(H)_3(C))+(1\times C_t-(H))+(1\times C_t-(C))+(1\times C-(C)_3(C_t))+(3\times -CH_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Liquid Phase				
Δ_fH° =	78.45	78.45	0.00	77KUP/SHI

3,3-Dimethylpenta-1,4-diyne C_7H_8

$(2\times C-(H)_3(C))+(2\times C_t-(H))+(2\times C_t-(C))+(1\times C-(C)_2(C_t)_2)$

	Literature	Calculated	Residual	Reference
Liquid Phase				
Δ_fH° =	348.69	348.69	0.00	77KUP/SHI

3,3,6,6,-Tetramethylocta-1,7-diyne $C_{12}H_{18}$

$(4\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(2\times C_t-(H))+(2\times C_t-(C))+(2\times C-(C)_3(C_t))+(4\times -CH_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Liquid Phase				
Δ_fH° =	211.08	209.44	1.64	77KUP/SHI

2,2,7,7-Tetramethylocta-3,5-diyne $C_{12}H_{18}$

$(6\times C-(H)_3(C))+(2\times C-(C)_3(C_t))+(2\times C_t-(C))+(2\times C_t-(C_t))+(6\times -CH_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Liquid Phase				
Δ_fH° =		157.56		
Solid Phase				
Δ_fH° =	156.10	156.10	0.00	77KUP/SHI

TABLE 10. Aromatic CH-01 (42)

Benzene C_6H_6

$(6\times C_B-(H)(C_B)_2)$, $\sigma = 12$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	82.80	82.86	−0.06	47OSB/GIN
C_p° =	81.67	81.66	0.01	69STU/WES
S° =	269.20	269.20	0.00	69STU/WES
$\Delta_f S^\circ$ =		−156.95		
$\Delta_f G^\circ$ =		129.66		
$\ln K_f$ =		−52.30		
Liquid phase				
$\Delta_f H^\circ$ =	48.95	48.96	−0.01	69GOO/SMI
C_p° =	136.06	136.08	−0.02	48OLI/EAT
S° =	173.26	173.22	0.04	48OLI/EAT
$\Delta_f S^\circ$ =		−252.93		
$\Delta_f G^\circ$ =		124.37		
$\ln K_f$ =		−50.17		
Solid phase				
$\Delta_f H^\circ$ =	39.08	39.18	−0.10	48OLI/EAT
C_p° =		120.78		
S° =		136.50		
$\Delta_f S^\circ$ =		−289.65		
$\Delta_f G^\circ$ =		125.54		
$\ln K_f$ =		−50.64		

Toluene C_7H_8

$(1\times C-(H)_3(C)) + (5\times C_B-(H)(C_B)_2) + (1\times C_B-(C)(C_B)_2)$, $\sigma = 6$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	50.00	50.43	−0.43	47OSB/GIN
C_p° =	103.64	103.53	0.11	69STU/WES
S° =	320.66	318.36	2.30	69STU/WES
$\Delta_f S^\circ$ =		−244.10		
$\Delta_f G^\circ$ =		123.21		
$\ln K_f$ =		−49.70		
Liquid phase				
$\Delta_f H^\circ$ =	12.01	12.35	−0.34	69GOO/SMI
C_p° −	157.23	159.98	−2.75	62SCO/GUT
S° =	220.96	208.15	12.81	62SCO/GUT
$\Delta_f S^\circ$ =		−354.31		
$\Delta_f G^\circ$ =		117.99		
$\ln K_f$ −		47.60		

TABLE 10. Aromatic CH-01 (42) – Continued

1,2-Dimethylbenzene C_8H_{10}

$(2\times C-(H)_3(C)) + (4\times C_B-(H)(C_B)_2) + (2\times C_B-(C)(C_B)_2) + (1\times \textit{ortho}\ \text{corr})$, $\sigma = 18$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	19.08	19.26	−0.18	47OSB/GIN
C_p° =	133.26	131.80	1.46	69STU/WES
S° =	352.75	350.13	2.62	69STU/WES
$\Delta_f S^\circ$ =		−348.65		
$\Delta_f G^\circ$ =		123.21		
$\ln K_f$ =		−49.70		
Liquid phase				
$\Delta_f H^\circ$ =	−24.35	−21.00	−3.35	45PRO/GIL
C_p° =	187.82	187.38	0.44	43PIT/SCO
S° =	246.02	243.08	2.94	43PIT/SCO
$\Delta_f S^\circ$ =		−455.69		
$\Delta_f G^\circ$ =		114.87		
$\ln K_f$ =		−46.34		

1,3-Dimethylbenzene C_8H_{10}

$(2\times C-(H)_3(C)) + (4\times C_B-(H)(C_B)_2) + (2\times C_B-(C)(C_B)_2) + (1\times \textit{meta}\ \text{corr})$, $\sigma = 18$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	17.32	17.37	−0.05	47OSB/GIN
C_p° =	127.57	126.11	1.46	69STU/WES
S° =	357.69	352.63	5.06	69STU/WES
$\Delta_f S^\circ$ =		−346.15		
$\Delta_f G^\circ$ =		120.57		
$\ln K_f$ =		−48.64		
Liquid phase				
$\Delta_f H^\circ$ =	−25.36	−24.26	−1.10	45PRO/GIL
C_p° =	183.18	183.88	−0.70	43PIT/SCO
S° =	253.80	243.08	10.72	43PIT/SCO
$\Delta_f S^\circ$ =		−455.69		
$\Delta_f G^\circ$ =		111.61		
$\ln K_f$ =		−45.02		

1,4-Dimethylbenzene C_8H_{10}

$(2\times C-(H)_3(C)) + (4\times C_B-(H)(C_B)_2) + (2\times C_B-(C)(C_B)_2)$, $\sigma = 18$

	Literature	Calculated	− Residual	Reference
Gas phase				
$\Delta_f H^\circ$ −	18.03	18.00	0.03	47OSD/GIN
C_p° =	126.86	125.40	1.46	69STU/WES
S° =	352.42	352.63	−0.21	69STU/WES
$\Delta_f S^\circ$ =		−346.15		
$\Delta_f G^\circ$ −		121.20		
$\ln K_f$ =		−48.89		

TABLE 10. Aromatic CH-01 (42) – Continued

1,4-Dimethylbenzene C_8H_{10}

$(2\times C\text{-}(H)_3(C))+(4\times C_B\text{-}(H)(C_B)_2)+(2\times C_B\text{-}(C)(C_B)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−24.35	−24.26	−0.09	45PRO/GIL
$C_p°$ =	183.76	183.88	−0.12	43PIT/SCO
$S°$ =	243.51	243.08	0.43	43PIT/SCO
$\Delta_f S°$ =		−455.69		
$\Delta_f G°$ =		111.61		
$\ln K_f$ =		−45.02		

1,2,3-Trimethylbenzene C_9H_{12}

$(3\times C\text{-}(H)_3(C))+(3\times C_B\text{-}(H)(C_B)_2)+(3\times C_B\text{-}(C)(C_B)_2)+(2\times ortho\text{ corr})+(1\times meta\text{ corr})$, $\sigma = 54$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−9.46	−12.54	3.08	47OSB/GIN
$C_p°$ =	154.18	160.78	−6.60	69STU/WES
$S°$ =	384.84	381.89	2.95	69STU/WES
$\Delta_f S°$ =		−453.19		
$\Delta_f G°$ =		122.58		
$\ln K_f$ =		−49.45		
Liquid phase				
$\Delta_f H°$ =	−58.53	−54.35	−4.18	45JOH/PRO
$C_p°$ =	216.44	214.78	1.66	55TAY/JOH
$S°$ =	267.94	278.01	−10.07	55TAY/JOH
$\Delta_f S°$ =		−557.08		
$\Delta_f G°$ =		111.74		
$\ln K_f$ =		−45.08		

1,2,4-Trimethylbenzene C_9H_{12}

$(3\times C\text{-}(H)_3(C))+(3\times C_B\text{-}(H)(C_B)_2)+(3\times C_B\text{-}(C)(C_B)_2)+(1\times ortho\text{ corr})+(1\times meta\text{ corr})$, $\sigma = 27$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−13.85	−13.80	−0.05	47OSB/GIN
$C_p°$ =	154.01	154.38	−0.37	69STU/WES
$S°$ =	395.76	390.16	5.60	69STU/WES
$\Delta_f S°$ =		−444.93		
$\Delta_f G°$ =		118.86		
$\ln K_f$ =		−47.95		
Liquid phase				
$\Delta_f H°$ =	−61.80	−57.61	−4.19	45JOH/PRO
$C_p°$ =	214.97	211.28	3.69	57PUT/KIL
$S°$ =	283.38	278.01	5.37	57PUT/KIL
$\Delta_f S°$ =		−557.08		
$\Delta_f G°$ =		108.48		
$\ln K_f$ =		−43.76		

TABLE 10. Aromatic CH-01 (42) – Continued

1,3,5-Trimethylbenzene C_9H_{12}

$(3\times C\text{-}(H)_3(C))+(3\times C_B\text{-}(H)(C_B)_2)+(3\times C_B\text{-}(C)(C_B)_2)+(3\times meta\text{ corr})$, $\sigma = 162$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−15.94	−16.32	0.38	47OSB/GIN
$C_p°$ =	150.25	149.40	0.85	69STU/WES
$S°$ =	385.30	377.76	7.54	69STU/WES
$\Delta_f S°$ =		−457.33		
$\Delta_f G°$ =		120.03		
$\ln K_f$ =		−48.42		
Liquid phase				
$\Delta_f H°$ =	−63.43	−60.87	−2.56	45JOH/PRO
$C_p°$ =	209.53	207.78	1.75	55TAY/KIL
$S°$ =	273.55	278.01	−4.46	55TAY/KIL
$\Delta_f S°$ =		−557.08		
$\Delta_f G°$ =		105.22		
$\ln K_f$ =		−42.45		

1,2,3,4-Tetramethylbenzene $C_{10}H_{14}$

$(4\times C\text{-}(H)_3(C))+(2\times C_B\text{-}(H)(C_B)_2)+(4\times C_B\text{-}(C)(C_B)_2)+(3\times ortho\text{ corr})+(2\times meta\text{ corr})$, $\sigma = 162$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−41.92	−44.34	2.42	69STU/WES
$C_p°$ =	189.58	189.76	−0.18	69STU/WES
$S°$ =	416.52	413.66	2.86	69STU/WES
$\Delta_f S°$ =		−557.74		
$\Delta_f G°$ =		121.95		
$\ln K_f$ =		−49.19		
Liquid phase				
$\Delta_f H°$ =	−90.21	−87.70	−2.51	75GOO
$C_p°$ =	235.98	242.18	−6.20	31HUF/PAR
$S°$ =	290.79	312.94	−22.15	31HUR/PAR
$\Delta_f S°$ =		−658.46		
$\Delta_f G°$ =		108.62		
$\ln K_f$ =		−43.82		

1,2,3,5-Tetramethylbenzene $C_{10}H_{14}$

$(4\times C\text{-}(H)_3(C))+(2\times C_B\text{-}(H)(C_B)_2)+(4\times C_B\text{-}(C)(C_B)_2)+(2\times ortho\text{ corr})+(2\times meta\text{ corr})$, $\sigma = 162$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−44.81	−45.60	0.79	69STU/WES
$C_p°$ =	185.73	183.36	2.37	69STU/WES
$S°$ =	422.54	416.16	6.38	69STU/WES
$\Delta_f S°$ =		−555.24		
$\Delta_f G°$ =		119.94		
$\ln K_f$ =		−48.38		

TABLE 10. Aromatic CH-01 (42) – Continued

1,2,3,5-Tetramethylbenzene (Continued) $C_{10}H_{14}$
(4 × C–(H)$_3$(C)) + (2 × C$_B$–(H)(C$_B$)$_2$) + (4 × C$_B$–(C)(C$_B$)$_2$) + (2 × *ortho* corr) + (2 × *meta* corr), σ = 162

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−96.36	−90.96	−5.40	75GOO
$C_p°$ =	240.16	238.68	1.48	31HUF/PAR
$S°$ =	310.03	312.94	−2.91	31HUF/PAR
$\Delta_f S°$ =		−658.46		
$\Delta_f G°$ =		105.36		
$\ln K_f$ =		−42.50		

1,2,4,5-Tetramethylbenzene $C_{10}H_{14}$
(4 × C–(H)$_3$(C)) + (2 × C$_B$–(H)(C$_B$)$_2$) + (4 × C$_B$–(C)(C$_B$)$_2$) + (2 × *ortho* corr) + (2 × *meta* corr), σ = 324

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−45.27	−45.60	0.33	69STU/WES
$C_p°$ =	186.52	183.36	3.16	69STU/WES
$S°$ =	418.53	410.40	8.13	69STU/WES
$\Delta_f S°$ =		−561.00		
$\Delta_f G°$ =		121.66		
$\ln K_f$ =		−49.08		
Liquid phase				
$\Delta_f H°$ =	−98.99	−90.96	−8.03	75GOO
$C_p°$ =		238.68		
$S°$ =		312.94		
$\Delta_f S°$ =		−658.46		
$\Delta_f G°$ =		105.36		
$\ln K_f$ =		−42.50		
Solid phase				
$\Delta_f H°$ =	−119.87	−104.30	−15.57	75GOO
$C_p°$ =	220.08	217.02	3.06	44EIB
$S°$ =	245.60	250.26	−4.66	31HUF/PAR
$\Delta_f S°$ =		−721.14		
$\Delta_f G°$ =		110.71		
$\ln K_f$ =		−44.66		

Pentamethylbenzene $C_{11}H_{16}$
(5 × C–(H)$_3$(C)) + (1 × C$_B$–(H)(C$_B$)$_2$) + (5 × C$_B$–(C)(C$_B$)$_2$) + (4 × *ortho* corr) + (4 × *meta* corr), σ = 486

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−74.48	−76.77	2.29	69STU/WES
$C_p°$ =	216.48	219.45	−2.97	69STU/WES
$S°$ =	443.88	445.42	−1.54	69STU/WES
$\Delta_f S°$ =		−662.28		
$\Delta_f G°$ =		120.69		
$\ln K_f$ =		−48.69		

TABLE 10. Aromatic CH-01 (42) – Continued

Pentamethylbenzene (Continued) $C_{11}H_{16}$
(5 × C–(H)$_3$(C)) + (1 × C$_B$–(H)(C$_B$)$_2$) + (5 × C$_B$–(C)(C$_B$)$_2$) + (4 × *ortho* corr) + (4 × *meta* corr), σ = 486

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−122.97	−121.05	−1.92	33FER/THO
$C_p°$ =		269.58		
$S°$ =		347.87		
$\Delta_f S°$ =		−759.84		
$\Delta_f G°$ =		105.50		
$\ln K_f$ =		−42.56		
Solid phase				
$\Delta_f H°$ =	−133.64	−129.67	−3.97	64BON/COL
$C_p°$ =	270.29	241.08	29.21	44EIB
$S°$ =	294.14	278.70	15.44	31HUF/PAR
$\Delta_f S°$ =		−829.01		
$\Delta_f G°$ =		117.50		
$\ln K_f$ =		−47.40		

Hexamethylbenzene $C_{12}H_{18}$
(6 × C–(H)$_3$(C)) + (6 × C$_B$–(C)(C$_B$)$_2$) + (6 × *ortho* corr) + (5 × *meta* corr), σ = 8748

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−86.82	−107.31	20.49	67FRA/AST
$C_p°$ =	248.61	254.83	−6.22	69STU/WES
$S°$ =	452.37	459.79	−7.42	69STU/WES
$\Delta_f S°$ =		−784.23		
$\Delta_f G°$ =		126.51		
$\ln K_f$ =		−51.03		
Liquid phase				
$\Delta_f H°$ =	−139.14	−151.14	12.00	32SPA/THO
$C_p°$ =		300.48		
$S°$ =		382.80		
$\Delta_f S°$ =		−861.22		
$\Delta_f G°$ =		105.63		
$\ln K_f$ =		−42.61		
Solid phase				
$\Delta_f H°$ =	−161.54	−157.04	−4.50	64BON/COL
$C_p°$ =	245.64	265.14	−19.50	65FRA/AST
$S°$ =	306.31	307.14	−0.83	65FRA/AST
$\Delta_f S°$ =		−936.88		
$\Delta_f G°$ =		122.29		
$\ln K_f$ =		−49.33		

TABLE 10. Aromatic CH-01 (42) — Continued

Ethylbenzene C_8H_{10}

$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(5\times C_B-(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	29.92	29.09	0.83	47OSB/GIN
$C_p°$ =	128.41	129.14	−0.73	69STU/WES
$S°$ =	360.45	360.95	−0.50	69STU/WES
$\Delta_f S°$ =		−337.82		
$\Delta_f G°$ =		129.81		
$\ln K_f$ =		−52.37		
Liquid phase				
$\Delta_f H°$ =	−12.34	−12.46	0.12	45PRO/GIL
$C_p°$ =	185.81	182.88	2.93	44GUT/SPI
$S°$ =	255.01	255.55	−0.54	44GUT/SPI
$\Delta_f S°$ =		−443.22		
$\Delta_f G°$ =		119.69		
$\ln K_f$ =		−48.28		

Propylbenzene C_9H_{12}

$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(5\times C_B-(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	7.91	8.46	−0.55	47OSB/GIN
$C_p°$ =	152.34	152.03	0.31	69STU/WES
$S°$ =	400.66	400.11	0.55	69STU/WES
$\Delta_f S°$ =		−434.97		
$\Delta_f G°$ =		138.15		
$\ln K_f$ =		−55.73		
Liquid phase				
$\Delta_f H°$ =	−38.33	−38.19	−0.14	45PRO/GIL
$C_p°$ =	214.72	213.30	1.42	65MES/TOD
$S°$ =	287.78	287.93	−0.15	65MES/TOD
$\Delta_f S°$ =		−547.16		
$\Delta_f G°$ =		124.94		
$\ln K_f$ =		−50.40		

Butylbenzene $C_{10}H_{14}$

$(1\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(5\times C_B-(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−13.05	−12.17	−0.88	46PRO/JOH
$C_p°$ =	175.10	174.92	0.18	69STU/WES
$S°$ =	439.49	439.27	0.22	69STU/WES
$\Delta_f S°$ =		−532.12		
$\Delta_f G°$ =		146.48		
$\ln K_f$ =		−59.09		

TABLE 10. Aromatic CH-01 (42) — Continued

Butylbenzene (Continued) $C_{10}H_{14}$

$(1\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(5\times C_B-(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−63.85	−63.92	0.07	46PRO/JOH
$C_p°$ =	243.34	243.72	−0.38	65MES/TOD
$S°$ =	321.21	320.31	0.90	65MES/TOD
$\Delta_f S°$ =		−651.09		
$\Delta_f G°$ =		130.20		
$\ln K_f$ =		−52.52		

Pentylbenzene $C_{11}H_{16}$

$(1\times C-(H)_3(C))+(3\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(5\times C_B-(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−34.43	−32.80	−1.63	69STU/WES
$C_p°$ =	197.99	197.81	0.18	69STU/WES
$S°$ =	478.94	478.43	0.51	69STU/WES
$\Delta_f S°$ =		−629.28		
$\Delta_f G°$ =		154.82		
$\ln K_f$ =		−62.45		
Liquid phase				
$\Delta_f H°$ =		−89.65		
$C_p°$ =		274.14		
$S°$ =		352.69		
$\Delta_f S°$ =		−755.02		
$\Delta_f G°$ =		135.46		
$\ln K_f$ =		−54.64		

Hexylbenzene $C_{12}H_{18}$

$(1\times C-(H)_3(C))+(4\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(5\times C_B-(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−55.02	−53.43	−1.59	69STU/WES
$C_p°$ =	220.87	220.70	0.17	69STU/WES
$S°$ =	517.90	517.59	0.31	69STU/WES
$\Delta_f S°$ =		−726.43		
$\Delta_f G°$ =		163.15		
$\ln K_f$ =		−65.82		
Liquid phase				
$\Delta_f H°$ =		−115.38		
$C_p°$ =		304.56		
$S°$ =		385.07		
$\Delta_f S°$ =		−858.95		
$\Delta_f G°$ =		140.72		
$\ln K_f$ =		−56.76		

TABLE 10. Aromatic CH-01 (42) – Continued

Heptylbenzene $C_{13}H_{20}$

$(1\times C\text{-}(H)_3(C)) + (5\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(C_B)) + (1\times C_B\text{-}(C)(C_B)_2) + (5\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−75.65	−74.06	−1.59	69STU/WES
C_p° =	243.72	243.59	0.13	69STU/WES
S° =	556.85	556.75	0.10	69STU/WES
$\Delta_f S^\circ$ =		−823.58		
$\Delta_f G^\circ$ =		171.49		
$\ln K_f$ =		−69.18		
Liquid phase				
$\Delta_f H^\circ$ =		−141.11		
C_p° =		334.98		
S° =		417.45		
$\Delta_f S^\circ$ =		−962.88		
$\Delta_f G^\circ$ =		145.97		
$\ln K_f$ =		−58.88		

Octylbenzene $C_{14}H_{22}$

$(1\times C\text{-}(H)_3(C)) + (6\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(C_B)) + (1\times C_B\text{-}(C)(C_B)_2) + (5\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−96.23	−94.69	−1.54	69STU/WES
C_p° =	266.60	266.48	0.12	69STU/WES
S° =	595.80	595.91	−0.11	69STU/WES
$\Delta_f S^\circ$ =		−920.73		
$\Delta_f G^\circ$ =		179.83		
$\ln K_f$ =		−72.54		
Liquid phase				
$\Delta_f H^\circ$ =		−166.84		
C_p° =		365.40		
S° =		449.83		
$\Delta_f S^\circ$ =		−1066.81		
$\Delta_f G^\circ$ =		151.23		
$\ln K_f$ =		−61.01		

Nonylbenzene $C_{15}H_{24}$

$(1\times C\text{-}(H)_3(C)) + (7\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(C_B)) + (1\times C_B\text{-}(C)(C_B)_2) + (5\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−116.86	−115.32	−1.54	69STU/WES
C_p° =	289.45	289.37	0.08	69STU/WES
S° =	634.75	635.07	−0.32	69STU/WES
$\Delta_f S^\circ$ =		−1017.88		
$\Delta_f G^\circ$ =		188.16		
$\ln K_f$ =		−75.90		

TABLE 10. Aromatic CH-01 (42) – Continued

Nonylbenzene (Continued) $C_{15}H_{24}$

$(1\times C\text{-}(H)_3(C)) + (7\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(C_B)) + (1\times C_B\text{-}(C)(C_B)_2) + (5\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H^\circ$ =		−192.57		
C_p° =		395.82		
S° =		482.21		
$\Delta_f S^\circ$ =		−1170.74		
$\Delta_f G^\circ$ =		156.49		
$\ln K_f$ =		−63.13		

Decylbenzene $C_{16}H_{26}$

$(1\times C\text{-}(H)_3(C)) + (8\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(C_B)) + (1\times C_B\text{-}(C)(C_B)_2) + (5\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−137.49	−135.95	−1.54	69STU/WES
C_p° =	312.34	312.26	0.08	69STU/WES
S° =	673.71	674.23	−0.52	69STU/WES
$\Delta_f S^\circ$ =		−1115.03		
$\Delta_f G^\circ$ =		196.50		
$\ln K_f$ =		−79.27		
Liquid phase				
$\Delta_f H^\circ$ =		−218.30		
C_p° =		426.24		
S° =		514.59		
$\Delta_f S^\circ$ =		−1274.67		
$\Delta_f G^\circ$ =		161.74		
$\ln K_f$ =		−65.25		

Undecylbenzene $C_{17}H_{28}$

$(1\times C\text{-}(H)_3(C)) + (9\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(C_B)) + (1\times C_B\text{-}(C)(C_B)_2) + (5\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−158.07	−156.58	−1.49	69STU/WES
C_p° =	335.22	335.15	0.07	69STU/WES
S° =	712.62	713.39	−0.77	69STU/WES
$\Delta_f S^\circ$ =		−1212.18		
$\Delta_f G^\circ$ =		204.83		
$\ln K_f$ =		−82.63		
Liquid phase				
$\Delta_f H^\circ$ =		−244.03		
C_p° =		456.66		
S° =		546.97		
$\Delta_f S^\circ$ =		−1378.60		
$\Delta_f G^\circ$ =		167.00		
$\ln K_f$ =		−67.37		

TABLE 10. Aromatic CH-01 (42) – Continued

Dodecylbenzene $C_{18}H_{30}$

$(1\times C-(H)_3(C))+(10\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(5\times C_B-(H)(C_B)_2)$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−178.70	−177.21	−1.49	69STU/WES
$C_p°$ =	358.07	358.04	0.03	69STU/WES
$S°$ =	751.57	752.55	−0.98	69STU/WES
$\Delta_fS°$ =		−1309.33		
$\Delta_fG°$ =		213.17		
$\ln K_f$ =		−85.99		
Liquid phase				
$\Delta_fH°$ =		−269.76		
$C_p°$ =		487.08		
$S°$ =		579.35		
$\Delta_fS°$ =		−1482.54		
$\Delta_fG°$ =		172.26		
$\ln K_f$ =		−69.49		

1-Methyl-2-ethylbenzene C_9H_{12}

$(2\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(2\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times$ *ortho* corr), $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	1.21	−2.08	3.29	69STU/WES
$C_p°$ =	157.90	157.41	0.49	69STU/WES
$S°$ =	399.24	398.48	0.76	69STU/WES
$\Delta_fS°$ =		−436.60		
$\Delta_fG°$ =		128.09		
$\ln K_f$ =		−51.67		
Liquid phase				
$\Delta_fH°$ =	−46.40	−45.81	−0.59	45JOH/PRO
$C_p°$ =		210.28		
$S°$ =		290.48		
$\Delta_fS°$ =		−544.61		
$\Delta_fG°$ =		116.56		
$\ln K_f$ =		−47.02		

1-Methyl-3-ethylbenzene C_9H_{12}

$(2\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(2\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times$ *meta* corr), $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−1.92	−3.97	2.05	69STU/WES
$C_p°$ =	152.21	151.72	0.49	69STU/WES
$S°$ =	404.17	400.98	3.19	69STU/WES
$\Delta_fS°$ =		−434.10		
$\Delta_fG°$ =		125.46		
$\ln K_f$ =		−50.61		

TABLE 10. Aromatic CH-01 (42) – Continued

1-Methyl-3-ethylbenzene (Continued) C_9H_{12}

$(2\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(2\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times$ *meta* corr), $\sigma = 9$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−48.70	−49.07	0.37	45JOH/PRO
$C_p°$ =		206.78		
$S°$ =		290.48		
$\Delta_fS°$ =		−544.61		
$\Delta_fG°$ =		113.30		
$\ln K_f$ =		−45.71		

1-Methyl-4-ethylbenzene C_9H_{12}

$(2\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(2\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−3.26	−3.34	0.08	69STU/WES
$C_p°$ =	151.54	151.01	0.53	69STU/WES
$S°$ =	398.90	395.22	3.68	69STU/WES
$\Delta_fS°$ =		−439.87		
$\Delta_fG°$ =		127.81		
$\ln K_f$ =		−51.56		
Liquid phase				
$\Delta_fH°$ =	−49.79	−49.07	−0.72	45JOH/PRO
$C_p°$ =		206.78		
$S°$ =		290.48		
$\Delta_fS°$ =		−544.61		
$\Delta_fG°$ =		113.30		
$\ln K_f$ =		−45.71		

1-Methyl-2-propylbenzene $C_{10}H_{14}$

$(2\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_B))+(2\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times$ *ortho* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−22.71		
$C_p°$ =		180.30		
Liquid phase				
$\Delta_fH°$ =	−72.47	−71.54	−0.93	73GOO
$C_p°$ =		240.70		
$S°$ =		322.86		
$\Delta_fS°$ =		−648.54		
$\Delta_fG°$ =		121.82		
$\ln K_f$ =		−49.14		

TABLE 10. Aromatic CH-01 (42) – Continued

1-Methyl-3-propylbenzene $C_{10}H_{14}$

$(2\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_B))+(2\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times$ *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−24.60		
$C_p°$ =		174.61		
Liquid phase				
$\Delta_fH°$ =	−76.23	−74.80	−1.43	73GOO
$C_p°$ =		237.20		
$S°$ =		322.86		
$\Delta_fS°$ =		−648.54		
$\Delta_fG°$ =		118.56		
$\ln K_f$ =		−47.83		

1-Methyl-4-propylbenzene $C_{10}H_{14}$

$(2\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(C_B))+(2\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−23.97		
$C_p°$ =		173.90		
Liquid phase				
$\Delta_fH°$ =	−75.06	−74.80	−0.26	73GOO
$C_p°$ =		237.20		
$S°$ =		322.86		
$\Delta_fS°$ =		−648.54		
$\Delta_fG°$ =		118.56		
$\ln K_f$ =		−47.83		

1-Methyl-2-isopropylbenzene $C_{10}H_{14}$

$(3\times C-(H)_3(C))+(1\times C-(H)(C)_2(C_B))+(2\times -CH_3$ corr (tertiary)$)+(2\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times$ *ortho* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−32.04		
$C_p°$ =		179.98		
Liquid phase				
$\Delta_fH°$ =	−73.30	−78.79	5.49	73GOO
$C_p°$ =		241.36		
$S°$ =		312.48		
$\Delta_fS°$ =		−658.92		
$\Delta_fG°$ =		117.67		
$\ln K_f$ =		−47.47		

TABLE 10. Aromatic CH-01 (42) – Continued

1-Methyl-3-isopropylbenzene $C_{10}H_{14}$

$(3\times C-(H)_3(C))+(1\times C-(H)(C)_2(C_B))+(2\times -CH_3$ corr (tertiary)$)+(2\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times$ *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−33.93		
$C_p°$ =		174.29		
Liquid phase				
$\Delta_fH°$ =	−78.62	−82.05	3.43	73GOO
$C_p°$ =		237.86		
$S°$ =		312.48		
$\Delta_fS°$ =		−658.92		
$\Delta_fG°$ =		114.41		
$\ln K_f$ =		−46.15		

1-Methyl-4-isopropylbenzene $C_{10}H_{14}$

$(3\times C-(H)_3(C))+(1\times C-(H)(C)_2(C_B))+(2\times -CH_3$ corr (tertiary)$)+(2\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−33.30		
$C_p°$ =		173.58		
Liquid phase				
$\Delta_fH°$ =	−78.03	−82.05	4.02	73GOO
$C_p°$ =	236.40	237.86	−1.46	31HUF/PAR
$S°$ =	306.69	312.48	−5.79	31HUF/PAR
$\Delta_fS°$ =		−658.92		
$\Delta_fG°$ =		114.41		
$\ln K_f$ =		−46.15		

3-Ethyl-1,2-dimethylbenzene $C_{10}H_{14}$

$(3\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(3\times C_B-(C)(C_B)_2)+(3\times C_B-(H)(C_B)_2)+(2\times$ *ortho* corr$)+(1\times$ *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−33.88		
$C_p°$ =		186.39		
Liquid phase				
$\Delta_fH°$ =	−80.50	−79.16	−1.34	75GOO
$C_p°$ =		237.68		
$S°$ =		325.41		
$\Delta_fS°$ =		−645.99		
$\Delta_fG°$ =		113.44		
$\ln K_f$ =		−45.76		

TABLE 10. Aromatic CH-01 (42) – Continued

4-Ethyl-1,2-dimethylbenzene $C_{10}H_{14}$

$(3\times C-(H)_3(C)) + (1\times C-(H)_2(C)(C_B)) + (3\times C_B-(C)(C_B)_2) + (3\times C_B-(H)(C_B)_2) + (1\times ortho\ corr) + (1\times meta\ corr)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−35.14		
C_p° =		179.99		
Liquid phase				
Δ_fH° =	−86.02	−82.42	−3.60	75GOO
C_p° =		234.18		
S° =		325.41		
Δ_fS° =		−645.99		
Δ_fG° =		110.18		
$\ln K_f$ =		−44.45		

2-Ethyl-1,3-dimethylbenzene $C_{10}H_{14}$

$(3\times C-(H)_3(C)) + (1\times C-(H)_2(C)(C_B)) + (3\times C_B-(C)(C_B)_2) + (3\times C_B-(H)(C_B)_2) + (2\times ortho\ corr) + (1\times meta\ corr)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−33.88		
C_p° =		186.39		
Liquid phase				
Δ_fH° =	−80.12	−79.16	−0.96	75GOO
C_p° =		237.68		
S° =		325.41		
Δ_fS° =		−645.99		
Δ_fG° =		113.44		
$\ln K_f$ =		−45.76		

4-Ethyl-1,3-dimethylbenzene $C_{10}H_{14}$

$(3\times C-(H)_3(C)) + (1\times C-(H)_2(C)(C_B)) + (3\times C_B-(C)(C_B)_2) + (3\times C_B-(H)(C_B)_2) + (1\times ortho\ corr) + (1\times meta\ corr)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−35.14		
C_p° =		179.99		
Liquid phase				
Δ_fH° =	−84.10	−82.42	−1.68	75GOO
C_p° =		234.18		
S° =		325.41		
Δ_fS° =		−645.99		
Δ_fG° =		110.18		
$\ln K_f$ =		−44.45		

TABLE 10. Aromatic CH-01 (42) – Continued

5-Ethyl-1,3-dimethylbenzene $C_{10}H_{14}$

$(3\times C-(H)_3(C)) + (1\times C-(H)_2(C)(C_B)) + (3\times C_B-(C)(C_B)_2) + (3\times C_B-(H)(C_B)_2) + (3\times meta\ corr)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−37.66		
C_p° =		175.01		
Liquid phase				
Δ_fH° =	−87.78	−85.68	−2.10	75GOO
C_p° =		230.68		
S° =		325.41		
Δ_fS° =		−645.99		
Δ_fG° =		106.92		
$\ln K_f$ =		−43.13		

2-Ethyl-1,4-dimethylbenzene $C_{10}H_{14}$

$(3\times C-(H)_3(C)) + (1\times C-(H)_2(C)(C_B)) + (3\times C_B-(C)(C_B)_2) + (3\times C_B-(H)(C_B)_2) + (1\times ortho\ corr) + (1\times meta\ corr)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−35.14		
C_p° =		179.99		
Liquid phase				
Δ_fH° =	−84.81	−82.42	−2.39	75GOO
C_p° =		234.18		
S° =		325.41		
Δ_fS° =		−645.99		
Δ_fG° =		110.18		
$\ln K_f$ =		−44.45		

1,2-Diethylbenzene $C_{10}H_{14}$

$(2\times C-(H)_3(C)) + (2\times C-(H)_2(C)(C_B)) + (2\times C_B-(C)(C_B)_2) + (4\times C_B-(H)(C_B)_2) + (1\times ortho\ corr)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−23.42		
C_p° =		183.02		
Liquid phase				
Δ_fH° =	−68.49	−70.62	2.13	75GOO
C_p° =		233.18		
S° =		337.88		
Δ_fS° =		−633.52		
Δ_fG° =		118.26		
$\ln K_f$ =		−47.71		

TABLE 10. Aromatic CH-01 (42) – Continued

1,3-Diethylbenzene $C_{10}H_{14}$

(2 × C–(H)$_3$(C)) + (2 × C–(H)$_2$(C)(C$_B$)) + (2 × C$_B$–(C)(C$_B$)$_2$) + (4 × C$_B$–(H)(C$_B$)$_2$) + (1 × *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−25.31		
$C_p°$ =		177.33		
Liquid phase				
$\Delta_f H°$ =	−73.51	−73.88	0.37	73GOO
$C_p°$ =		229.68		
$S°$ =		337.88		
$\Delta_f S°$ =		−633.52		
$\Delta_f G°$ =		115.00		
$\ln K_f$ =		−46.39		

1,4-Diethylbenzene $C_{10}H_{14}$

(2 × C–(H)$_3$(C)) + (2 × C–(H)$_2$(C)(C$_B$)) + (2 × C$_B$–(C)(C$_B$)$_2$) + (4 × C$_B$–(H)(C$_B$)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−24.68		
$C_p°$ =	176.15	176.62	−0.47	69STU/WES
$S°$ =	434.01	437.81	−3.80	69STU/WES
$\Delta_f S°$ =		−533.59		
$\Delta_f G°$ =		134.41		
$\ln K_f$ =		−54.22		
Liquid phase				
$\Delta_f H°$ =	−72.84	−73.88	1.04	73GOO
$C_p°$ =		229.68		
$S°$ =		337.88		
$\Delta_f S°$ =		−633.52		
$\Delta_f G°$ =		115.00		
$\ln K_f$ =		−46.39		

TABLE 11. Aromatic CH-02 (80)

1,2,3-Triethylbenzene $C_{12}H_{18}$

(3 × C–(H)$_3$(C)) + (3 × C–(H)$_2$(C)(C$_B$)) + (3 × C$_B$–(C)(C$_B$)$_2$) + (3 × C$_B$–(H)(C$_B$)$_2$) + (2 × *ortho* corr) + (1 × *meta* corr), σ = 54

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−67.99	−76.56	8.57	69STU/WES
$C_p°$ =	228.11	237.61	−9.50	69STU/WES
$S°$ =	507.23	509.66	−2.43	69STU/WES
$\Delta_f S°$ =		−734.36		
$\Delta_f G°$ =		142.39		
$\ln K_f$ =		−57.44		
Liquid phase				
$\Delta_f H°$ =		−128.78		
$C_p°$ =		283.48		
$S°$ =		420.21		
$\Delta_f S°$ =		−823.81		
$\Delta_f G°$ =		116.84		
$\ln K_f$ =		−47.13		

1,2,4-Triethylbenzene $C_{12}H_{18}$

(3 × C–(H)$_3$(C)) + (3 × C–(H)$_2$(C)(C$_B$)) + (3 × C$_B$–(C)(C$_B$)$_2$) + (3 × C$_B$–(H)(C$_B$)$_2$) + (1 × *ortho* corr) + (1 × *meta* corr), σ = 27

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−71.09	−77.82	6.73	69STU/WES
$C_p°$ =	227.94	231.21	−3.27	69STU/WES
$S°$ =	518.15	517.93	0.22	69STU/WES
$\Delta_f S°$ =		−726.09		
$\Delta_f G°$ =		138.66		
$\ln K_f$ =		−55.94		
Liquid phase				
$\Delta_f H°$ =		−132.04		
$C_p°$ =		279.98		
$S°$ =		420.21		
$\Delta_f S°$ =		−823.81		
$\Delta_f G°$ =		113.58		
$\ln K_f$ =		−45.82		

1,3,5-Triethylbenzene $C_{12}H_{18}$

(3 × C–(H)$_3$(C)) + (3 × C–(H)$_2$(C)(C$_B$)) + (3 × C$_B$–(C)(C$_B$)$_2$) + (3 × C$_B$–(H)(C$_B$)$_2$) + (3 × *meta* corr), σ = 162

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−74.73	−80.34	5.61	69STU/WES
$C_p°$ =	224.18	226.23	−2.05	69STU/WES
$S°$ =	507.69	505.53	2.16	69STU/WES
$\Delta_f S°$ =		−738.49		
$\Delta_f G°$ =		139.84		
$\ln K_f$ =		−56.41		

TABLE 11. Aromatic CH-02 (80) — Continued

1,3,5-Triethylbenzene (Continued) $C_{12}H_{18}$

(3×C–(H)$_3$(C)) + (3×C–(H)$_2$(C)(C$_B$)) + (3×C$_B$–(C)(C$_B$)$_2$) + (3×C$_B$–(H)(C$_B$)$_2$) + (3×*meta* corr), σ = 162

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−135.30		
$C_p°$ =		276.48		
$S°$ =		420.21		
$\Delta_fS°$ =		−823.81		
$\Delta_fG°$ =		110.32		
lnK_f =		−44.50		

Pentaethylbenzene $C_{16}H_{26}$

(5×C–(H)$_3$(C)) + (5×C–(H)$_2$(C)(C$_B$)) + (5×C$_B$–(C)(C$_B$)$_2$) + (1×C$_B$–(H)(C$_B$)$_2$) + (4×*ortho* corr) + (4×*meta* corr), σ = 486

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−175.18	−183.47	8.29	69STU/WES
$C_p°$ =	339.70	347.50	−7.80	69STU/WES
$S°$ =	647.89	658.37	−10.48	69STU/WES
$\Delta_fS°$ =		−1130.89		
$\Delta_fG°$ =		153.70		
lnK_f =		−62.00		
Liquid phase				
$\Delta_fH°$ =		−245.10		
$C_p°$ =		384.08		
$S°$ =		584.87		
$\Delta_fS°$ =		−1204.39		
$\Delta_fG°$ =		113.99		
lnK_f =		−45.98		

Hexaethylbenzene $C_{18}H_{30}$

(6×C–(H)$_3$(C)) + (6×C–(H)$_2$(C)(C$_B$)) + (6×C$_B$–(C)(C$_B$)$_2$) + (6×*ortho* corr) + (5×*meta* corr), σ = 8748

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−224.26	−235.35	11.09	69STU/WES
$C_p°$ =	396.48	408.49	−12.01	69STU/WES
$S°$ =	697.14	715.33	−18.19	69STU/WES
$\Delta_fS°$ =		−1346.55		
$\Delta_fG°$ =		166.12		
lnK_f =		−67.01		
Liquid phase				
$\Delta_fH°$ =		−300.00		
$C_p°$ =		437.88		
$S°$ =		667.20		
$\Delta_fS°$ =		−1394.68		
$\Delta_fG°$ =		115.83		
lnK_f =		−46.72		

TABLE 11. Aromatic CH-02 (80) — Continued

Hexaethylbenzene $C_{18}H_{30}$

(6×C–(H)$_3$(C)) + (6×C–(H)$_2$(C)(C$_B$)) + (6×C$_B$–(C)(C$_B$)$_2$) + (6×*ortho* corr) + (5×*meta* corr), σ = 8748

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =		−289.64		
$C_p°$ =		561.42		
$S°$ =		468.54		
$\Delta_fS°$ =		−1593.34		
$\Delta_fG°$ =		185.42		
lnK_f =		−74.80		

Isopropylbenzene; Cumene C_9H_{12}

(2×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(C$_B$)) + (2×–CH$_3$ corr (tertiary)) + (1×C$_B$–(C)(C$_B$)$_2$) + (5×C$_B$–(H)(C$_B$)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	4.02	−0.87	4.89	47OSB/GIN
$C_p°$ =	151.71	151.71	0.00	69STU/WES
$S°$ =	388.57	388.55	0.02	69STU/WES
$\Delta_fS°$ =		−446.54		
$\Delta_fG°$ =		132.27		
lnK_f =		−53.35		
Liquid phase				
$\Delta_fH°$ =	−41.13	−45.44	4.31	45JOH/PRO
$C_p°$ =	215.40	213.96	1.44	73KIS/SUG
$S°$ =	277.57	277.55	0.02	73KIS/SUG
$\Delta_fS°$ =		−557.54		
$\Delta_fG°$ =		120.79		
lnK_f =		−48.73		

(1-Methylpropyl)benzene; sec-Butylbenzene $C_{10}H_{14}$

(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(C$_B$)) + (1×–CH$_3$ corr (tertiary)) + (1×C$_B$–(C)(C$_B$)$_2$) + (5×C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−17.36	−19.24	1.88	46PRO/JOH
$C_p°$ =		174.60		
Liquid phase				
$\Delta_fH°$ =	−66.40	−68.99	2.59	46PRO/JOH
$C_p°$ =		244.38		
$S°$ =		309.93		
$\Delta_fS°$ =		−661.47		
$\Delta_fG°$ =		128.23		
lnK_f =		−51.73		

TABLE 11. Aromatic CH-02 (80) — Continued

(2-Methylpropyl)benzene; Isobutylbenzene $C_{10}H_{14}$
(2×C–(H)$_3$(C))+(1×C–(H)(C)$_3$)+(2×–CH$_3$ corr (tertiary))+(1×C–(H)$_2$(C)(C$_B$))+(1×C$_B$–(C)(C$_B$)$_2$)+(5×C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−21.51	−18.86	−2.65	46PRO/JOH
$C_p°$ =		174.95		
Liquid phase				
$\Delta_fH°$ =	−69.79	−69.20	−0.59	46PRO/JOH
$C_p°$ =		240.74		
$S°$ =		314.96		
$\Delta_fS°$ =		−656.44		
$\Delta_fG°$ =		126.52		
$\ln K_f$ =		−51.04		

***tert*-Butylbenzene** $C_{10}H_{14}$
(3×C–(H)$_3$(C))+(1×C–(C$_B$)(C)$_3$)+(1×C$_B$–(C)(C$_B$)$_2$)+(5×C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−22.59	−15.81	−6.78	46PRO/JOH
$C_p°$ =		173.27		
Liquid phase				
$\Delta_fH°$ =	−70.71	−64.17	−6.54	46PRO/JOH
$C_p°$ =	238.11	238.11	0.00	30HUF/PAR
$S°$ =	278.65	278.65	0.00	30HUF/PAR
$\Delta_fS°$ =		−692.75		
$\Delta_fG°$ =		142.37		
$\ln K_f$ =		−57.43		

Styrene C_8H_8
(1×C$_d$–(H)$_2$)+(1×C$_d$–(H)(C$_B$))+(1×C$_B$–(C$_d$)(C$_B$)$_2$)+(5×C$_B$–(H)(C$_B$)$_2$), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	147.82	147.82	0.00	46PIT/GUT
$C_p°$ =	122.09	122.09	0.00	69STU/WES
$S°$ =	345.10	345.20	−0.10	69STU/WES
$\Delta_fS°$ =		−223.01		
$\Delta_fG°$ =		214.31		
$\ln K_f$ =		−86.45		
Liquid phase				
$\Delta_fH°$ =	103.47	103.85	−0.38	45PRO/GIL
$C_p°$ =	182.88	182.88	0.00	46PIT/GUT
$S°$ =	237.57	234.80	2.77	46PIT/GUT
$\Delta_fS°$ =		−333.40		
$\Delta_fG°$ =		203.25		
$\ln K_f$ =		−81.99		

TABLE 11. Aromatic CH-02 (80) — Continued

***ortho*-Methylstyrene** C_9H_{10}
(1×C–(H)$_3$(C))+(1×C$_d$–(H)$_2$)+(1×C$_d$–(H)(C$_B$))+(1×C$_B$–(C$_d$)(C$_B$)$_2$)+(1×C$_B$–(C)(C$_B$)$_2$)+(1×*ortho* corr)+(4×C$_B$–(H)(C$_B$)$_2$), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	118.41	116.65	1.76	69STU/WES
$C_p°$ =	145.18	150.36	−5.18	69STU/WES
$S°$ =	383.67	382.73	0.94	69STU/WES
$\Delta_fS°$ =		−321.79		
$\Delta_fG°$ =		212.59		
$\ln K_f$ =		−85.76		
Liquid phase				
$\Delta_fH°$ =		70.50		
$C_p°$ =		210.28		
$S°$ =		269.73		
$\Delta_fS°$ =		−434.78		
$\Delta_fG°$ =		200.13		
$\ln K_f$ =		−80.73		

***meta*-Methylstyrene** C_9H_{10}
(1×C–(H)$_3$(C))+(1×C$_d$–(H)$_2$)+(1×C$_d$–(H)(C$_B$))+(1×C$_B$–(C$_d$)(C$_B$)$_2$)+(1×C$_B$–(C)(C$_B$)$_2$)+(1×*meta* corr)+(4×C$_B$–(H)(C$_B$)$_2$), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	115.48	114.76	0.72	69STU/WES
$C_p°$ =	145.18	144.67	0.51	69STU/WES
$S°$ =	389.53	385.23	4.30	69STU/WES
$\Delta_fS°$ =		−319.29		
$\Delta_fG°$ =		209.96		
$\ln K_f$ =		−84.69		
Liquid phase				
$\Delta_fH°$ =		67.24		
$C_p°$ =		206.78		
$S°$ =		269.73		
$\Delta_fS°$ =		−434.78		
$\Delta_fG°$ =		196.87		
$\ln K_f$ =		−79.42		

para-Methylstyrene C_9H_{10}
(1×C–(H)$_3$(C))+(1×C$_d$–(H)$_2$)+(1×C$_d$–(H)(C$_B$))+(1×C$_B$–(C$_d$)(C$_B$)$_2$)+(1×C$_B$–(C)(C$_B$)$_2$)+(4×C$_B$–(H)(C$_B$)$_2$), σ = 6

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	114.64	115.39	−0.75	69STU/WES
$C_p°$ =	145.18	143.96	1.22	69STU/WES
$S°$ =	383.67	379.46	4.21	69STU/WES
$\Delta_fS°$ =		−325.05		
$\Delta_fG°$ =		212.30		
$\ln K_f$ =		−85.64		

TABLE 11. Aromatic CH-02 (80) – Continued

para-Methylstyrene (Continued) C_9H_{10}

$(1\times C-(H)_3(C)) + (1\times C_d-(H)_2) + (1\times C_d-(H)(C_B)) + (1\times C_B-(C_d)(C_B)_2) + (1\times C_B-(C)(C_B)_2) + (4\times C_B-(H)(C_B)_2)$, $\sigma = 6$

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_f H^\circ$ =		67.24		
C_p° =		206.78		
S° =		269.73		
$\Delta_f S^\circ$ =		–434.78		
$\Delta_f G^\circ$ =		196.87		
$\ln K_f$ =		–79.42		

Isopropenylbenzene; α-Methylstyrene C_9H_{10}

$(1\times C-(H)_3(C)) + (1\times C_d-(C)(C_B)) + (1\times C_d-(H)_2) + (1\times C_B-(C_d)(C_B)_2) + (5\times C_B-(H)(C_B)_2) + (1\times -CH_3$ corr (tertiary)), $\sigma = 6$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	112.97	112.97	0.00	69STU/WES
C_p° =	145.18	145.18	0.00	69STU/WES
S° =	383.67	383.67	0.00	69STU/WES
$\Delta_f S^\circ$ =		–320.84		
$\Delta_f G^\circ$ =		208.63		
$\ln K_f$ =		–84.16		
Liquid phase				
$\Delta_f H^\circ$ =	70.46	70.46	0.00	51ROB/JES

***cis*-1-Propenylbenzene; *cis*-β-Methylstyrene** C_9H_{10}

$(1\times C-(H)_3(C)) + (1\times C_d-(H)(C)) + (1\times cis$ (unsat) corr) $+ (1\times C_d-(H)(C_B)) + (1\times C_B-(C_d)(C_B)_2) + (5\times C_B-(H)(C_B)_2)$, $\sigma = 6$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	121.34	120.41	0.93	69STU/WES
C_p° =	145.18	137.15	8.03	69STU/WES
S° =	383.67	385.97	–2.30	69STU/WES
$\Delta_f S^\circ$ =		–318.54		
$\Delta_f G^\circ$ =		215.38		
$\ln K_f$ =		–86.88		
Liquid phase				
$\Delta_f H^\circ$ =		70.81		
C_p° =		215.59		
S° =		260.49		
$\Delta_f S^\circ$ =		–444.02		
$\Delta_f G^\circ$ =		203.20		
$\ln K_f$ =		–81.97		

TABLE 11. Aromatic CH-02 (80) – Continued

***trans*-1-Propenylbenzene; *trans*-β-Methylstyrene** C_9H_{10}

$(1\times C-(H)_3(C)) + (1\times C_d-(H)(C)) + (1\times C_d-(H)(C_B)) + (1\times C_B-(C_d)(C_B)_2) + (5\times C_B-(H)(C_B)_2)$, $\sigma = 6$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	117.15	115.56	1.59	69STU/WES
C_p° =	146.02	145.18	0.84	69STU/WES
S° =	380.33	380.91	–0.58	69STU/WES
$\Delta_f S^\circ$ =		–323.60		
$\Delta_f G^\circ$ =		212.04		
$\ln K_f$ =		–85.54		
Liquid phase				
$\Delta_f H^\circ$ =		65.54		
C_p° =		215.59		
S° =		260.49		
$\Delta_f S^\circ$ =		–444.02		
$\Delta_f G^\circ$ =		197.93		
$\ln K_f$ =		–79.84		

2-Propenylbenzene C_9H_{10}

$(1\times C_d-(H)_2) + (1\times C_d-(H)(C)) + (1\times C-(H)_2(C_d)(C_B)) + (1\times C_B-(C)(C_B)_2) + (5\times C_B-(H)(C_B)_2)$

	Literature	-Calculated	= Residual	Reference
Liquid phase				
$\Delta_f H^\circ$ =	88.03	88.03	0.00	71ROC/MCL

1-Methyl-2-propenylbenzene $C_{10}H_{12}$

$(1\times C-(H)_3(C)) + (1\times C_d-(H)_2) + (1\times C_d-(H)(C)) + (1\times C-(H)(C)(C_d)(C_B)) + (1\times -CH_3$ corr (tertiary)) $+ (1\times C_B-(C)(C_B)_2) + (5\times C_B-(H)(C_B)_2)$

	Literature	-Calculated	= Residual	Reference
Liquid phase				
$\Delta_f H^\circ$ =	56.07	56.07	0.00	71ROC/MCL

Ethynylbenzene C_8H_6

$(1\times C_t-(H)) + (1\times C_t-(C_B)) + (1\times C_B-(C_t)(C_B)_2) + (5\times C_B-(H)(C_B)_2)$, $\sigma = 2$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	327.27	327.48	–0.21	69STU/WES
C_p° =	114.89	114.89	0.00	69STU/WES
S° =	321.67	321.67	0.00	69STU/WES
$\Delta_f S^\circ$ =		–115.97		
$\Delta_f G^\circ$ =		362.06		
$\ln K_f$ =		–146.05		

TABLE 11. Aromatic CH-02 (80) – Continued

Ethynylbenzene (Continued) C_8H_6

$(1 \times C_t-(H)) + (1 \times C_t-(C_B)) + (1 \times C_B-(C_t)(C_B)_2) + (5 \times C_B-(H)(C_B)_2)$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	282.88	283.39	−0.51	58FLI/SKI

Diphenylmethane $C_{13}H_{12}$

$(1 \times C-(H)_2(C_B)_2) + (2 \times C_B-(C)(C_B)_2) + (10 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	138.95	138.95	0.00	59AIH
Liquid phase				
$\Delta_f H°$ =	89.66	93.42	−3.76	50PAR/MOS2
$C_p°$ =	279.91	279.91	0.00	50KUR
$S°$ =	301.67	301.67	0.00	30HUF/PAR
$\Delta_f S°$ =		−556.38		
$\Delta_f G°$ =		259.30		
$\ln K_f$ =		−104.60		
Solid phase				
$\Delta_f H°$ =	71.09	71.66	−0.57	30HUF/PAR
$C_p°$ =	223.84	223.84	0.00	30HUF/PAR
$S°$ =	239.32	239.35	−0.03	30HUF/PAR
$\Delta_f S°$ =		−618.70		
$\Delta_f G°$ =		256.12		
$\ln K_f$ =		−103.32		

4-Methyldiphenylmethane $C_{14}H_{14}$

$(1 \times C-(H)_3(C)) + (3 \times C_B-(C)(C_B)_2) + (9 \times C_B-(H)(C_B)_2) + (1 \times C-(H)_2(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		106.52		
Liquid phase				
$\Delta_f H°$ =	61.55	56.81	4.74	76GOO/LEE
$C_p°$ =		303.81		
$S°$ =		336.60		
$\Delta_f S°$ =		−657.76		
$\Delta_f G°$ =		252.92		
$\ln K_f$ =		−102.03		

2,5-Dimethyldiphenylmethane $C_{15}H_{16}$

$(2 \times C-(H)_3(C)) + (4 \times C_B-(C)(C_B)_2) + (1 \times C-(H)_2(C_B)_2) + (8 \times C_B-(H)(C_B)_2) + (1 \times$ *ortho* corr$) + (2 \times$ *meta* corr$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		74.09		
Liquid phase				
$\Delta_f H°$ =	24.69	23.46	1.23	76GOO/LEE
$C_p°$ =		331.21		
$S°$ =		371.53		
$\Delta_f S°$ =		−759.14		
$\Delta_f G°$ =		249.80		
$\ln K_f$ =		−100.77		

1,1-Diphenylethane $C_{14}H_{14}$

$(1 \times C-(H)_3(C)) + (1 \times C-(H)(C)(C_B)_2) + (1 \times -CH_3$ corr (tertiary)$) + (2 \times C_B-(C)(C_B)_2) + (10 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	48.66	48.66	0.00	53COO/MUL
$C_p°$ =	294.97	294.98	−0.01	31SMI/AND
$S°$ =		361.12		
$\Delta_f S°$ =		−633.24		
$\Delta_f G°$ =		237.46		
$\ln K_f$ =		−95.79		

1,1-Diphenyldodecane $C_{24}H_{34}$

$(1 \times C-(H)_3(C)) + (10 \times C-(H)_2(C)_2) + (1 \times C-(H)(C)(C_B)_2) + (2 \times C_B-(C)(C_B)_2) + (10 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		−206.46		
$C_p°$ =	593.71	599.18	−5.47	60KAR/STR2
$S°$ =	684.92	684.92	0.00	60KAR/STR2
$\Delta_f S°$ =		−1672.55		
$\Delta_f G°$ =		292.21		
$\ln K_f$ =		−117.88		

1,1-Diphenylethylene $C_{14}H_{12}$

$(1 \times C_d-(H)_2) + (1 \times C_d-(C_B)_2) + (2 \times C_B-(C_d)(C_B)_2) + (10 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	245.64	245.64	0.00	56HOL/TYR

TABLE 11. Aromatic CH-02 (80) — Continued

1,1-Diphenylethylene $C_{14}H_{12}$
$(1\times C_d-(H)_2)+(1\times C_d-(C_B)_2)+(2\times C_B-(C_d)(C_B)_2)+(10\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	172.42	172.42	0.00	50COO/HOI
$C_p°$ =	299.16	299.15	0.01	31SMI/AND

cis-**Stilbene** $C_{14}H_{12}$
$(2\times C_d-(H)(C_B))+(2\times C_B-(C_d)(C_B)_2)+(10\times C_B-(H)(C_B)_2)+(1\times cis\text{(unsat) corr})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	252.55	247.85	4.70	52BRA/PLE
$C_p°$ =		193.39		
Liquid phase				
$\Delta_fH°$ =	183.51	169.47	14.04	50COO/HOI
$C_p°$ =		309.02		
$S°$ =		297.22		
$\Delta_fS°$ =		−566.57		
$\Delta_fG°$ =		338.39		
$\ln K_f$ =		−136.50		

trans-**Stilbene** $C_{14}H_{12}$
$(2\times C_d-(H)(C_B))+(2\times C_B-(C_d)(C_B)_2)+(10\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	239.70	243.00	−3.30	72MOR2
$C_p°$ =		201.42		
Liquid phase				
$\Delta_fH°$ =		164.20		
$C_p°$ =		309.02		
$S°$ =		297.22		
$\Delta_fS°$ =		−566.57		
$\Delta_fG°$ =		333.12		
$\ln K_f$ =		−134.38		
Solid phase				
$\Delta_fH°$ =	140.50	140.90	−0.40	50COO/HOI
$C_p°$ =	232.60	232.60	0.00	31SMI/AND
$S°$ =	251.00	251.00	0.00	30PAR/HUF2
$\Delta_fS°$ =		−612.79		
$\Delta_fG°$ =		323.60		
$\ln K_f$ =		−130.54		

TABLE 11. Aromatic CH-02 (80) — Continued

1,2-Diphenylethane; Bibenzyl $C_{14}H_{14}$
$(2\times C-(H)_2(C)(C_B))+(2\times C_B-(C)(C_B)_2)+(10\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	142.93	142.70	0.23	59AIH
$C_p°$ =		206.82		
Liquid phase				
$\Delta_fH°$ =		70.30		
$C_p°$ =		292.80		
$S°$ =		344.50		
$\Delta_fS°$ =		−649.86		
$\Delta_fG°$ =		264.05		
$\ln K_f$ =		−106.52		
Solid phase				
$\Delta_fH°$ =	51.51	48.90	2.61	66COL/PIL
$C_p°$ =	253.55	253.54	0.01	31SMI/AND
$S°$ =	270.29	270.30	−0.01	30HUF/PAR
$\Delta_fS°$ =		−724.06		
$\Delta_fG°$ =		264.78		
$\ln K_f$ =		−106.81		

Triphenylmethane $C_{19}H_{16}$
$(1\times C-(H)(C_B)_3)+(3\times C_B-(C)(C_B)_2)+(15\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		271.21		
Solid phase				
$\Delta_fH°$ =		174.13		
$C_p°$ =	295.39	295.81	−0.42	31SMI/AND
$S°$ =	312.13	312.13	0.00	30HUF/PAR
$\Delta_fS°$ =		−841.50		
$\Delta_fG°$ =		425.02		
$\ln K_f$ =		−171.45		

Tetraphenylmethane $C_{25}H_{20}$
$(1\times C-(C_B)_4)+(4\times C_B-(C)(C_B)_2)+(20\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		397.80		
Solid phase				
$\Delta_fH°$ =		251.09		
$C_p°$ =	368.19	368.30	−0.11	31SMI/AND

TABLE 11. Aromatic CH-02 (80) – Continued

1,1,2-Triphenylethane $C_{20}H_{18}$
$(1\times C\text{-}(H)_2(C)(C_B))+(1\times C\text{-}(H)(C)(C_B)_2)+(3\times C_B\text{-}(C)(C_B)_2)+(15\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		133.60		
$C_p°$ =		404.90		
$S°$ =		450.07		
$\Delta_f S°$ =		−839.87		
$\Delta_f G°$ =		384.01		
$\ln K_f$ =		−154.91		
Solid phase				
$\Delta_f H°$ =		133.95		
$C_p°$ =	319.66	325.10	−5.44	31SMI/AND

1,1,1-Triphenylethane $C_{20}H_{18}$
$(1\times C\text{-}(H)_3(C))+(1\times C\text{-}(C_B)_3(C))+(1\times \text{-}CH_3 \text{ corr (tertiary)})+(3\times C_B\text{-}(C)(C_B)_2)+(15\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =		206.82		
$C_p°$ =	316.73	339.45	−22.72	31SMI/AND

1,1,1,2-Tetraphenylethane $C_{26}H_{22}$
$(1\times C\text{-}(C_B)_3(C))+(1\times C\text{-}(H)_2(C)(C_B))+(4\times C_B\text{-}(C)(C_B)_2)+(20\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =		280.35		
$C_p°$ =	395.39	398.77	−3.38	31SMI/AND

1,1,2,2-Tetraphenylethane $C_{26}H_{22}$
$(2\times C\text{-}(H)(C)(C_B)_2)+(4\times C_B\text{-}(C)(C_B)_2)+(20\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		196.90		
$C_p°$ =		517.00		
$S°$ =		555.64		
$\Delta_f S°$ =		−1029.88		
$\Delta_f G°$ =		503.96		
$\ln K_f$ =		−203.29		
Solid phase				
$\Delta_f H°$ =		219.00		
$C_p°$ =	396.64	396.66	−0.02	31SMI/AND

TABLE 11. Aromatic CH-02 (80) – Continued

Pentaphenylethane $C_{32}H_{26}$
$(1\times C\text{-}(C_B)_3(C))+(1\times C\text{-}(H)(C)(C_B)_2)+(5\times C_B\text{-}(C)(C_B)_2)+(25\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =		365.40		
$C_p°$ =	473.63	470.33	3.30	31SMI/AND

Triphenylethylene $C_{20}H_{16}$
$(1\times C_d\text{-}(C_B)_2)+(1\times C_d\text{-}(H)(C_B))+(3\times C_B\text{-}(C_d)(C_B)_2)+(15\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		340.82		
Liquid phase				
$\Delta_f H°$ =		232.77		
$C_p°$ =		425.29		
Solid phase				
$\Delta_f H°$ =	233.38	226.20	7.18	50COO/HOI
$C_p°$ =	309.20	310.10	−0.90	31SMI/AND

Diphenylacetylene $C_{14}H_{10}$
$(2\times C_t\text{-}(C_B))+(2\times C_B\text{-}(C_t)(C_B)_2)+(10\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		427.96		
$C_p°$ =		184.68		
Liquid phase				
$\Delta_f H°$ =		357.84		
Solid phase				
$\Delta_f H°$ =	312.40	312.00	0.40	53COO/HOI
$C_p°$ =	225.90	225.90	0.00	31SMI/AND

Biphenyl $C_{12}H_{10}$
$(2\times C_B\text{-}(C_B)_3)+(10\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 8$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	182.03	181.42	0.61	89CHI/KNI
$C_p°$ =	162.34	162.34	0.00	69STU/WES
$S°$ =	392.67	392.67	0.00	69STU/WES
$\Delta_f S°$ =		−329.06		
$\Delta_f G°$ =		279.53		
$\ln K_f$ =		−112.76		

TABLE 11. Aromatic CH-02 (80) — Continued

Biphenyl (Continued) $C_{12}H_{10}$
$(2\times C_B-(C_B)_3)+(10\times C_B-(H)(C_B)_2)$, $\sigma = 8$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H^\circ$ =	119.12	116.02	3.10	89CHI/KNI
C_p° =		260.94		
Solid phase				
$\Delta_f H^\circ$ =	100.54	99.36	1.18	66COL/PIL
C_p° =	198.39	197.86	0.53	89CHI/KNI
S° =	209.38	215.50	−6.12	89CHI/KNI
$\Delta_f S^\circ$ =		−506.23		
$\Delta_f G^\circ$ =		250.29		
$\ln K_f$ =		−100.97		

Naphthalene $C_{10}H_8$
$(2\times C_{BF}-(C_{BF})(C_B)_2)+(8\times C_B-(H)(C_B)_2)+$
$(2\times$ naphthalene 0 sub), $\sigma = 4$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	150.63	150.68	−0.05	63MIL
C_p° =	132.55	132.54	0.01	69STU/WES
S° =	335.64	335.63	0.01	69STU/WES
$\Delta_f S^\circ$ =		−244.05		
$\Delta_f G^\circ$ =		223.44		
$\ln K_f$ =		−90.14		
Liquid phase				
$\Delta_f H^\circ$ =	95.97	96.94	−0.97	57MCC/FIN
C_p° =		200.48		
S° =		219.88		
$\Delta_f S^\circ$ =		−359.80		
$\Delta_f G^\circ$ =		204.22		
$\ln K_f$ =		−82.38		
Solid phase				
$\Delta_f H^\circ$ =	77.74	80.44	−2.70	66COL/PIL
C_p° =	165.69	165.64	0.05	57MCC/FIN
S° =	167.40	170.00	−2.60	57MCC/FIN
$\Delta_f S^\circ$ =		−409.68		
$\Delta_f G^\circ$ =		202.59		
$\ln K_f$ =		−81.72		

2-Methylbiphenyl $C_{13}H_{12}$
$(1\times C-(H)_3(C))+(1\times C_B-(C)(C_B)_2)+(1\times$ *ortho* corr$)+$
$(2\times C_B-(C_B)_3)+(9\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		150.25		
C_p° =		190.61		

TABLE 11. Aromatic CH-02 (80) — Continued

2-Methylbiphenyl (Continued) $C_{13}H_{12}$
$(1\times C-(H)_3(C))+(1\times C_B-(C)(C_B)_2)+(1\times$ *ortho* corr$)+$
$(2\times C_B-(C_B)_3)+(9\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H^\circ$ =	108.16	82.67	25.49	35BRU
C_p° =		288.34		

3-Methylbiphenyl $C_{13}H_{12}$
$(1\times C-(H)_3(C))+(1\times C_B-(C)(C_B)_2)+(1\times$ *meta* corr$)+$
$(2\times C_B-(C_B)_3)+(9\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		148.36		
C_p° =		184.92		
Liquid phase				
$\Delta_f H^\circ$ =	85.56	79.41	6.15	35BRU
C_p° =		284.84		

4-Methylbiphenyl $C_{13}H_{12}$
$(1\times C-(H)_3(C))+(1\times C_B-(C)(C_B)_2)+(2\times C_B-(C_B)_3)+$
$(9\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		148.99		
C_p° =		184.21		
Liquid phase				
$\Delta_f H^\circ$ =		79.41		
C_p° =		284.84		
Solid phase				
$\Delta_f H^\circ$ =	55.44	59.99	−4.55	35BRU
C_p° =		221.92		
S° =		243.94		
$\Delta_f S^\circ$ =		−614.11		
$\Delta_f G^\circ$ =		243.09		
$\ln K_f$ =		−98.06		

TABLE 11. Aromatic CH-02 (80) – Continued

Isopropylbiphenyl $C_{15}H_{16}$

$(2\times C\text{–}(H)_3(C))+(1\times C\text{–}(H)(C)_2(C_B))+(2\times\text{–}CH_3 \text{ corr (tertiary)})+(1\times C_B\text{–}(C)(C_B)_2)+(1\times \textit{ortho} \text{ corr})+(9\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(C_B)_3)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		98.95		
$C_p°$ =		238.79		
Liquid phase				
$\Delta_fH°$ =		24.88		
$C_p°$ =	338.49	342.32	−3.83	64VUK/RAS

1-Methylnaphthalene $C_{11}H_{10}$

$(1\times C\text{–}(H)_3(C))+(1\times C_B\text{–}(C)(C_B)_2)+(2\times C_{BF}\text{–}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 1 sub})+(7\times C_B\text{–}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	116.86	118.25	−1.39	69STU/WES
$C_p°$ =	159.54	159.53	0.01	69STU/WES
$S°$ =	377.44	377.75	−0.31	69STU/WES
$\Delta_fS°$ =		−338.25		
$\Delta_fG°$ =		219.10		
$\ln K_f$ =		−88.38		
Liquid phase				
$\Delta_fH°$ =	56.19	60.33	−4.14	60SPE/ROS
$C_p°$ =	224.39	224.38	0.01	57MCC/FIN
$S°$ =	254.81	254.81	0.00	57MCC/FIN
$\Delta_fS°$ =		−461.18		
$\Delta_fG°$ =		197.83		
$\ln K_f$ =		−79.80		

4,4′-Dimethylbiphenyl $C_{14}H_{14}$

$(2\times C\text{–}(H)_3(C))+(2\times C_B\text{–}(C)(C_B)_2)+(2\times C_B\text{–}(C_B)_3)+(8\times C_B\text{–}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		116.56		
$C_p°$ =		206.08		
Liquid phase				
$\Delta_fH°$ =		42.80		
$C_p°$ =		308.74		
Solid phase				
$\Delta_fH°$ =	14.14	20.62	−6.48	35BRU
$C_p°$ =		245.98		
$S°$ =		272.38		
$\Delta_fS°$ =		−721.98		
$\Delta_fG°$ =		235.88		
$\ln K_f$ =		−95.15		

TABLE 11. Aromatic CH-02 (80) – Continued

***ortho*-Terphenyl** $C_{18}H_{14}$

$(4\times C_B\text{–}(C_B)_3)+(14\times C_B\text{–}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		279.98		
$C_p°$ =		243.02		
Liquid phase				
$\Delta_fH°$ =		183.08		
$C_p°$ =		385.80		
Solid phase				
$\Delta_fH°$ =		159.54		
$C_p°$ =	274.34	274.94	−0.60	72CHA/BES
$S°$ =	298.82	294.50	4.32	72CHA/BES
$\Delta_fS°$ =		−722.82		
$\Delta_fG°$ =		375.05		
$\ln K_f$ =		−151.29		

1,3,5-Triphenylbenzene $C_{24}H_{18}$

$(6\times C_B\text{–}(C_B)_3)+(18\times C_B\text{–}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		378.54		
$C_p°$ =		323.70		
Liquid phase				
$\Delta_fH°$ =		250.14		
$C_p°$ =		510.66		
Solid phase				
$\Delta_fH°$ =		219.72		
$C_p°$ =	358.32	352.02	6.30	36PAR/TOD
$S°$ =	367.36	373.50	−6.14	36PAR/TOD
$\Delta_fS°$ =		−939.40		
$\Delta_fG°$ =		499.80		
$\ln K_f$ =		−201.62		

2-Methylnaphthalene $C_{11}H_{10}$

$(1\times C\text{–}(H)_3(C))+(1\times C_B\text{–}(C)(C_B)_2)+(2\times C_{BF}\text{–}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 1 sub})+(7\times C_B\text{–}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	116.11	118.25	−2.14	69STU/WES
$C_p°$ =	159.79	159.53	0.26	69STU/WES
$S°$ =	380.03	377.75	2.28	69STU/WES
$\Delta_fS°$ =		−338.25		
$\Delta_fG°$ =		219.10		
$\ln K_f$ =		−88.38		

TABLE 11. Aromatic CH-02 (80) — Continued

2-Methylnaphthalene (Continued) $C_{11}H_{10}$

$(1\times C\text{-}(H)_3(C))+(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	62.58	60.33	2.25	57MCC/FIN
$C_p°$ =		224.38		
$S°$ =		254.81		
$\Delta_fS°$ =		−461.18		
$\Delta_fG°$ =		197.83		
$\ln K_f$ =		−79.80		
Solid phase				
$\Delta_fH°$ =	44.85	41.07	3.78	60SPE/ROS
$C_p°$ =	195.98	189.70	6.28	57MCC/FIN
$S°$ =	219.99	198.44	21.55	57MCC/FIN
$\Delta_fS°$ =		−517.55		
$\Delta_fG°$ =		195.38		
$\ln K_f$ =		−78.81		

1-Ethylnaphthalene $C_{12}H_{12}$

$(1\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)(C_B))+(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	96.65	96.91	−0.26	69STU/WES
$C_p°$ =	184.18	185.14	−0.96	69STU/WES
$S°$ =	418.15	420.34	−2.19	69STU/WES
$\Delta_fS°$ =		−431.97		
$\Delta_fG°$ =		225.70		
$\ln K_f$ =		−91.05		
Liquid phase				
$\Delta_fH°$ =		35.52		
$C_p°$ =		247.28		
$S°$ =		302.21		
$\Delta_fS°$ =		−550.10		
$\Delta_fG°$ =		199.53		
$\ln K_f$ =		−80.49		

2-Ethylnaphthalene $C_{12}H_{12}$

$(1\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)(C_B))+(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	95.90	96.91	−1.01	69STU/WES
$C_p°$ =	184.43	185.14	−0.71	69STU/WES
$S°$ =	420.74	420.34	0.40	69STU/WES
$\Delta_fS°$ =		−431.97		
$\Delta_fG°$ =		225.70		
$\ln K_f$ =		−91.05		

TABLE 11. Aromatic CH-02 (80) — Continued

2-Ethylnaphthalene (Continued) $C_{12}H_{12}$

$(1\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)(C_B))+(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		35.52		
$C_p°$ =		247.28		
$S°$ =		302.21		
$\Delta_fS°$ =		−550.10		
$\Delta_fG°$ =		199.53		
$\ln K_f$ =		−80.49		

1-Propylnaphthalene $C_{13}H_{14}$

$(1\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_2(C)(C_B))+(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	74.68	76.28	−1.60	69STU/WES
$C_p°$ =	208.11	208.03	0.08	69STU/WES
$S°$ =	458.36	459.50	−1.14	69STU/WES
$\Delta_fS°$ =		−529.12		
$\Delta_fG°$ =		234.04		
$\ln K_f$ =		−94.41		
Liquid phase				
$\Delta_fH°$ =		9.79		
$C_p°$ =		277.70		
$S°$ =		334.59		
$\Delta_fS°$ =		−654.03		
$\Delta_fG°$ =		204.79		
$\ln K_f$ =		−82.61		

2-Propylnaphthalene $C_{13}H_{14}$

$(1\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_2(C)(C_B))+(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	73.85	76.28	2.43	69STU/WES
$C_p°$ =	208.36	208.03	0.33	69STU/WES
$S°$ =	460.99	459.50	1.49	69STU/WES
$\Delta_fS°$ =		−529.12		
$\Delta_fG°$ =		234.04		
$\ln K_f$ =		−94.41		
Liquid phase				
$\Delta_fH°$ =		9.79		
$C_p°$ =		277.70		
$S°$ =		334.59		
$\Delta_fS°$ =		−654.03		
$\Delta_fG°$ =		204.79		
$\ln K_f$ =		−82.61		

TABLE 11. Aromatic CH-02 (80) – Continued

1-Butylnaphthalene $C_{14}H_{16}$

$(1\times C\text{-}(H)_3(C))+(2\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_2(C)(C_B))+$
$(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+$
$(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	53.05	55.65	−2.60	69STU/WES
$C_p°$ =	230.87	230.92	−0.05	69STU/WES
$S°$ =	497.18	498.66	−1.48	69STU/WES
$\Delta_f S°$ =		−626.27		
$\Delta_f G°$ =		242.37		
$\ln K_f$ =		−97.77		
Liquid phase				
$\Delta_f H°$ =		−15.94		
$C_p°$ =		308.12		
$S°$ =		366.97		
$\Delta_f S°$ =		−757.96		
$\Delta_f G°$ =		210.05		
$\ln K_f$ =		−84.73		

2-Butylnaphthalene $C_{14}H_{16}$

$(1\times C\text{-}(H)_3(C))+(2\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_2(C)(C_B))+$
$(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+$
$(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	52.30	55.65	−3.35	69STU/WES
$C_p°$ =	231.12	230.92	0.20	69STU/WES
$S°$ =	499.82	498.66	1.16	69STU/WES
$\Delta_f S°$ =		−626.27		
$\Delta_f G°$ =		242.37		
$\ln K_f$ =		−97.77		
Liquid phase				
$\Delta_f H°$ =		−15.94		
$C_p°$ =		308.12		
$S°$ =		366.97		
$\Delta_f S°$ =		−757.96		
$\Delta_f G°$ =		210.05		
$\ln K_f$ =		−84.73		

1-Pentylnaphthalene $C_{15}H_{18}$

$(1\times C\text{-}(H)_3(C))+(3\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_2(C)(C_B))+$
$(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+$
$(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	32.43	35.02	−2.59	69STU/WES
$C_p°$ =	253.76	253.81	−0.05	69STU/WES
$S°$ =	536.64	537.82	−1.18	69STU/WES
$\Delta_f S°$ =		−723.42		
$\Delta_f G°$ =		250.71		
$\ln K_f$ =		−101.13		

TABLE 11. Aromatic CH-02 (80) – Continued

1-Pentylnaphthalene (Continued) $C_{15}H_{18}$

$(1\times C\text{-}(H)_3(C))+(3\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_2(C)(C_B))+$
$(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+$
$(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		−41.67		
$C_p°$ =		338.54		
$S°$ =		399.35		
$\Delta_f S°$ =		−861.89		
$\Delta_f G°$ =		215.30		
$\ln K_f$ =		−86.85		

2-Pentylnaphthalene $C_{15}H_{18}$

$(1\times C\text{-}(H)_3(C))+(3\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_2(C)(C_B))+$
$(1\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+$
$(2\times \text{naphthalene 1 sub})+(7\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	31.67	35.02	−3.35	69STU/WES
$C_p°$ =	254.01	253.81	0.20	69STU/WES
$S°$ =	539.28	537.82	1.46	69STU/WES
$\Delta_f S°$ =		−723.42		
$\Delta_f G°$ =		250.71		
$\ln K_f$ =		−101.13		
Liquid phase				
$\Delta_f H°$ =		−41.67		
$C_p°$ =		338.54		
$S°$ =		399.35		
$\Delta_f S°$ =		−861.89		
$\Delta_f G°$ =		215.30		
$\ln K_f$ =		−86.85		

1,2-Dimethylnaphthalene $C_{12}H_{12}$

$(2\times C\text{-}(H)_3(C))+(2\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+$
$(2\times \text{naphthalene 2 sub})+(6\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	83.55	85.82	−2.27	69STU/WES
$C_p°$ =	184.85	185.58	−0.73	69STU/WES
$S°$ =	406.81	409.01	−2.20	69STU/WES
$\Delta_f S°$ =		−443.29		
$\Delta_f G°$ =		217.99		
$\ln K_f$ =		−87.94		
Liquid phase				
$\Delta_f H°$ =		23.72		
$C_p°$ =		248.28		
$S°$ =		289.74		
$\Delta_f S°$ =		−562.57		
$\Delta_f G°$ =		191.45		
$\ln K_f$ =		−77.23		

TABLE 11. Aromatic CH-02 (80) — Continued

1,3-Dimethylnaphthalene $C_{12}H_{12}$

$(2\times C\text{-}(H)_3(C)) + (2\times C_B\text{-}(C)(C_B)_2) + (2\times C_{BF}\text{-}(C_{BF})(C_B)_2) + (2\times \text{naphthalene 2 sub}) + (6\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	81.80	85.82	−4.02	69STU/WES
$C_p°$ =	185.10	185.58	−0.48	69STU/WES
$S°$ =	409.45	409.01	0.44	69STU/WES
$\Delta_f S°$ =		−443.29		
$\Delta_f G°$ =		217.99		
$\ln K_f$ =		−87.94		
Liquid phase				
$\Delta_f H°$ =		23.72		
$C_p°$ =		248.28		
$S°$ =		289.74		
$\Delta_f S°$ =		−562.57		
$\Delta_f G°$ =		191.45		
$\ln K_f$ =		−77.23		

1,4-Dimethylnaphthalene $C_{12}H_{12}$

$(2\times C\text{-}(H)_3(C)) + (2\times C_B\text{-}(C)(C_B)_2) + (2\times C_{BF}\text{-}(C_{BF})(C_B)_2) + (2\times \text{naphthalene 2 sub}) + (6\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	82.51	85.82	−3.31	69STU/WES
$C_p°$ =	184.85	185.58	−0.73	69STU/WES
$S°$ =	401.08	403.25	−2.17	69STU/WES
$\Delta_f S°$ =		−449.06		
$\Delta_f G°$ =		219.71		
$\ln K_f$ =		−88.63		
Liquid phase				
$\Delta_f H°$ =		23.72		
$C_p°$ =		248.28		
$S°$ =		289.74		
$\Delta_f S°$ =		−562.57		
$\Delta_f G°$ =		191.45		
$\ln K_f$ =		−77.23		

1,5-Dimethylnaphthalene $C_{12}H_{12}$

$(2\times C\text{-}(H)_3(C)) + (2\times C_B\text{-}(C)(C_B)_2) + (2\times C_{BF}\text{-}(C_{BF})(C_B)_2) + (2\times \text{naphthalene 2 sub}) + (6\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	81.80	85.82	−4.02	69STU/WES
$C_p°$ =	184.85	185.58	−0.73	69STU/WES
$S°$ =	401.08	409.01	−7.93	69STU/WES
$\Delta_f S°$ =		−443.29		
$\Delta_f G°$ =		217.99		
$\ln K_f$ =		−87.94		

TABLE 11. Aromatic CH-02 (80) — Continued

1,5-Dimethylnaphthalene (Continued) $C_{12}H_{12}$

$(2\times C\text{-}(H)_3(C)) + (2\times C_B\text{-}(C)(C_B)_2) + (2\times C_{BF}\text{-}(C_{BF})(C_B)_2) + (2\times \text{naphthalene 2 sub}) + (6\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		23.72		
$C_p°$ =		248.28		
$S°$ =		289.74		
$\Delta_f S°$ =		−562.57		
$\Delta_f G°$ =		191.45		
$\ln K_f$ =		−77.23		

1,6-Dimethylnaphthalene $C_{12}H_{12}$

$(2\times C\text{-}(H)_3(C)) + (2\times C_B\text{-}(C)(C_B)_2) + (2\times C_{BF}\text{-}(C_{BF})(C_B)_2) + (2\times \text{naphthalene 2 sub}) + (6\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	82.51	85.82	−3.31	69STU/WES
$C_p°$ =	185.10	185.58	−0.48	69STU/WES
$S°$ =	409.45	409.01	0.44	69STU/WES
$\Delta_f S°$ =		−443.29		
$\Delta_f G°$ =		217.99		
$\ln K_f$ =		−87.94		
Liquid phase				
$\Delta_f H°$ =		23.72		
$C_p°$ =		248.28		
$S°$ =		289.74		
$\Delta_f S°$ =		−562.57		
$\Delta_f G°$ =		191.45		
$\ln K_f$ =		−77.23		

1,7-Dimethylnaphthalene $C_{12}H_{12}$

$(2\times C\text{-}(H)_3(C)) + (2\times C_B\text{-}(C)(C_B)_2) + (2\times C_{BF}\text{-}(C_{BF})(C_B)_2) + (2\times \text{naphthalene 2 sub}) + (6\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	81.80	85.82	−4.02	69STU/WES
$C_p°$ =	185.10	185.58	−0.48	69STU/WES
$S°$ =	409.45	409.01	0.44	69STU/WES
$\Delta_f S°$ =		−443.29		
$\Delta_f G°$ =		217.99		
$\ln K_f$ =		−87.94		
Liquid phase				
$\Delta_f H°$ =		23.72		
$C_p°$ =		248.28		
$S°$ =		289.74		
$\Delta_f S°$ =		−562.57		
$\Delta_f G°$ =		191.45		
$\ln K_f$ =		−77.23		

TABLE 11. Aromatic CH-02 (80) – Continued

1,8-Dimethylnaphthalene $C_{12}H_{12}$
$(2\times C-(H)_3(C))+(2\times C_B-(C)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(2\times \text{naphthalene 2 sub})+(6\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	108.66	85.82	22.84	74MAN
$C_p°$ =		185.58		
Liquid phase				
$\Delta_fH°$ =	41.76	23.72	18.04	74MAN
$C_p°$ =		248.28		
$S°$ =		289.74		
$\Delta_fS°$ =		−562.57		
$\Delta_fG°$ =		191.45		
$\ln K_f$ =		−77.23		
Solid phase				
$\Delta_fH°$ =	26.10	1.70	24.40	74MAN
$C_p°$ =	242.80	213.76	29.04	77FIN/MES
$S°$ =	224.72	226.88	−2.16	77FIN/MES
$\Delta_fS°$ =		−625.43		
$\Delta_fG°$ =		188.17		
$\ln K_f$ =		−75.91		

2,3-Dimethylnaphthalene $C_{12}H_{12}$
$(2\times C-(H)_3(C))+(2\times C_B-(C)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(2\times \text{naphthalene 2 sub})+(6\times C_B-(H)(C_B)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	83.55	85.82	−2.27	69STU/WES
$C_p°$ =	185.81	185.58	0.23	69STU/WES
$S°$ =	410.95	403.25	7.70	69STU/WES
$\Delta_fS°$ =		−449.06		
$\Delta_fG°$ =		219.71		
$\ln K_f$ =		−88.63		
Liquid phase				
$\Delta_fH°$ =		23.72		
$C_p°$ =		248.28		
$S°$ =		289.74		
$\Delta_fS°$ =		−562.57		
$\Delta_fG°$ =		191.45		
$\ln K_f$ =		−77.23		
Solid phase				
$\Delta_fH°$ =	−2.34	1.70	−4.04	73GOO2
$C_p°$ =		213.76		
$S°$ =		226.88		
$\Delta_fS°$ =		−625.43		
$\Delta_fG°$ =		188.17		
$\ln K_f$ =		−75.91		

2,6-Dimethylnaphthalene $C_{12}H_{12}$
$(2\times C-(H)_3(C))+(2\times C_B-(C)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(2\times \text{naphthalene 2 sub})+(6\times C_B-(H)(C_B)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	82.51	85.82	−3.31	69STU/WES
$C_p°$ =	187.07	185.58	1.49	69STU/WES
$S°$ =	408.69	409.01	−0.32	69STU/WES
$\Delta_fS°$ =		−443.29		
$\Delta_fG°$ =		217.99		
$\ln K_f$ =		−87.94		
Liquid phase				
$\Delta_fH°$ =		23.72		
$C_p°$ =		248.28		
$S°$ =		289.74		
$\Delta_fS°$ =		−562.57		
$\Delta_fG°$ =		191.45		
$\ln K_f$ =		−77.23		
Solid phase				
$\Delta_fH°$ =	−5.73	1.70	−7.43	73GOO2
$C_p°$ =	203.55	213.76	−10.21	77FIN/MES
$S°$ =	227.86	226.88	0.98	77FIN/MES
$\Delta_fS°$ =		−625.43		
$\Delta_fG°$ =		188.17		
$\ln K_f$ =		−75.91		

2,7-Dimethylnaphthalene $C_{12}H_{12}$
$(2\times C-(H)_3(C))+(2\times C_B-(C)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(2\times \text{naphthalene 2 sub})+(6\times C_B-(H)(C_B)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	82.51	85.82	−3.31	69STU/WES
$C_p°$ =	187.07	185.58	1.49	69STU/WES
$S°$ =	408.69	403.25	5.44	69STU/WES
$\Delta_fS°$ =		−449.06		
$\Delta_fG°$ =		219.71		
$\ln K_f$ =		−88.63		
Liquid phase				
$\Delta_fH°$ =		23.72		
$C_p°$ =		248.28		
$S°$ =		289.74		
$\Delta_fS°$ =		−562.57		
$\Delta_fG°$ =		191.45		
$\ln K_f$ =		−77.23		
Solid phase				
$\Delta_fH°$ =	−5.44	1.70	−7.14	73GOO2
$C_p°$ =	204.39	213.76	−9.37	77FIN/MES
$S°$ =	228.57	226.88	1.69	77FIN/MES
$\Delta_fS°$ =		−625.43		
$\Delta_fG°$ =		188.17		
$\ln K_f$ =		−75.91		

TABLE 11. Aromatic CH-02 (80) – Continued

2-Ethyl-3-methylnaphthalene $C_{13}H_{14}$

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)(C_B))+(2\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 2 sub})+(6\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	65.77	64.48	1.29	69STU/WES
C_p° =	210.46	211.19	−0.73	69STU/WES
S° =	457.44	451.60	5.84	69STU/WES
Δ_fS° =		−537.02		
Δ_fG° =		224.59		
$\ln K_f$ =		−90.60		
Liquid phase				
Δ_fH° =		−1.09		
C_p° =		271.18		
S° =		337.14		
Δ_fS° =		−651.48		
Δ_fG° =		193.15		
$\ln K_f$ =		−77.91		

2-Ethyl-6-methylnaphthalene $C_{13}H_{14}$

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)(C_B))+(2\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 2 sub})+(6\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	61.30	64.48	−3.18	69STU/WES
C_p° =	211.71	211.19	0.52	69STU/WES
S° =	455.18	451.60	3.58	69STU/WES
Δ_fS° =		−537.02		
Δ_fG° =		224.59		
$\ln K_f$ =		−90.60		
Liquid phase				
Δ_fH° =		−1.09		
C_p° =		271.18		
S° =		337.14		
Δ_fS° =		−651.48		
Δ_fG° =		193.15		
$\ln K_f$ =		−77.91		
Solid phase				
Δ_fH° =		−20.40		
C_p° =		263.14		
S° =		253.78		
Δ_fS° =		−734.84		
Δ_fG° =		198.69		
$\ln K_f$ =		−80.15		

TABLE 11. Aromatic CH-02 (80) – Continued

2-Ethyl-7-methylnaphthalene $C_{13}H_{14}$

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)_2(C)(C_B))+(2\times C_B\text{-}(C)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(2\times \text{naphthalene 2 sub})+(6\times C_B\text{-}(H)(C_B)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	61.30	64.48	−3.18	69STU/WES
C_p° =	211.71	211.19	0.52	69STU/WES
S° =	455.18	451.60	3.58	69STU/WES
Δ_fS° =		−537.02		
Δ_fG° =		224.59		
$\ln K_f$ =		−90.60		
Liquid phase				
Δ_fH° =		−1.09		
C_p° =		271.18		
S° =		337.14		
Δ_fS° =		−651.48		
Δ_fG° =		193.15		
$\ln K_f$ =		−77.91		

Tetraphenylethylene $C_{26}H_{20}$

$(2\times C_d\text{-}(C_B)_2)+(4\times C_B\text{-}(C_d)(C_B)_2)+(20\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		438.64		
Liquid phase				
Δ_fH° =		301.34		
C_p° =		541.56		
Solid phase				
Δ_fH° =	311.50	311.50	0.00	50COO/HOI
C_p° =	387.60	387.60	0.00	31SMI/AND

Anthracene $C_{14}H_{10}$

$(4\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(10\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	230.96	218.50	12.46	64KEL/RIC
C_p° =		136.10		
Liquid phase				
Δ_fH° =	158.57	144.92	13.65	70GOU/GIR
C_p° =		264.88		
S° =		266.54		
Δ_fS° =		−466.67		
Δ_fG° =		284.06		
$\ln K_f$ =		−114.59		

TABLE 11. Aromatic CH-02 (80) – Continued

Anthracene (Continued) $C_{14}H_{10}$
$(4 \times C_{BF}-(C_{BF})(C_B)_2) + (10 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H^\circ$ =	129.20	121.70	7.50	66COL/PIL
C_p° =	210.50	210.50	0.00	70GOU/GIR
S° =	207.15	203.50	3.65	70GOU/GIR
$\Delta_f S^\circ$ =		−529.71		
$\Delta_f G^\circ$ =		279.63		
$\ln K_f$ =		−112.80		

Naphthacene $C_{18}H_{12}$
$(6 \times C_{BF}-(C_{BF})(C_B)_2) + (12 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	283.50	286.32	−2.82	67WAK/INO
C_p° =		163.32		
Liquid phase				
$\Delta_f H^\circ$ =		192.90		
C_p° =		329.28		
S° =		313.20		
$\Delta_f S^\circ$ =		−573.55		
$\Delta_f G^\circ$ =		363.90		
$\ln K_f$ =		−146.80		
Solid phase				
$\Delta_f H^\circ$ =	158.78	162.96	−4.18	51MAG/HAR
C_p° =	236.56	255.36	−18.80	80WON/WES
S° =	215.39	237.00	−21.61	80WON/WES
$\Delta_f S^\circ$ =		−649.75		
$\Delta_f G^\circ$ =		356.68		
$\ln K_f$ =		−143.88		

Phenanthrene $C_{14}H_{10}$
$(2 \times C_{BF}-(C_{BF})(C_B)_2) + (2 \times C_{BF}-(C_B)(C_{BF})_2) + (10 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	209.10	210.30	−1.20	59AIH
Liquid phase				
$\Delta_f H^\circ$ =	132.66	136.26	−3.60	77FIN/MES
Solid phase				
$\Delta_f H^\circ$ =	116.20	117.50	−1.30	66COL/PIL
C_p° =	220.62	217.44	3.18	77FIN/MES
S° =	215.06	219.50	−4.44	77FIN/MES
$\Delta_f S^\circ$ =		−513.71		
$\Delta_f G^\circ$ =		270.66		
$\ln K_f$ =		−109.18		

TABLE 11. Aromatic CH-02 (80) – Continued

Triphenylene $C_{18}H_{12}$
$(6 \times C_{BF}-(C_B)(C_{BF})_2) + (12 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	269.80	261.72	8.08	58HOY/PEP
Liquid phase				
$\Delta_f H^\circ$ =	176.52	166.92	9.60	71WON/WES
Solid phase				
$\Delta_f H^\circ$ =	151.80	150.36	1.44	78GOO
C_p° =	259.20	276.18	−16.98	71WON/WES
S° =	254.68	285.00	−30.32	71WON/WES
$\Delta_f S^\circ$ =		601.75		
$\Delta_f G^\circ$ =		329.77		
$-\ln K_f$ =		−133.03		

Chrysene $C_{18}H_{12}$
$(2 \times C_{BF}-(C_{BF})(C_B)_2) + (4 \times C_{BF}-(C_B)(C_{BF})_2) + (12 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	276.30	269.92	6.38	80KRU
Liquid phase				
$\Delta_f H^\circ$ =		175.58		
Solid phase				
$\Delta_f H^\circ$ =	145.30	154.56	−9.26	51MAG/HAR
C_p° =		269.24		
S° =		269.00		
$\Delta_f S^\circ$ =		−617.75		
$\Delta_f G^\circ$ =		338.74		
$\ln K_f$ =		−136.65		

Pyrene $C_{16}H_{10}$
$(2 \times C_{BF}-(C_{BF})_3) + (4 \times C_{BF}-(C_{BF})(C_B)_2) + (10 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	225.68	225.68	0.00	80SMI/STE
Liquid phase				
$\Delta_f H^\circ$ =	143.13	143.12	0.01	71WON/WES
Solid phase				
$\Delta_f H^\circ$ =	125.48	125.58	−0.10	80SMI/STE
C_p° =	227.65	226.50	1.15	71WON/WES
S° =	224.89	217.50	7.39	71WON/WES
$\Delta_f S^\circ$ =		−527.20		
$\Delta_f G^\circ$ =		282.76		
$\ln K_f$ =		−114.06		

TABLE 11. Aromatic CH-02 (80) — Continued

1,2-Benzanthracene $C_{18}H_{12}$

$(4\times C_{BF}-(C_{BF})(C_B)_2)+(2\times C_{BF}-(C_B)(C_{BF})_2)+(12\times C_B-(H)(C_B)_2)$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	294.14	278.12	16.02	80KRU
Liquid phase				
$\Delta_f H°$ =	170.83	184.24	−13.41	51MAG/HAR
Solid phase				
$\Delta_f H°$ =		158.76		
$C_p°$ =		262.30		
$S°$ =		253.00		
$\Delta_f S°$ =		−633.75		
$\Delta_f G°$ =		347.71		
$\ln K_f$ =		−140.26		

Fluoranthene $C_{16}H_{10}$

$(1\times C_{BF}-(C_{BF})_3)+(1\times C_{BF}-(C_{BF})(C_B)_2)+(4\times C_{BF}-(C_B)(C_{BF})_2)+(10\times C_B-(H)(C_B)_2)+(1\times \text{fluoranthene rsc})$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	289.00	289.00	0.00	72MOR2
Liquid phase				
$\Delta_f H°$ =	205.00	205.00	0.00	71WON/WES
Solid phase				
$\Delta_f H°$ =	189.00	189.00	0.00	67WES/WON
$C_p°$ =	230.25	230.25	0.00	71WON/WES
$S°$ =	230.58	230.58	0.00	71WON/WES
$\Delta_f S°$ =		−514.11		
$\Delta_f G°$ =		342.28		
$\ln K_f$ =		−138.07		

Perylene $C_{20}H_{12}$

$(2\times C_{BF}-(C_{BF})_3)+(4\times C_{BF}-(C_B)(C_{BF})_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(12\times C_B-(H)(C_B)_2)$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		277.10		

TABLE 11. Aromatic CH-02 (80) — Continued

Perylene (Continued) $C_{20}H_{12}$

$(2\times C_{BF}-(C_{BF})_3)+(4\times C_{BF}-(C_B)(C_{BF})_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(12\times C_B-(H)(C_B)_2)$

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_f H°$ =		173.78		
Solid phase				
$\Delta_f H°$ =	182.67	158.44	24.23	67WES/WON
$C_p°$ =	274.93	285.24	−10.31	80WON/WES
$S°$ =	264.55	283.00	−18.45	80WON/WES
$\Delta_f S°$ =		−615.23		
$\Delta_f G°$ =		341.87		
$\ln K_f$ =		−137.91		

Coronene $C_{24}H_{12}$

$(6\times C_{BF}-(C_{BF})_3)+(6\times C_{BF}-(C_{BF})(C_B)_2)+(12\times C_B-(H)(C_B)_2)$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		307.86		
Liquid phase				
$\Delta_f H°$ =		187.50		
Solid phase				
$\Delta_f H°$ =		174.60		
$C_p°$ =	313.76	303.36	10.40	80WON/WES
$S°$ =	280.87	279.00	1.87	80WON/WES
$\Delta_f S°$ =		−642.19		
$\Delta_f G°$ =		366.07		
$\ln K_f$ =		−147.67		

TABLE 12. Cyclic CH-01 (40)

Cyclopropane C_3H_6

$(3\times C\text{-}(H)_2(C)_2) + (1\times \text{Cyclopropane rsc})$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	53.26	53.26	0.00	49KNO/ROS
$C_p°$ =	55.94	55.94	0.00	69STU/WES
$S°$ =	237.44	237.44	0.00	69STU/WES
$\Delta_f S°$ =		−171.49		
$\Delta_f G°$ =		104.39		
$\ln K_f$ =		−42.11		
Liquid Phase				
$\Delta_f H°$ =		34.39		
$C_p°$ =		62.73		

Cyclobutane C_4H_8

$(4\times C\text{-}(H)_2(C)_2) + (1\times \text{Cyclobutane rsc})$, $\sigma = 8$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	28.37	28.37	0.00	50COO/KAR
$C_p°$ =	72.22	72.22	0.00	69STU/WES
$S°$ =	265.39	265.39	0.00	69STU/WES
$\Delta_f S°$ =		−279.85		
$\Delta_f G°$ =		111.81		
$\ln K_f$ =		−45.10		

Cyclopentane C_5H_{10}

$(5\times C\text{-}(H)_2(C)_2) + (1\times \text{Cyclopentane rsc (unsub)})$, $\sigma = 10$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−76.40	−76.40	0.00	59MCC/PEN
$C_p°$ =	83.01	83.01	0.00	69STU/WES
$S°$ =	292.88	292.88	0.00	69STU/WES
$\Delta_f S°$ =		−388.68		
$\Delta_f G°$ =		39.48		
$\ln K_f$ =		−15.93		
Liquid Phase				
$\Delta_f H°$ =	−105.81	−105.81	0.00	46JOH/PRO
$C_p°$ =	128.78	128.78	0.00	46DOU/HUF2
$S°$ =	204.14	204.14	0.00	46DOU/HUF2
$\Delta_f S°$ =		−477.41		
$\Delta_f G°$ =		36.53		
$\ln K_f$ =		−14.74		

TABLE 12. Cyclic CH-01 (40) – Continued

Cyclohexane C_6H_{12}

$(6\times C\text{-}(H)_2(C)_2) + (1\times \text{Cyclohexane rsc (unsub)})$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−123.10	−123.10	0.00	47OSB/GIN
$C_p°$ =	106.27	106.27	0.00	69STU/WES
$S°$ =	298.24	298.24	0.00	69STU/WES
$\Delta_f S°$ =		−519.62		
$\Delta_f G°$ =		31.83		
$\ln K_f$ =		−12.84		
Liquid Phase				
$\Delta_f H°$ =	−156.15	−156.15	0.00	69GOO/SMI
$C_p°$ =	156.31	156.31	0.00	43RUE/HUF
$S°$ =	204.35	204.35	0.00	43RUE/HUF
$\Delta_f S°$ =		−613.52		
$\Delta_f G°$ =		26.77		
$\ln K_f$ =		−10.80		

Cycloheptane C_7H_{14}

$(7\times C\text{-}(H)_2(C)_2) + (1\times \text{Cycloheptane rsc})$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−118.07	−118.07	0.00	56FIN/SCO
$C_p°$ =	123.09	123.09	0.00	69STU/WES
$S°$ =	342.33	342.33	0.00	69STU/WES
$\Delta_f S°$ =		−611.85		
$\Delta_f G°$ =		64.35		
$\ln K_f$ =		−25.96		
Liquid Phase				
$\Delta_f H°$ =	−156.61	−156.61	0.00	52KAA/COO
$C_p°$ =	180.75	180.75	0.00	56FIN/SCO
$S°$ =	242.55	242.55	0.00	56FIN/SCO
$\Delta_f S°$ =		−711.63		
$\Delta_f G°$ =		55.56		
$\ln K_f$ =		−22.41		

Cyclooctane C_8H_{16}

$(8\times C\text{-}(H)_2(C)_2) + (1\times \text{Cyclooctane rsc})$, $\sigma = 8$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−124.39	−124.39	0.00	56FIN/SCO
$C_p°$ =	139.95	139.95	0.00	69STU/WES
$S°$ =	366.77	366.77	0.00	69STU/WES
$\Delta_f S°$ =		−723.72		
$\Delta_f G°$ =		91.39		
$\ln K_f$ =		−36.86		
Liquid Phase				
$\Delta_f H°$ =	−167.74	−167.74	0.00	52KAA/COO
$C_p°$ =	215.48	215.48	0.00	56FIN/SCO
$S°$ =	262.00	262.00	0.00	56FIN/SCO
$\Delta_f S°$ =		−828.49		
$\Delta_f G°$ =		79.27		
$\ln K_f$ =		−31.98		

TABLE 12. Cyclic CH-01 (40) – Continued

Cyclononane C_9H_{18}
(9 × C–(H)$_2$(C)$_2$) + (1 × Cyclononane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase $\Delta_fH°$ =	−132.76	−132.76	0.00	57KAM
Liquid Phase $\Delta_fH°$ =	−181.17	−181.17	0.00	52KAA/COO

Cyclodecane $C_{10}H_{20}$
(10 × C–(H)$_2$(C)$_2$) + (1 × Cyclodecane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase $\Delta_fH°$ =	−154.31	−154.31	0.00	57KAM
Liquid Phase $\Delta_fH°$ =	−206.69	−206.69	0.00	60COO/KAM

Cycloundecane $C_{11}H_{22}$
(11 × C–(H)$_2$(C)$_2$) + (1 × Cycloundecane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase $\Delta_fH°$ =	−179.37	−179.37	0.00	57KAM
Liquid Phase $\Delta_fH°$ =	−235.48	−235.48	0.00	60COO/KAM

Cyclododecane $C_{12}H_{24}$
(12 × C–(H)$_2$(C)$_2$) + (1 × Cyclododecane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase $\Delta_fH°$ =	−230.25	−230.25	0.00	57KAM
Solid Phase $\Delta_fH°$ =	−306.65	−306.65	0.00	60COO/KAM

Cyclotridecane $C_{13}H_{26}$
(13 × C–(H)$_2$(C)$_2$) + (1 × Cyclotridecane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase $\Delta_fH°$ =	−246.35	−246.35	0.00	57KAM

TABLE 12. Cyclic CH-01 (40) – Continued

Cyclotridecane (Continued) $C_{13}H_{26}$
(13 × C–(H)$_2$(C)$_2$) + (1 × Cyclotridecane rsc)

	Literature	Calculated	Residual	Reference
Liquid Phase $\Delta_fH°$ =	−309.66	−309.66	0.00	60COO/KAM

Cyclotetradecane $C_{14}H_{28}$
(14 × C–(H)$_2$(C)$_2$) + (1 × Cyclotetradecane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase $\Delta_fH°$ =	−239.45	−239.45	0.00	57KAM
Solid Phase $\Delta_fH°$ =	−374.26	−374.26	0.00	60COO/KAM

Cyclopentadecane $C_{15}H_{30}$
(15 × C–(H)$_2$(C)$_2$) + (1 × Cyclopentadecane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase $\Delta_fH°$ =	−301.42	−301.42	0.00	57KAM
Solid Phase $\Delta_fH°$ =	−376.06	−376.06	0.00	60COO/KAM

Cyclohexadecane $C_{16}H_{32}$
(16 × C–(H)$_2$(C)$_2$) + (1 × Cyclohexadecane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase $\Delta_fH°$ =	−321.67	−321.67	0.00	57KAM
Solid Phase $\Delta_fH°$ =	−403.42	−403.42	0.00	60COO/KAM

Cycloheptadecane $C_{17}H_{34}$
(17 × C–(H)$_2$(C)$_2$) + (1 × Cycloheptadecane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase $\Delta_fH°$ =	−364.30	−364.30	0.00	57KAM
Solid Phase $\Delta_fH°$ =	−430.41	−430.41	0.00	60COO/KAM

TABLE 12. Cyclic CH-01 (40) — Continued

Cyclopropene C_3H_4
(2 × C_d–(H)(C)) + (1 × C–(H)$_2$(C_d)$_2$) + (1 × Cyclopropene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	276.98	276.98	0.00	62WIL/BAR

Cyclobutene C_4H_6
(2 × C_d–(H)(C)) + (2 × C–(H)$_2$(C)(C_d)) + (1 × Cyclobutene rsc), σ = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	156.69	156.69	0.00	68WIB/FEN
$C_p°$ =	67.07	67.07	0.00	69STU/WES
$S°$ =	263.51	263.51	0.00	69STU/WES
$\Delta_fS°$ =		−151.17		
$\Delta_fG°$ =		201.76		
$\ln K_f$ =		−81.39		

Cyclopentene C_5H_8
(1 × C–(H)$_2$(C)$_2$) + (2 × C_d–(H)(C)) + (2 × C–(H)$_2$(C)(C_d)) + (1 × Cyclopentene rsc (unsub)), σ = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	34.43	34.43	0.00	50FOR/CAM
$C_p°$ =	75.10	75.10	0.00	69STU/WES
$S°$ =	289.66	289.66	0.00	69STU/WES
$\Delta_fS°$ =		−261.33		
$\Delta_fG°$ =		112.34		
$\ln K_f$ =		−45.32		
Liquid Phase				
$\Delta_fH°$ =	6.36	6.36	0.00	37DOL/GRE
$C_p°$ =	122.38	122.38	0.00	48HUF/EAT
$S°$ =	201.25	201.25	0.00	48HUF/EAT
$\Delta_fS°$ =		−349.73		
$\Delta_fG°$ =		110.63		
$\ln K_f$ =		−44.63		

Cyclohexene C_6H_{10}
(2 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(C)(C_d)) + (2 × C_d–(H)(C)) + (1 × Cyclohexene rsc), σ = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−4.73	−4.77	0.04	50FOR/CAM
$C_p°$ =	105.02	105.02	0.00	69STU/WES
$S°$ =	310.75	310.75	0.00	69STU/WES
$\Delta_fS°$ =		−376.55		
$\Delta_fG°$ =		107.50		
$\ln K_f$ =		−43.36		

TABLE 12. Cyclic CH-01 (40) — Continued

Cyclohexene (Continued) C_6H_{10}
(2 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(C)(C_d)) + (2 × C_d–(H)(C)) + (1 × Cyclohexene rsc), σ = 2

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	−38.20	−38.78	0.58	69GOO/SMI
$C_p°$ =	148.36	148.36	0.00	77HAI/SUG2
$S°$ =	214.60	214.60	0.00	77HAI/SUG2
$\Delta_fS°$ =		−472.69		
$\Delta_fG°$ =		102.15		
$\ln K_f$ =		−41.21		

Cycloheptene C_7H_{12}
(3 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(C)(C_d)) + (2 × C_d–(H)(C)) + (1 × Cycloheptene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−9.20	−9.20	0.00	39CON/KIS

Cyclooctene C_8H_{14}
(4 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(C)(C_d)) + (2 × C_d–(H)(C)) + (1 × Cyclooctene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−26.99	−26.99	0.00	39CON/KIS
Liquid Phase				
$\Delta_fH°$ =	−74.02	−74.02	0.00	71ROG/MCL

1,3-Cyclopentadiene C_5H_6
(2 × C_d–(H)(C)) + (1 × C–(H)$_2$(C_d)$_2$) + (2 × C_d–(H)(C_d)) + (1 × 1,3-Cyclopentadiene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	134.35	134.35	0.00	36KIS/RUE2
Liquid Phase				
$\Delta_fH°$ =	105.98	105.98	0.00	65HUL/REI

1,3-Cyclohexadiene C_6H_8
(2 × C–(H)$_2$(C)(C_d)) + (2 × C_d–(H)(C)) + (2 × C_d–(H)(C_d)) + (1 × 1,3-Cyclohexadiene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	104.58	104.58	0.00	89STE/CHI

TABLE 12. Cyclic CH-01 (40) – Continued

1,3-Cyclohexadiene (Continued) C_6H_8

(2×C–(H)$_2$(C)(C$_d$))+(2×C$_d$–(H)(C))+(2×C$_d$–(H)(C$_d$))+(1×1,3-Cyclohexadiene rsc)

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	71.41	71.41	0.00	89STE/CHI
$C_p°$ =	144.56	144.56	0.00	76GEI/WOL
$S°$ =	197.28	197.28	0.00	76GEI/WOL
$\Delta_fS°$ =		−359.44		
$\Delta_fG°$ =		178.58		
$\ln K_f$ =		−72.04		

1,3-Cycloheptadiene C_7H_{10}

(1×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(C$_d$))+(2×C$_d$–(H)(C))+(2×C$_d$–(H)(C$_d$))+(1×1,3-Cycloheptadiene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	94.35	94.35	0.00	39CON/KIS

1,4-Cyclohexadiene C_6H_8

(4×C$_d$–(H)(C))+(2×C–(H)$_2$(C$_d$)$_2$)+(1×1,4-Cyclohexadiene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	104.75	104.75	0.00	89STE/CHI
Liquid Phase				
$\Delta_fH°$ =	69.70	69.70	0.00	89STE/CHI
$C_p°$ =	145.94	145.94	0.00	76GEI/WOL
$S°$ =	189.37	189.37	0.00	76GEI/WOL
$\Delta_fS°$ =		−367.35		
$\Delta_fG°$ =		179.23		
$\ln K_f$ =		−72.30		

1,5-Cyclooctadiene C_8H_{12}

(4×C$_d$–(H)(C))+(4×C–(H)$_2$(C)(C$_d$))+(1×1,5-Cyclooctadiene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	101.10	101.10	0.00	76KOZ/TIM
Liquid Phase				
$\Delta_fH°$ =	57.70	57.70	0.00	76KOZ/TIM
$C_p°$ =	208.11	208.11	0.00	75LEB/TSV
$S°$ =	264.35	264.35	0.00	75LEB/TSV
$\Delta_fS°$ =		−565.00		
$\Delta_fG°$ =		226.15		
$\ln K_f$ =		−91.23		

TABLE 12. Cyclic CH-01 (40) – Continued

1,3,5-Cycloheptatriene C_7H_8

(1×C–(H)$_2$(C$_d$)$_2$)+(2×C$_d$–(H)(C))+(4×C$_d$–(H)(C$_d$))+(1×1,3,5-Cycloheptatriene rsc), σ = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	183.68	183.68	0.00	39CON/KIS
$C_p°$ =	117.78	117.78	0.00	69STU/WES
$S°$ =	315.64	315.64	0.00	69STU/WES
$\Delta_fS°$ =		−246.83		
$\Delta_fG°$ =		257.27		
$\ln K_f$ =		−103.78		
Liquid Phase				
$\Delta_fH°$ =	144.98	144.98	0.00	56FIN/SCO
$C_p°$ =	162.76	162.76	0.00	56FIN/SCO
$S°$ =	214.64	214.64	0.00	56FIN/SCO
$\Delta_fS°$ =		−347.82		
$\Delta_fG°$ =		248.68		
$\ln K_f$ =		−100.32		

Cyclooctatetraene C_8H_8

(8×C$_d$–(H)(C$_d$))+(1×Cyclooctatetraene rsc), σ = 4

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	297.61	297.61	0.00	49SCO/GRO
$C_p°$ =	122.01	122.01	0.00	69STU/WES
$S°$ =	326.77	326.77	0.00	69STU/WES
$\Delta_fS°$ =		−241.43		
$\Delta_fG°$ =		369.59		
$\ln K_f$ =		−149.09		
Liquid Phase				
$\Delta_fH°$ =	254.51	254.51	0.00	50PRO/JOH
$C_p°$ =	185.18	185.18	0.00	49SCO/GRO
$S°$ =	220.29	220.29	0.00	49SCO/GRO
$\Delta_fS°$ =		−347.91		
$\Delta_fG°$ =		358.24		
$\ln K_f$ =		−144.51		

Spiropentane C_5H_8

(4×C–(H)$_2$(C)$_2$)+(1×C–(C)$_4$)+(1×Spiropentane rsc), σ = 4

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	185.18	185.18	0.00	50SCO/FIN2
$C_p°$ =	88.12	88.12	0.00	69STU/WES
$S°$ =	282.21	282.21	0.00	69STU/WES
$\Delta_fS°$ =		−268.77		
$\Delta_fG°$ =		265.31		
$\ln K_f$ =		−107.03		

TABLE 12. Cyclic CH-01 (40) — Continued

Spiropentane (Continued) C_5H_8
(4 × C–(H)$_2$(C)$_2$) + (1 × C–(C)$_4$) + (1 × Spiropentane rsc), σ = 4

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_f H°$ =	157.65	157.65	0.00	55FRA/PRO
$C_p°$ =	134.52	134.52	0.00	50SCO/FIN2
$S°$ =	193.68	193.68	0.00	50SCO/FIN2
$\Delta_f S°$ =		−357.30		
$\Delta_f G°$ =		264.18		
$\ln K_f$ =		−106.57		

Methylenecyclobutane C_5H_8
(3 × C–(H)$_2$(C)$_2$) + (1 × C$_d$–(H)$_2$) + (1 × C$_d$–(C)$_2$) + (1 × Cyclobutane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	121.55	119.46	2.09	74GOO/MOO
$C_p°$ =		85.81		
Liquid Phase				
$\Delta_f H°$ =	93.85	90.36	3.49	74GOO/MOO
$C_p°$ =	131.13	132.17	−1.04	81FIN/MES
$S°$ =	210.20	204.98	5.22	81FIN/MES
$\Delta_f S°$ =		−346.00		
$\Delta_f G°$ =		193.52		
$\ln K_f$ =		−78.07		

Methylcyclobutane C_5H_{10}
(1 × C–(H)$_3$(C)) + (3 × C–(H)$_2$(C)$_2$) + (1 × C–(H)(C)$_3$) + (1 × Cyclobutane rsc) + (1 × –CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		3.31		
$C_p°$ =		95.14		
Liquid Phase				
$\Delta_f H°$ =	−44.48	−25.11	−19.37	50HUM/SPI
$C_p°$ =		138.44		
$S°$ =		208.03		
$\Delta_f S°$ =		−473.52		
$\Delta_f G°$ =		116.07		
$\ln K_f$ =		−46.82		

Ethylcyclobutane C_6H_{12}
(1 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(H)(C)$_3$) + (1 × Cyclobutane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−26.32	−15.06	−11.26	74GOO/MOO
$C_p°$ =		118.03		

TABLE 12. Cyclic CH-01 (40) — Continued

Ethylcyclobutane (Continued) C_6H_{12}
(1 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(H)(C)$_3$) + (1 × Cyclobutane rsc)

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_f H°$ =	−58.95	−48.66	−10.29	74GOO/MOO
$C_p°$ =		168.86		
$S°$ =		240.41		
$\Delta_f S°$ =		−577.46		
$\Delta_f G°$ =		123.51		
$\ln K_f$ =		−49.82		

Methylcyclopentane C_6H_{12}
(1 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(H)(C)$_3$) + (1 × –CH$_3$ corr (tertiary)) + (1 × Cyclopentane (sub) rsc), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−106.03	−108.66	2.63	47OSB/GIN
$C_p°$ =	109.79	109.50	0.29	69STU/WES
$S°$ =	339.91	339.62	0.29	69STU/WES
$\Delta_f S°$ =		−478.25		
$\Delta_f G°$ =		33.93		
$\ln K_f$ =		−13.69		
Liquid Phase				
$\Delta_f H°$ =	−137.74	−133.89	−3.85	69GOO/SMI
$C_p°$ =	158.70	156.22	2.48	46DOU/HUF2
$S°$ =	247.78	245.58	2.20	46DOU/HUF2
$\Delta_f S°$ =		−572.29		
$\Delta_f G°$ =		36.74		
$\ln K_f$ =		−14.82		

Methylenecyclopentane C_6H_{10}
(1 × C$_d$–(H)$_2$) + (2 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(C)(C$_d$)) + (1 × C$_d$–(C)$_2$) + (1 × Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	12.01	6.99	5.02	75YUR/KAB
$C_p°$ =		95.65		
Liquid Phase				
$\Delta_f H°$ =	−20.08	−18.42	−1.66	61LAB/ROS
$C_p°$ =		147.69		
$S°$ =		241.11		
$\Delta_f S°$ =		−446.18		
$\Delta_f G°$ =		114.61		
$\ln K_f$ =		−46.23		

TABLE 12. Cyclic CH-01 (40) – Continued

1,1-Dimethylcyclopentane C_7H_{14}
(2×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(1×C–(C)$_4$)+
(2×–CH_3 corr (quaternary))+
(1×Cyclopentane (sub) rsc), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−138.24	−137.41	−0.83	86TRC
$C_p°$ =	133.30	131.68	1.62	69STU/WES
$S°$ =	359.28	356.15	3.13	69STU/WES
$\Delta_fS°$ =		−598.03		
$\Delta_fG°$ =		40.89		
$\ln K_f$ =		−16.50		
Liquid Phase				
$\Delta_fH°$ =	−172.05	−165.34	−6.71	49JOH/PRO
$C_p°$ =	187.36	181.56	5.80	53GRO/OLI
$S°$ =	265.01	254.12	10.89	53GRO/OLI
$\Delta_fS°$ =		−700.06		
$\Delta_fG°$ =		43.38		
$\ln K_f$ =		−17.50		

***cis*-1,2-Dimethylcyclopentane** C_7H_{14}
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(2×C–(H)(C)$_3$)+
(2×–CH_3 corr (tertiary))+
(1×Cyclopentane (sub) rsc), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−129.49	−133.72	4.23	86TRC
$C_p°$ =	134.14	132.42	1.72	69STU/WES
$S°$ =	366.14	359.28	6.86	69STU/WES
$\Delta_fS°$ =		−594.90		
$\Delta_fG°$ =		43.65		
$\ln K_f$ =		−17.61		
Liquid Phase				
$\Delta_fH°$ =	−165.27	−162.72	−2.55	49JOH/PRO
$C_p°$ =	188.74	183.66	5.08	53GRO/OLI
$S°$ =	269.16	272.61	−3.45	53GRO/OLI
$\Delta_fS°$ =		−681.57		
$\Delta_fG°$ =		40.49		
$\ln K_f$ =		−16.33		

***trans*-1,2-Dimethylcyclopentane** C_7H_{14}
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(2×C–(H)(C)$_3$)+
(2×–CH_3 corr (tertiary))+
(1×Cyclopentane (sub) rsc), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−136.65	−133.72	−2.93	86TRC
$C_p°$ =	134.47	132.42	2.05	69STU/WES
$S°$ =	366.81	359.28	7.53	69STU/WES
$\Delta_fS°$ =		−594.90		
$\Delta_fG°$ =		43.65		
$\ln K_f$ =		−17.61		

TABLE 12. Cyclic CH-01 (40) – Continued

***trans*-1,2-Dimethylcyclopentane (Continued)** C_7H_{14}
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(2×C–(H)(C)$_3$)+
(2×–CH_3 corr (tertiary))+
(1×Cyclopentane (sub) rsc), σ = 18

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	−171.21	−162.72	−8.49	49JOH/PRO
$C_p°$ =	187.40	183.66	3.74	53GRO/OLI
$S°$ =	269.90	272.61	−2.71	53GRO/OLI
$\Delta_fS°$ =		−681.57		
$\Delta_fG°$ =		40.49		
$\ln K_f$ =		−16.33		

***trans*-1,3-Dimethylcyclopentane** C_7H_{14}
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(2×C–(H)(C)$_3$)+
(2×–CH_3 corr (tertiary))+
(1×Cyclopentane (sub) rsc), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−133.55	−133.72	0.17	86TRC
$C_p°$ =	134.47	132.42	2.05	69STU/WES
$S°$ =	366.81	359.28	7.53	69STU/WES
$\Delta_fS°$ =		−594.90		
$\Delta_fG°$ =		43.65		
$\ln K_f$ =		−17.61		
Liquid Phase				
$\Delta_fH°$ =	−168.07	−162.72	−5.35	49JOH/PRO
$C_p°$ =	189.32	183.66	5.66	53GRO/OLI
$S°$ =	271.54	272.61	−1.07	53GRO/OLI
$\Delta_fS°$ =		−681.57		
$\Delta_fG°$ =		40.49		
$\ln K_f$ =		−16.33		

Ethylcyclopentane C_7H_{14}
(1×C–(H)$_3$(C))+(5×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+
(1×Cyclopentane (sub) rsc), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−126.94	−127.03	0.09	86TRC
$C_p°$ =	131.75	132.39	−0.64	69STU/WES
$S°$ =	378.32	378.78	−0.46	69STU/WES
$\Delta_fS°$ =		−575.40		
$\Delta_fG°$ =		44.53		
$\ln K_f$ =		−17.96		
Liquid Phase				
$\Delta_fH°$ =	−163.43	−157.44	−5.99	46JOH/PRO
$C_p°$ =	185.31	186.64	−1.33	53GRO/OLI
$S°$ =	279.91	277.96	1.95	53GRO/OLI
$\Delta_fS°$ =		−676.22		
$\Delta_fG°$ =		44.17		
$\ln K_f$ =		−17.82		

TABLE 12. Cyclic CH-01 (40) – Continued

Propylcyclopentane C_8H_{16}
(1×C–(H)$_3$(C))+(6×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+
(1×Cyclopentane (sub) rsc), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_fH°$ =	–147.74	–147.66	–0.08	47OSB/GIN
$C_p°$ =	154.64	155.28	–0.64	69STU/WES
$S°$ =	417.27	417.94	–0.67	69STU/WES
$\Delta_fS°$ =		–672.55		
$\Delta_fG°$ =		52.86		
$\ln K_f$ =		–21.32		
Liquid Phase				
$\Delta_fH°$ =	–189.07	–183.17	–5.90	46JOH/PRO
$C_p°$ =	216.27	217.06	–0.79	65MES/TOD2
$S°$ =	310.83	310.34	0.49	65MES/TOD2
$\Delta_fS°$ =		–780.15		
$\Delta_fG°$ =		49.43		
$\ln K_f$ =		–19.94		

TABLE 13. Cyclic CH-02 (48)

Butylcyclopentane C_9H_{18}
(1×C–(H)$_3$(C))+(7×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+
(1×Cyclopentane (sub) rsc), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_fH°$ =	–168.28	–168.29	0.01	69STU/WES
$C_p°$ =	177.49	178.17	–0.68	69STU/WES
$S°$ =	456.22	457.10	–0.88	69STU/WES
$\Delta_fS°$ =		–769.70		
$\Delta_fG°$ =		61.20		
$\ln K_f$ =		–24.69		
Liquid Phase				
$\Delta_fH°$ =		–208.90		
$C_p°$ =	245.35	247.48	–2.13	65MES/TOD2
$S°$ =	343.84	342.72	1.12	65MES/TOD2
$\Delta_fS°$ =		–884.08		
$\Delta_fG°$ =		54.69		
$\ln K_f$ =		–22.06		

Pentylcyclopentane $C_{10}H_{20}$
(1×C–(H)$_3$(C))+(8×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+
(1×Cyclopentane (sub) rsc), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_fH°$ =	–188.91	–188.92	0.01	69STU/WES
$C_p°$ =	200.37	201.06	–0.69	69STU/WES
$S°$ =	495.18	496.26	–1.08	69STU/WES
$\Delta_fS°$ =		–866.85		
$\Delta_fG°$ =		69.53		
$\ln K_f$ =		–28.05		
Liquid Phase				
$\Delta_fH°$ =		–234.63		
$C_p°$ =		277.90		
$S°$ =		375.10		
$\Delta_fS°$ =		–988.01		
$\Delta_fG°$ =		59.95		
$\ln K_f$ =		–24.18		

Hexylcyclopentane $C_{11}H_{22}$
(1×C–(H)$_3$(C))+(9×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+
(1×Cyclopentane (sub) rsc), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_fH°$ =	–209.49	–209.55	0.06	69STU/WES
$C_p°$ =	223.22	223.95	–0.73	69STU/WES
$S°$ =	534.13	535.42	–1.29	69STU/WES
$\Delta_fS°$ =		–964.01		
$\Delta_fG°$ =		77.87		
$\ln K_f$ =		–31.41		

TABLE 13. Cyclic CH-02 (48) – Continued

Hexylcyclopentane (Continued) $C_{11}H_{22}$
(1×C–(H)$_3$(C)) + (9×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_3$) + (1×Cyclopentane (sub) rsc), σ = 3

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =		−260.36		
$C_p°$ =		308.32		
$S°$ =		407.48		
$\Delta_fS°$ =		−1091.94		
$\Delta_fG°$ =		65.20		
lnK_f =		−26.30		

Heptylcyclopentane $C_{12}H_{24}$
(1×C–(H)$_3$(C)) + (10×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_3$) + (1×Cyclopentane (sub) rsc), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−230.12	−230.18	0.06	69STU/WES
$C_p°$ =	246.10	246.84	−0.74	69STU/WES
$S°$ =	573.04	574.58	−1.54	69STU/WES
$\Delta_fS°$ =		−1061.16		
$\Delta_fG°$ =		86.20		
lnK_f =		−34.77		
Liquid Phase				
$\Delta_fH°$ =		−286.09		
$C_p°$ =		338.74		
$S°$ =		439.86		
$\Delta_fS°$ =		−1195.87		
$\Delta_fG°$ =		70.46		
lnK_f =		−28.42		

Octylcyclopentane $C_{13}H_{26}$
(1×C–(H)$_3$(C)) + (11×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_3$) + (1×Cyclopentane (sub) rsc), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−250.71	−250.81	0.10	69STU/WES
$C_p°$ =	268.99	269.73	−0.74	69STU/WES
$S°$ =	611.99	613.74	−1.75	69STU/WES
$\Delta_fS°$ =		−1158.31		
$\Delta_fG°$ =		94.54		
lnK_f =		−38.14		
Liquid Phase				
$\Delta_fH°$ =		−311.82		
$C_p°$ =		369.16		
$S°$ =		472.24		
$\Delta_fS°$ =		−1299.80		
$\Delta_fG°$ =		75.72		
lnK_f =		−30.54		

TABLE 13. Cyclic CH-02 (48) – Continued

Nonylcyclopentane $C_{14}H_{28}$
(1×C–(H)$_3$(C)) + (12×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_3$) + (1×Cyclopentane (sub) rsc), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−271.33	−271.44	0.11	69STU/WES
$C_p°$ =	291.83	292.62	−0.79	69STU/WES
$S°$ =	650.95	652.90	−1.95	69STU/WES
$\Delta_fS°$ =		−1255.46		
$\Delta_fG°$ =		102.87		
lnK_f =		−41.50		
Liquid Phase				
$\Delta_fH°$ =		−337.55		
$C_p°$ =		399.58		
$S°$ =		504.62		
$\Delta_fS°$ =		−1403.73		
$\Delta_fG°$ =		80.97		
lnK_f =		−32.66		

Decylcyclopentane $C_{15}H_{30}$
(1×C–(H)$_3$(C)) + (13×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_3$) + (1×Cyclopentane (sub) rsc), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−292.33	−292.07	−0.26	86TRC
$C_p°$ =	314.72	315.51	−0.79	69STU/WES
$S°$ =	689.90	692.06	−2.16	69STU/WES
$\Delta_fS°$ =		−1352.61		
$\Delta_fG°$ =		111.21		
lnK_f =		−44.86		
Liquid Phase				
$\Delta_fH°$ =	−367.98	−363.28	−4.70	55FRA/PRO2
$C_p°$ =		430.00		
$S°$ =		537.00		
$\Delta_fS°$ =		−1507.66		
$\Delta_fG°$ =		86.23		
lnK_f =		−34.78		

Ethylidenecyclopentane C_7H_{12}

(1×C–(H)$_3$(C)) + (1×C_d–(H)(C)) + (1×C_d–(C)$_2$) + (4×C–(H)$_2$(C)$_2$) + (1×Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−24.77		
$C_p°$ =		123.26		

TABLE 13. Cyclic CH-02 (48) – Continued

Ethylidenecyclopentane (Continued) C_7H_{12}

(1 × C–(H)$_3$(C)) + (1 × C$_d$–(H)(C)) + (1 × C$_d$–(C)$_2$) + (4 × C–(H)$_2$(C)$_2$) + (1 × Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_f H°$ =	−56.74	−56.73	−0.01	61LAB/ROS
$C_p°$ =	181.17	182.66	−1.49	79FUC/PEA
$S°$ =		268.22		
$\Delta_f S°$ =		−555.39		
$\Delta_f G°$ =		108.86		
$\ln K_f$ =		−43.91		

Ethenylcyclopentane C_7H_{12}

(1 × C$_d$–(H)$_2$) + (1 × C$_d$–(H)(C)) + (1 × C–(H)(C)$_2$(C$_d$)) + (4 × C–(H)$_2$(C)$_2$) + (1 × Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−1.96		
$C_p°$ =		131.30		
Liquid Phase				
$\Delta_f H°$ =	−34.81	−31.55	−3.26	61LAB/ROS
$C_p°$ =		181.45		
$S°$ =		272.87		
$\Delta_f S°$ =		−550.74		
$\Delta_f G°$ =		132.65		
$\ln K_f$ =		−53.51		

11-Cyclopentylheneicosane $C_{26}H_{52}$

(2 × C–(H)$_3$(C)) + (22 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) + (1 × Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−521.17		
$C_p°$ =		567.33		
Liquid Phase				
$\Delta_f H°$ =	−648.52	−647.23	−1.29	44KNO/HUF
$C_p°$ =		761.64		
$S°$ =		887.83		
$\Delta_f S°$ =		−2656.26		
$\Delta_f G°$ =		144.73		
$\ln K_f$ =		−58.38		

TABLE 13. Cyclic CH-02 (48) – Continued

Bicyclopentyl $C_{10}H_{18}$

(8 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) + (2 × Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−128.28		
$C_p°$ =		167.54		
Liquid Phase				
$\Delta_f H°$ =	−179.33	−168.20	−11.13	76GOO/LEE
$C_p°$ =	238.91	239.48	−0.57	76GOO/LEE
$S°$ =		324.56		
$\Delta_f S°$ =		−907.98		
$\Delta_f G°$ =		102.51		
$\ln K_f$ =		−41.35		

1-Methylcyclopentene C_6H_{10}

(1 × C–(H)$_3$(C)) + (1 × C$_d$–(C)$_2$) + (1 × C$_d$–(H)(C)) + (2 × C–(H)$_2$(C)(C$_d$)) + (1 × C–(H)$_2$(C)$_2$) + (1 × Cyclopentene (sub) rsc), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−3.81	0.12	−3.93	79FUC/PEA
$C_p°$ =	100.83	99.22	1.61	69STU/WES
$S°$ =	326.35	333.07	−6.72	69STU/WES
$\Delta_f S°$ =		−354.23		
$\Delta_f G°$ =		105.73		
$\ln K_f$ =		−42.65		
Liquid Phase				
$\Delta_f H°$ =	−36.44	−34.77	−1.67	69GOO/SMI
$C_p°$ =	153.10	157.48	−4.38	79FUC/PEA
$S°$ =		226.14		
$\Delta_f S°$ =		−461.15		
$\Delta_f G°$ =		102.72		
$\ln K_f$ =		−41.44		

3-Methylcyclopentene C_6H_{10}

(2 × C$_d$–(H)(C)) + (1 × C–(H)$_2$(C)(C$_d$)) + (1 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_3$(C)) + (1 × C–(H)(C)$_2$(C$_d$)) + (1 × –CH$_3$ corr (tertiary)) + (1 × Cyclopentene (sub) rsc), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	7.36	9.29	−1.93	79FUC/PEA
$C_p°$ =	100.00	109.72	−9.72	69STU/WES
$S°$ =	330.54	328.38	2.16	69STU/WES
$\Delta_f S°$ =		−358.92		
$\Delta_f G°$ =		116.30		
$\ln K_f$ =		−46.92		

TABLE 13. Cyclic CH-02 (48) – Continued

3-Methylcyclopentene (Continued) C_6H_{10}

$(2\times C_d\text{-(H)(C)}) + (1\times C\text{-(H)}_2\text{(C)(C}_d)) + (1\times C\text{-(H)}_2\text{(C)}_2) + (1\times C\text{-(H)}_3\text{(C)}) + (1\times C\text{-(H)(C)}_2\text{(C}_d)) + (1\times\text{-CH}_3\text{ corr (tertiary)}) + (1\times\text{Cyclopentene (sub) rsc}), \sigma = 3$

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	−23.68	−24.35	0.67	61LAB/ROS
$C_p°$ =		159.69		
$S°$ =		224.81		
$\Delta_fS°$ =		−462.48		
$\Delta_fG°$ =		113.54		
$\ln K_f$ =		−45.80		

4-Methylcyclopentene C_6H_{10}

$(2\times C_d\text{-(H)(C)}) + (2\times C\text{-(H)}_2\text{(C)(C}_d)) + (1\times C\text{-(H)}_3\text{(C)}) + (1\times C\text{-(H)(C)}_3) + (1\times\text{-CH}_3\text{ corr (tertiary)}) + (1\times\text{Cyclopentene (sub) rsc}), \sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	14.77	9.50	5.27	69STU/WES
$C_p°$ =	100.00	100.05	−0.05	69STU/WES
$S°$ =	328.86	324.20	4.66	69STU/WES
$\Delta_fS°$ =		−363.10		
$\Delta_fG°$ =		117.76		
$\ln K_f$ =		−47.50		
Liquid Phase				
$\Delta_fH°$ =	−17.57	−24.10	6.53	61LAB/ROS
$C_p°$ =		149.82		
$S°$ =		228.28		
$\Delta_fS°$ =		−459.01		
$\Delta_fG°$ =		112.76		
$\ln K_f$ =		−45.48		

1-Ethylcyclopentene C_7H_{12}

$(1\times C\text{-(H)}_3\text{(C)}) + (3\times C\text{-(H)}_2\text{(C)(C}_d)) + (1\times C\text{-(H)}_2\text{(C)}_2) + (1\times C_d\text{-(H)(C)}) + (1\times C_d\text{-(C)}_2) + (1\times\text{Cyclopentene (sub) rsc})$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−19.75	−20.76	1.01	79FUC/PEA
$C_p°$ =		119.85		
Liquid Phase				
$\Delta_fH°$ =	−58.28	−60.50	2.22	61LAB/ROS
$C_p°$ =	188.28	186.77	1.51	79FUC/PEA
$S°$ =		257.81		
$\Delta_fS°$ =		−565.80		
$\Delta_fG°$ =		108.19		
$\ln K_f$ =		−43.64		

TABLE 13. Cyclic CH-02 (48) – Continued

Methylcyclohexane C_7H_{14}

$(1\times C\text{-(H)}_3\text{(C)}) + (1\times C\text{-(H)(C)}_3) + (1\times\text{-CH}_3\text{ corr (tertiary)}) + (5\times C\text{-(H)}_2\text{(C)}_2) + (1\times\text{Cyclohexane (sub) rsc}), \sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−154.72	−149.23	−5.49	47OSB/GIN
$C_p°$ =	135.02	137.44	−2.42	69STU/WES
$S°$ =	343.34	344.36	−1.02	69STU/WES
$\Delta_fS°$ =		−609.82		
$\Delta_fG°$ =		32.59		
$\ln K_f$ =		−13.15		
Liquid Phase				
$\Delta_fH°$ =	−190.08	−185.27	−4.81	46JOH/PRO
$C_p°$ =	184.51	183.75	0.76	46DOU/HUF2
$S°$ =	247.90	246.41	1.49	46DOU/HUF2
$\Delta_fS°$ =		−707.77		
$\Delta_fG°$ =		25.75		
$\ln K_f$ =		−10.39		

Allylcyclopentane; 3-Cyclopentyl-1-propene C_8H_{14}

$(1\times C_d\text{-(H)}_2) + (1\times C_d\text{-(H)(C)}) + (1\times C\text{-(H)}_2\text{(C)(C}_d)) + (1\times C\text{-(H)(C)}_3) + (4\times C\text{-(H)}_2\text{(C)}_2) + (1\times\text{Cyclopentane (sub) rsc})$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−19.10	−22.38	3.28	79FUC/PEA
$C_p°$ =		144.52		
Liquid Phase				
$\Delta_fH°$ =	−59.50	−57.03	−2.47	71ROG/MCL
$C_p°$ =	202.92	202.00	0.92	79FUC/PEA
$S°$ =		308.72		
$\Delta_fS°$ =		−651.20		
$\Delta_fG°$ =		137.12		
$\ln K_f$ =		−55.32		

Methylenecyclohexane C_7H_{12}

$(1\times C_d\text{-(H)}_2) + (1\times C_d\text{-(C)}_2) + (2\times C\text{-(H)}_2\text{(C)(C}_d)) + (3\times C\text{-(H)}_2\text{(C)}_2) + (1\times\text{Cyclohexane (sub) rsc})$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−25.23	−33.58	8.35	79FUC/PEA
$C_p°$ =		123.59		
Liquid Phase				
$\Delta_fH°$ =	−61.30	−69.80	8.50	63PAS/ALM
$C_p°$ =	177.40	175.22	2.18	79FUC/PEA
$S°$ =		241.94		
$\Delta_fS°$ =		−581.67		
$\Delta_fG°$ =		103.62		
$\ln K_f$ =		−41.80		

TABLE 13. Cyclic CH-02 (48) – Continued

1,1-Dimethylcyclohexane C_8H_{16}
(2×C–(H)$_3$(C))+(1×C–(C)$_4$)+(2×–CH$_3$ corr (quaternary))+(5×C–(H)2(C)$_2$)+(1×Cyclohexane (sub) rsc), σ = 9

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−180.87	−177.98	−2.89	86TRC
$C_p°$ =	154.39	159.62	−5.23	69STU/WES
$S°$ =	365.01	366.65	−1.64	69STU/WES
$\Delta_fS°$ =		−723.84		
$\Delta_fG°$ =		37.83		
$\ln K_f$ =		−15.26		
Liquid Phase				
$\Delta_fH°$ =	−218.74	−216.72	−2.02	47JOH/PRO2
$C_p°$ =	209.24	209.09	0.15	49HUF/TOD
$S°$ =	267.23	254.95	12.28	49HUF/TOD
$\Delta_fS°$ =		−835.54		
$\Delta_fG°$ =		32.40		
$\ln K_f$ =		−13.07		

***trans*-1,2-Dimethylcyclohexane** C_8H_{16}
(2×C–(H)$_3$(C))+(2×C–(H)(C)$_3$)+(2×–CH$_3$ corr (tertiary))+(4×C–(H)$_2$(C)$_2$)+(1×Cyclohexane (sub) rsc), σ = 9

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−179.87	−174.29	−5.58	47OSB/GIN
$C_p°$ =	158.99	160.36	−1.37	69STU/WES
$S°$ =	370.91	369.78	1.13	69STU/WES
$\Delta_fS°$ =		−720.71		
$\Delta_fG°$ =		40.59		
$\ln K_f$ =		−16.37		
Liquid Phase				
$\Delta_fH°$ =	−218.24	−214.10	−4.14	47JOH/PRO2
$C_p°$ =	209.41	211.19	−1.78	49HUF/TOD
$S°$ =	273.22	273.44	−0.22	49HUF/TOD
$\Delta_fS°$ =		−817.05		
$\Delta_fG°$ =		29.50		
$\ln K_f$ =		−11.90		

***trans*-1,3-Dimethylcyclohexane** C_8H_{16}
(2×C–(H)$_3$(C))+(2×C–(H)(C)$_3$)+(2×–CH$_3$ corr (tertiary))+(4×C–(H)$_2$(C)$_2$)+(1×Cyclohexane (sub) rsc), σ = 9

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−176.48	−174.29	−2.19	47OSB/GIN
$C_p°$ =	157.32	160.36	−3.04	69STU/WES
$S°$ =	376.23	369.78	6.45	69STU/WES
$\Delta_fS°$ =		−720.71		
$\Delta_fG°$ =		40.59		
$\ln K_f$ =		−16.37		

TABLE 13. Cyclic CH-02 (48) – Continued

***trans*-1,3-Dimethylcyclohexane (Continued)** C_8H_{16}
(2×C–(H)$_3$(C))+(2×C–(H)(C)$_3$)+(2×–CH$_3$ corr (tertiary))+(4×C–(H)$_2$(C)$_2$)+(1×Cyclohexane (sub) rsc), σ = 9

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	−215.69	−214.10	−1.59	47JOH/PRO2
$C_p°$ =	212.84	211.19	1.65	49HUF/TOD
$S°$ =	276.27	273.44	2.83	49HUF/TOD
$\Delta_fS°$ =		−817.05		
$\Delta_fG°$ =		29.50		
$\ln K_f$ =		−11.90		

***trans*-1,4-Dimethylcyclohexane** C_8H_{16}
(2×C–(H)$_3$(C))+(2×C–(H)(C)$_3$)+(2×–CH$_3$ corr (tertiary))+(4×C–(H)$_2$(C)$_2$)+(1×Cyclohexane (sub) rsc), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−184.51	−174.29	−10.22	47OSB/GIN
$C_p°$ =	157.74	160.36	−2.62	69STU/WES
$S°$ =	364.80	364.02	0.78	69STU/WES
$\Delta_fS°$ =		−726.47		
$\Delta_fG°$ =		42.31		
$\ln K_f$ =		−17.07		
Liquid Phase				
$\Delta_fH°$ =	−222.38	−214.10	−8.28	47JOH/PRO2
$C_p°$ =	210.25	211.19	−0.94	49HUF/TOD
$S°$ =	268.03	273.44	−5.41	47HUF/TOD
$\Delta_fS°$ =		−817.05		
$\Delta_fG°$ =		29.50		
$\ln K_f$ =		−11.90		

Ethylcyclohexane C_8H_{16}
(1×C–(H)$_3$(C))+(1×C–(H)(C)$_3$)+(6×C–(H)$_2$(C)$_2$)+(1×Cyclohexane (sub) rsc), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−171.63	−167.60	−4.03	47OSB/GIN
$C_p°$ =	158.82	160.33	−1.51	69STU/WES
$S°$ =	382.58	383.52	−0.94	69STU/WES
$\Delta_fS°$ =		−706.97		
$\Delta_fG°$ =		43.18		
$\ln K_f$ =		−17.42		
Liquid Phase				
$\Delta_fH°$ =	−212.13	−208.82	−3.31	46JOH/PRO2
$C_p°$ =	211.79	214.17	−2.38	49HUF/TOD
$S°$ =	280.91	278.79	2.12	49HUF/TOD
$\Delta_fS°$ =		−811.70		
$\Delta_fG°$ =		33.19		
$\ln K_f$ =		−13.39		

TABLE 13. Cyclic CH-02 (48) — Continued

Propylcyclohexane C_9H_{18}

$(1\times C-(H)_3(C))+(1\times C-(H)(C)_3)+(7\times C-(H)_2(C)_2)+(1\times \text{Cyclohexane (sub) rsc})$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−192.30	−188.23	−4.07	65FIN/MES
$C_p°$ =	184.22	183.22	1.00	69STU/WES
$S°$ =	419.53	422.68	−3.15	69STU/WES
$\Delta_fS°$ =		−804.12		
$\Delta_fG°$ =		51.52		
$\ln K_f$ =		−20.78		
Liquid Phase				
$\Delta_fH°$ =	−237.40	−234.55	−2.85	70GOO2
$C_p°$ =	242.04	244.59	−2.55	65FIN/MES
$S°$ =	311.88	311.17	0.71	65FIN/MES
$\Delta_fS°$ =		−915.63		
$\Delta_fG°$ =		38.44		
$\ln K_f$ =		−15.51		

Butylcyclohexane $C_{10}H_{20}$

$(1\times C-(H)_3(C))+(1\times C-(H)(C)_3)+(8\times C-(H)_2(C)_2)+(1\times \text{Cyclohexane (sub) rsc})$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−213.10	−208.86	−4.24	65FIN/MES
$C_p°$ =	207.11	206.11	1.00	69STU/WES
$S°$ =	458.48	461.84	−3.36	69STU/WES
$\Delta_fS°$ =		−901.27		
$\Delta_fG°$ =		59.85		
$\ln K_f$ =		−24.15		
Liquid Phase				
$\Delta_fH°$ =	−263.09	−260.28	−2.81	46JOH/PRO2
$C_p°$ =	271.04	275.01	−3.97	65FIN/MES
$S°$ =	344.97	343.55	1.42	65FIN/MES
$\Delta_fS°$ =		−1019.56		
$\Delta_fG°$ =		43.70		
$\ln K_f$ =		−17.63		

Pentylcyclohexane $C_{11}H_{22}$

$(1\times C-(H)_3(C))+(1\times C-(H)(C)_3)+(9\times C-(H)_2(C)_2)+(1\times \text{Cyclohexane (sub) rsc})$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−229.49		
$C_p°$ =	229.95	229.00	0.95	69STU/WES
$S°$ =	497.44	501.00	−3.56	69STU/WES
$\Delta_fS°$ =		−998.43		
$\Delta_fG°$ =		68.19		
$\ln K_f$ =		−27.51		

TABLE 13. Cyclic CH-02 (48) — Continued

Pentylcyclohexane (Continued) $C_{11}H_{22}$

$(1\times C-(H)_3(C))+(1\times C-(H)(C)_3)+(9\times C-(H)_2(C)_2)+(1\times \text{Cyclohexane (sub) rsc})$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =		−286.01		
$C_p°$ =		305.43		
$S°$ =		375.93		
$\Delta_fS°$ =		−1123.49		
$\Delta_fG°$ =		48.96		
$\ln K_f$ =		−19.75		

Dodecylcyclohexane $C_{18}H_{36}$

$(1\times C-(H)_3(C))+(1\times C-(H)(C)_3)+(16\times C-(H)_2(C)_2)+(1\times \text{Cyclohexane (sub) rsc})$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−378.70	−373.90	−4.80	78FUC/PEA
$C_p°$ =		389.23		
Liquid Phase				
$\Delta_fH°$ =	−467.56	−466.12	−1.44	40MOO/REN
$C_p°$ =		518.37		
$S°$ =	615.50	602.59	12.91	49PAR/MOO
$\Delta_fS°$ =		−1851.01		
$\Delta_fG°$ =		85.76		
$\ln K_f$ =		−34.59		

1-Methylcyclohexene C_7H_{12}

$(1\times C-(H)_3(C))+(1\times C_d-(C)_2)+(1\times -CH_3 \text{ corr (tertiary)})+(1\times C_d-(H)(C))+(2\times C-(H)_2(C)(C_d))+(2\times C-(H)_2(C)_2)+(1\times \text{Cyclohexene rsc})$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−43.26	−41.47	−1.79	60CAM/ROS
$C_p°$ =		127.11		
Liquid Phase				
$\Delta_fH°$ =	−81.17	−80.46	−0.71	61LAB/ROS
$C_p°$ =		183.46		
$S°$ =		239.49		
$\Delta_fS°$ =		−584.12		
$\Delta_fG°$ =		93.69		
$\ln K_f$ =		−37.80		

TABLE 13. Cyclic CH-02 (48) – Continued

1-Ethylcyclohexene C_8H_{14}
(1×C–(H)$_3$(C))+(3×C–(H)$_2$(C)(C$_d$))+(1×C$_d$–(C)$_2$)+
(1×C$_d$–(H)(C))+(2×C–(H)$_2$(C)$_2$)+(1×Cyclohexene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−63.43	−60.09	−3.34	60CAM/ROS
$C_p°$ =		147.74		
Liquid Phase				
$\Delta_f H°$ =	−106.69	−104.01	−2.68	61LAB/ROS
$C_p°$ =		212.75		
$S°$ =		271.16		
$\Delta_f S°$ =		−688.76		
$\Delta_f G°$ =		101.34		
$\ln K_f$ =		−40.88		

Allylcyclohexane C_9H_{16}
(1×C$_d$–(H)$_2$)+(1×C$_d$–(H)(C))+(1×C–(H)$_2$(C)(C$_d$))+
(1×C–(H)(C)$_3$)+(5×C–(H)$_2$(C)$_2$)+(1×Cyclohexane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−62.95		
$C_p°$ =		172.46		
Liquid Phase				
$\Delta_f H°$ =		−108.41		
$C_p°$ =	233.47	229.53	3.94	79FUC/PEA
$S°$ =		309.55		
$\Delta_f S°$ =		−786.68		
$\Delta_f G°$ =		126.14		
$\ln K_f$ =		−50.88		

Ethylidenecyclohexane C_8H_{14}
(1×C–(H)$_3$(C))+(1×C$_d$–(C)$_2$)+(1×C$_d$–(H)(C))+
(2×C–(H)$_2$(C)(C$_d$))+(3×C–(H)$_2$(C)$_2$)+
(1×Cyclohexane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−65.84		
$C_p°$ =		146.68		
Liquid Phase				
$\Delta_f H°$ =		−108.11		
$C_p°$ =	203.76	207.93	−4.17	79FUC/PEA
$S°$ =		267.63		
$\Delta_f S°$ =		−692.29		
$\Delta_f G°$ =		98.30		
$\ln K_f$ =		−39.65		

TABLE 13. Cyclic CH-02 (48) – Continued

3-Cyclohexyleicosane $C_{26}H_{52}$
(2×C–(H)$_3$(C))+(2×C–(H)(C)$_3$)+(22×C–(H)$_2$(C)$_2$)+
(1×Cyclohexane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−541.11		
$C_p°$ =		572.38		
Liquid Phase				
$\Delta_f H°$ =	−666.09	−672.88	6.79	44KNO/HUF
$C_p°$ =		758.75		
$S°$ =		856.28		
$\Delta_f S°$ =		−2687.81		
$\Delta_f G°$ =		128.49		
$\ln K_f$ =		−51.83		

9-Cyclohexyleicosane $C_{26}H_{52}$
(2×C–(H)$_3$(C))+(2×C–(H)(C)$_3$)+(22×C–(H)$_2$(C)$_2$)+
(1×Cyclohexane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−541.11		
$C_p°$ =		572.38		
Liquid Phase				
$\Delta_f H°$ =	−674.04	−672.88	−1.16	44KNO/HUF
$C_p°$ =		758.75		
$S°$ =		856.28		
$\Delta_f S°$ =		−2687.81		
$\Delta_f G°$ =		128.49		
$\ln K_f$ =		−51.83		

11-Cyclohexylheneicosane $C_{27}H_{54}$
(2×C–(H)$_3$(C))+(2×C–(H)(C)$_3$)+(23×C–(H)$_2$(C)$_2$)+
(1×Cyclohexane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−561.74		
$C_p°$ =		595.27		
Liquid Phase				
$\Delta_f H°$ =	−689.94	−698.61	8.67	44KNO/HUF
$C_p°$ =		789.17		
$S°$ =		888.66		
$\Delta_f S°$ =		−2791.74		
$\Delta_f G°$ =		133.75		
$\ln K_f$ =		−53.95		

TABLE 13. Cyclic CH-02 (48) — Continued

13-Cyclohexylpentacosane $C_{31}H_{62}$
(2×C-(H)$_3$(C))+(2×C-(H)(C)$_3$)+(27×C-(H)$_2$(C)$_2$)+
(1×Cyclohexane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−644.26		
$C_p°$ =		686.83		
Liquid Phase				
$\Delta_f H°$ =	−792.45	−801.53	9.08	46PAR/WES
$C_p°$ =		910.85		
$S°$ =		1018.18		
$\Delta_f S°$ =		−3207.46		
$\Delta_f G°$ =		154.77		
$\ln K_f$ =		−62.43		

***cis*-Hexahydroindan** C_9H_{16}
(2×C-(H)(C)$_3$)+(7×C-(H)$_2$(C)$_2$)+
(1×*cis*-Hexahydroindan rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−127.24	−127.24	0.00	60BRO/ROS
Liquid Phase				
$\Delta_f H°$ =	−173.26	−173.26	0.00	60BRO/ROS
$C_p°$ =	214.18	214.18	0.00	72FIN/MCC
$S°$ =	265.47	265.47	0.00	72FIN/MCC
$\Delta_f S°$ =		−830.76		
$\Delta_f G°$ =		74.43		
$\ln K_f$ =		−30.02		

***trans*-Hexahydroindan** C_9H_{16}
(2×C-(H)(C)$_3$)+(7×C-(H)$_2$(C)$_2$)+
(1×*trans*-Hexahydroindan rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−131.59	−131.59	0.00	60BRO/ROS
Liquid Phase				
$\Delta_f H°$ =	−176.36	−176.36	0.00	60BRO/ROS
$C_p°$ =	209.70	209.70	0.00	72FIN/MCC
$S°$ =	258.86	258.86	0.00	72FIN/MCC
$\Delta_f S°$ =		−837.37		
$\Delta_f G°$ =		73.30		
$\ln K_f$ =		−29.57		

TABLE 13. Cyclic CH-02 (48) — Continued

***cis*-Decalin** $C_{10}H_{18}$
(2×C-(H)(C)$_3$)+(8×C-(H)$_2$(C)$_2$)+(1×*cis*-Decalin rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−40.38	−40.38	0.00	69STU/WES
$C_p°$ =	39.84	39.84	0.00	69STU/WES
Liquid Phase				
$\Delta_f H°$ =	−219.40	−219.40	0.00	60SPE/ROS
$C_p°$ =	232.00	232.00	0.00	57MCC/FIN
$S°$ =	265.01	265.01	0.00	57MCC/FIN
$\Delta_f S°$ =		−967.53		
$\Delta_f G°$ =		69.07		
$\ln K_f$ =		−27.86		

***trans*-Decalin** $C_{10}H_{18}$
(2×C-(H)(C)$_3$)+(8×C-(H)$_2$(C)$_2$)+(1×*trans*-Decalin rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−43.57	−43.57	0.00	69STU/WES
$C_p°$ =	40.04	40.04	0.00	69STU/WES
Liquid Phase				
$\Delta_f H°$ =	−230.60	−230.60	0.00	60SPE/ROS
$C_p°$ =	228.49	228.49	0.00	57MCC/FIN
$S°$ =	264.93	264.93	0.00	57MCC/FIN
$\Delta_f S°$ =		−967.61		
$\Delta_f G°$ =		57.89		
$\ln K_f$ =		−23.35		

Bicyclo[2.2.2]octane C_8H_{14}
(2×C-(H)(C)$_3$)+(6×C-(H)$_2$(C)$_2$)+
(1×Bicyclo[2.2.2]octane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−99.00	−99.00	0.00	71WON/WES
Liquid Phase				
$C_p°$ =		157.69		
$S°$ =		83.05		
$\Delta_f S°$ =		−876.87		
Solid Phase				
$\Delta_f H°$ =	−146.90	−146.90	0.00	71WON/WES

TABLE 13. Cyclic CH-02 (48) – Continued

Adamantane; Tricyclo[3.3.1.1^{3,7}]decane $C_{10}H_{16}$
(4 × C–(H)(C)$_3$) + (6 × C–(H)$_2$(C)$_2$) + (1 × Adamantane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	–134.60	–134.60	0.00	70MAN/RAP
Solid Phase				
$\Delta_f H°$ =	–197.20	–197.20	0.00	70MAN/RAP

Bicyclo[3.3.3]undecane $C_{11}H_{20}$
(2 × C–(H)(C)$_3$) + (9 × C–(H)$_2$(C)$_2$) + (1 × Bicyclo[3.3.3]undecane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	–88.95	–88.95	0.00	75PAR/STE
Solid Phase				
$\Delta_f H°$ =	–152.55	–152.55	0.00	75PAR/STE

2,2-Metacyclophane $C_{16}H_{16}$
(8 × C$_B$–(H)(C$_B$)$_2$) + (4 × C$_B$–(C)(C$_B$)$_2$) + (4 × C–(H)$_2$(C)(C$_B$)) + (2 × *meta* corr) + (1 × 2,2-Metacyclophane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	170.50	170.50	0.00	69SHI/MCN
Solid Phase				
$\Delta_f H°$ =	78.50	78.50	0.00	69SHI/MCN
C_p° =	240.60	240.60	0.00	69SCH/MCN

2,2-Metaparacyclophane $C_{16}H_{16}$
(8 × C$_B$–(H)(C$_B$)$_2$) + (4 × C$_B$–(C)(C$_B$)$_2$) + (4 × C–(H)$_2$(C)(C$_B$)) + (1 × *meta* corr) + (1 × 2,2-Metaparacyclophane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	218.40	218.40	0.00	69SHI/MCN
Solid Phase				
$\Delta_f H°$ =	130.90	130.90	0.00	69SHI/MCN
C_p° =	261.50	261.50	0.00	69SHI/MCN

2,2-Paracyclophane $C_{16}H_{16}$
(8 × C$_B$–(H)(C$_B$)$_2$) + (4 × C$_B$–(C)(C$_B$)$_2$) + (4 × C–(H)$_2$(C)(C$_B$)) + (1 × 2,2-Paracyclophane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	244.70	244.77	–0.07	80NIS/SAK
Solid Phase				
$\Delta_f H°$ =	146.70	146.70	0.00	80NIS/SAK
C_p° =	252.34	252.34	0.00	70AND/WES2
$S°$ =	265.68	265.68	0.00	70AND/WES2
$\Delta_f S°$ =		–870.73		
$\Delta_f G°$ =		406.31		
$\ln K_f$ =		–163.90		

3,3-Paracyclophane $C_{18}H_{20}$
(8 × C$_B$–(H)(C$_B$)$_2$) + (4 × C$_B$–(C)(C$_B$)$_2$) + (4 × C–(H)$_2$(C)(C$_B$)) + (2 × C–(H)$_2$(C)$_2$) + (1 × 3,3-Paracyclophane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	129.37	129.37	0.00	69SHI/MCN
Solid Phase				
$\Delta_f H°$ =	26.15	26.15	0.00	69SHI/MCN
C_p° =	324.26	324.26	0.00	69SHI/MCN

Indane C_9H_{10}
(4 × C$_B$–(H)(C$_B$)$_2$) + (2 × C$_{BF}$–(C$_{BF}$)(C$_B$)$_2$) + (2 × C–(H)$_2$(C)(C$_B$)) + (1 × C–(H)$_2$(C)$_2$) + (1 × Cyclopentene rsc (unsub))

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	60.90	56.31	4.59	61STU/SIN
C_p° =		102.02		
Liquid Phase				
$\Delta_f H°$ =	10.71	10.40	0.31	61STU/SIN
C_p° =		170.16		
$S°$ =		279.95		
$\Delta_f S°$ =		–424.56		
$\Delta_f G°$ =		136.98		
$\ln K_f$ =		–55.26		

TABLE 13. Cyclic CH-02 (48) — Continued

Indene C_9H_8

$(4\times C_B-(H)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(1\times C_d-(H)(C_d))+(1\times C_d-(H)(C))+(1\times C-(H)_2(C_d)_2)+$ (1 × 1,3-Cyclopentadiene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	163.30	165.19	−1.89	37DOL/GRE
Liquid Phase				
$\Delta_fH°$ =	110.42	117.05	−6.63	61STU/SIN

TABLE 14. Cyclic CH-03 (47)

Bicyclo[1.1.0]butane C_4H_6

$(2\times C-(H)_2(C)_2)+(2\times C-(H)(C)_3)+$ (1 × Bicyclo[1.1.0]butane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	217.10	217.10	0.00	68WIB/FEN
Liquid Phase				
$\Delta_fH°$ =	193.70	193.70	0.00	73SUN/WUL

Bicyclopropyl C_6H_{10}

$(4\times C-(H)_2(C)_2)+(2\times C-(H)(C)_3)+$ (2 × cyclopropane(sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	129.40	127.04	2.36	66BEE/LUT
Liquid Phase				
$\Delta_fH°$ =	95.90	80.70	15.20	66BEE/LUT

Bicyclo[3.1.0]hexane C_6H_{10}

$(4\times C-(H)_2(C)_2)+(2\times C-(H)(C)_3)+$ (1 × Bicyclo[3.1.0]hexane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	38.30	38.30	0.00	70CHA/MCN
Liquid Phase				
$\Delta_fH°$ =	5.10	5.10	0.00	70CHA/MCN

Bicyclo[2.2.1]hepta-2,5-diene; Norbornadiene C_7H_8

$(4\times C_d-(H)(C))+(2\times C-(H)(C)(C_d)_2)+(1\times C-(H)_2(C)_2)+$ (1 × Bicyclo[2.2.1]hepta-2,5-diene rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	247.60	247.60	0.00	78STE4
Liquid Phase				
$\Delta_fH°$ =	213.80	213.80	0.00	78STE4

TABLE 14. Cyclic CH-03 (47) – Continued

Tetracyclo[3.2.0^{2,7}.0^{4,6}]heptane; Quadricyclane C_7H_8
(1 × C–(H)$_2$(C)$_2$) + (6 × C–(H)(C)$_3$) +
(1 × Tetracyclo[3.2.0^{2,7}.0^{4,6}]heptane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase $\Delta_f H°$ =	339.10	339.10	0.00	78STE4
Liquid Phase $\Delta_f H°$ =	302.10	302.10	0.00	78STE4

Tricyclo[2.2.1.0^{2,6}]heptane C_7H_{10}
(3 × C–(H)$_2$(C)$_2$) + (4 × C–(H)(C)$_3$) +
(1 × Tricyclo[2.2.1.0^{2,6}]heptane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase $\Delta_f H°$ =	82.10	82.10	0.00	78STE4
Liquid Phase $\Delta_f H°$ =	43.40	43.40	0.00	78STE4

Bicyclo[2.2.1]hept-2-ene; Norbornene C_7H_{10}
(2 × C_d–(H)(C)) + (3 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × Bicyclo[2.2.1]hept-2-ene rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase $\Delta_f H°$ =	91.20	91.20	0.00	78STE4
Liquid Phase $\Delta_f H°$ =		48.95		
Solid Phase $\Delta_f H°$ =	53.50	53.50	0.00	78STE4

Bicyclo[2.2.1]heptane; Norbornane C_7H_{12}
(5 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × Bicyclo[2.2.1]heptane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase $\Delta_f H°$ =	–61.60	–61.60	0.00	78STE4
Liquid Phase $\Delta_f H°$ =		–92.80		
Solid Phase $\Delta_f H°$ =	–102.00	–102.00	0.00	78STE4

TABLE 14. Cyclic CH-03 (47) – Continued

Bicyclo[4.1.0]heptane C_7H_{12}
(5 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × Bicyclo[4.1.0]heptane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase $\Delta_f H°$ =	1.50	1.50	0.00	67BOY/SHI
Liquid Phase $\Delta_f H°$ =	–36.80	–36.80	0.00	67BOY/SHI

1-Methylbicyclo[3.1.0]hexane C_7H_{12}
(1 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(H)(C)$_3$) +
(1 × Bicyclo[3.1.0]hexane rsc) + (1 × C–(C)$_4$) +
(1 × –CH_3 corr (quaternary))

	Literature	– Calculated	= Residual	Reference
Gas Phase $\Delta_f H°$ =	1.50	11.85	–10.35	71KOZ/TIM
Liquid Phase $\Delta_f H°$ =	–33.20	–24.14	–9.06	71KOZ/TIM

***cis*-1,2-Diethylcyclopropane** C_7H_{14}
(2 × C–(H)$_3$(C)) + (3 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × cyclopropane(sub) rsc) + (1 × *cis* (unsat) corr)

	Literature	– Calculated	= Residual	Reference
Gas Phase $\Delta_f H°$ =		–37.95		
Liquid Phase $\Delta_f H°$ =	–79.90	–80.10	0.20	70LUP

***trans*-1,2-Diethylcyclopropane** C_7H_{14}
(2 × C–(H)$_3$(C)) + (3 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × cyclopropane(sub) rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase $\Delta_f H°$ =		–42.80		
Liquid Phase $\Delta_f H°$ =	–83.30	–85.37	2.07	70LUP

TABLE 14. Cyclic CH-03 (47) — Continued

Pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane ; Cubane C_8H_8

(8 × C-(H)(C)$_3$) + (1 × Pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]-octane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	665.30	665.24	0.06	89KIR/CHU
Solid Phase				
$\Delta_f H°$ =	585.00	585.00	0.00	89KIR/CHU

Bicyclo[2.2.2]oct-2-ene C_8H_{12}

(2 × C_d-(H)(C)) + (4 × C-(H)$_2$(C)$_2$) + (2 × C-(H)(C)$_2$(C_d)) + (1 × Bicyclo[2.2.2]oct-2-ene rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	20.50	20.50	0.00	70WON/WES
Solid Phase				
$\Delta_f H°$ =	−23.30	−23.30	0.00	71WON/WES

2-Methylenebicyclo[2.2.1]heptane C_8H_{12}

(1 × C_d-(H)$_2$) + (1 × C_d-(C)$_2$) + (1 × C-(H)$_2$(C)(C_d)) + (1 × C-(H)(C)$_2$(C_d)) + (3 × C-(H)$_2$(C)$_2$) + (1 × C-(H)(C)$_3$) + (1 × Bicyclo[2.2.1]heptane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =		28.78		
Liquid Phase				
$\Delta_f H°$ =	−4.10	−6.41	2.31	69SKU/KOZ

2-Methylbicyclo[2.2.1]hept-2-ene C_8H_{12}

(1 × C-(H)$_3$(C)) + (3 × C-(H)$_2$(C)$_2$) + (1 × C_d-(C)$_2$) + (1 × C_d-(H)(C)) + (2 × C-(H)(C)$_2$(C_d)) + (1 × Bicyclo[2.2.1]hept-2-ene rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =		55.84		
Liquid Phase				
$\Delta_f H°$ =	4.50	8.95	−4.45	71KOZ/TIM

TABLE 14. Cyclic CH-03 (47) — Continued

Vinylcyclohexane C_8H_{14}

(1 × C_d-(H)$_2$) + (1 × C_d-(H)(C)) + (1 × C-(H)(C)$_2$(C_d)) + (5 × C-(H)$_2$(C)$_2$) + (1 × Cyclohexane (sub) rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−48.90	−42.53	−6.37	79FUC/PEA
$C_p°$ =		159.24		
Liquid Phase				
$\Delta_f H°$ =	−88.70	−82.93	−5.77	61LAB/ROS
$C_p°$ =		208.98		
$S°$ =		273.70		
$\Delta_f S°$ =		−686.22		
$\Delta_f G°$ =		121.67		
$\ln K_f$ =		−49.08		

Bicyclo[4.2.0]octane C_8H_{14}

(6 × C-(H)$_2$(C)$_2$) + (2 × C-(H)(C)$_3$) + (1 × Bicyclo[4.2.0]octane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−25.40	−25.40	0.00	70CHA/MCN
Liquid Phase				
$\Delta_f H°$ =	−68.20	−68.20	0.00	70CHA/MCN

Bicyclo[5.1.0]octane C_8H_{14}

(6 × C-(H)$_2$(C)$_2$) + (2 × C-(H)(C)$_3$) + (1 × Bicyclo[5.1.0]octane rsc)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−16.70	−16.70	0.00	70CHA/MCN
Liquid Phase				
$\Delta_f H°$ =	−60.30	−60.30	0.00	70CHA/MCN

***cis*-Bicyclo[3.3.0]octane** C_8H_{14}

(6 × C-(H)$_2$(C)$_2$) + (2 × C-(H)(C)$_3$) + (1 × *cis*-Bicyclo[3.3.0]octane)

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−92.90	−92.90	0.00	70CHA/MCN
Liquid Phase				
$\Delta_f H°$ =	−136.00	−136.00	0.00	70CHA/MCN

TABLE 14. Cyclic CH-03 (47) – Continued

***trans*-Bicyclo[3.3.0]octane** C_8H_{14}
(6 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × *trans*-Bicyclo[3.3.0]octane)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−66.60	−66.60	0.00	70CHA/MCN
Liquid Phase				
$\Delta_f H°$ =	−109.20	−109.20	0.00	70CHA/MCN

1-Methylbicyclo[4.1.0]heptane C_8H_{14}
(1 × C–(H)$_3$(C)) + (1 × C–(C)$_4$) + (1 × –CH_3 corr (quaternary)) +
(1 × C–(H)(C)$_3$) + (5 × C–(H)$_2$(C)$_2$) +
(1 × Bicyclo[4.1.0]heptane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−20.80	−24.95	4.15	71KOZ/TIM
Liquid Phase				
$\Delta_f H°$ =	−59.90	−66.04	6.14	71KOZ/TIM

***cis*-1-Ethyl-2-methylcyclopentane** C_8H_{16}
(2 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × –CH_3 corr (tertiary)) + (1 × Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−152.09		
$C_p°$ =		155.31		
Liquid Phase				
$\Delta_f H°$ =	−190.80	−186.27	−4.53	71GOO
$C_p°$ =		214.08		
$S°$ =		304.99		
$\Delta_f S°$ =		−785.50		
$\Delta_f G°$ =		47.93		
$\ln K_f$ =		−19.33		

***trans*-1-Ethyl-2-methylcyclopentane** C_8H_{16}
(2 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × –CH_3 corr (tertiary)) + (1 × Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−152.09		
$C_p°$ =		155.31		
Liquid Phase				
$\Delta_f H°$ =	−195.10	−186.27	−8.83	71GOO
$C_p°$ =		214.08		
$S°$ =		304.99		
$\Delta_f S°$ =		−785.50		

TABLE 14. Cyclic CH-03 (47) – Continued

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_f H°$ =	−195.10	−186.27	−8.83	71GOO
$C_p°$ =		214.08		
$S°$ =		304.99		
$\Delta_f S°$ =		−785.50		
$\Delta_f G°$ =		47.93		
$\ln K_f$ =		−19.33		

***cis*-1-Ethyl-3-methylcyclopentane** C_8H_{16}
(2 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × –CH_3 corr (tertiary)) + (1 × Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−152.09		
$C_p°$ =		155.31		
Liquid Phase				
$\Delta_f H°$ =	−194.40	−186.27	−8.13	71GOO
$C_p°$ =		214.08		
$S°$ =		304.99		
$\Delta_f S°$ =		−785.50		
$\Delta_f G°$ =		47.93		
$\ln K_f$ =		−19.33		

***trans*-1-Ethyl-3-methylcyclopentane** C_8H_{16}
(2 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × Cyclopentane (sub) rsc) + (1 × –CH_3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−152.09		
$C_p°$ =		155.31		
Liquid Phase				
$\Delta_f H°$ =	−196.00	−186.27	−9.73	71GOO
$C_p°$ =		214.08		
$S°$ =		304.99		
$\Delta_f S°$ =		−785.50		
$\Delta_f G°$ =		47.93		
$\ln K_f$ =		−19.33		

1-Ethyl-1-methylcyclopentane C_8H_{16}
(2 × C–(H)$_3$(C)) + (5 × C–(H)$_2$(C)$_2$) + (1 × C–(C)$_4$) +
(1 × –CH_3 corr (quaternary)) + (1 × Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−153.48		
$C_p°$ =		154.57		

TABLE 14. Cyclic CH-03 (47) — Continued

1-Ethyl-1-methylcyclopentane (Continued) C_8H_{16}
(2 × C–(H)$_3$(C)) + (5 × C–(H)$_2$(C)$_2$) + (1 × C–(C)$_4$) +
(1 × –CH_3 corr (quaternary)) + (1 × Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	−193.80	−186.68	−7.12	71GOO
C_p^o =		211.98		
$S°$ =		286.50		
$\Delta_fS°$ =		−803.99		
$\Delta_fG°$ =		53.03		
$\ln K_f$ =		−21.39		

Phenylcyclopropane C_9H_{10}
(2 × C–(H)$_2$(C)$_2$) + (5 × C_B–(H)(C_B)$_2$) + (1 × C_B–(C)(C_B)$_2$) +
(1 × C–(H)(C)$_2$(C_B)) + (1 × cyclopropane(sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	150.50	152.86	−2.36	82FUC/HAL
Liquid Phase				
$\Delta_fH°$ =	100.30	99.26	1.04	61KOS/LUK

***cis*-Bicyclo[6.1.0]nonane** C_9H_{16}
(7 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × *cis*-Bicyclo[6.1.0]nonane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−31.20	−31.20	0.00	78COR/PER
Liquid Phase				
$\Delta_fH°$ =	−80.30	−80.30	0.00	78COR/PER

***trans*-(+)-Bicyclo[6.1.0]nonane** C_9H_{16}
(7 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × *trans*-Bicyclo[6.1.0]nonane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−39.70	−39.70	0.00	78COR/PER
Liquid Phase				
$\Delta_fH°$ =	−82.40	−82.40	0.00	78COR/PER

TABLE 14. Cyclic CH-03 (47) — Continued

***trans*-2,3-Dimethylbicyclo[2.2.1]heptane** C_9H_{16}
(2 × C–(H)$_3$(C)) + (3 × C–(H)$_2$(C)$_2$) + (4 × C–(H)(C)$_3$) +
(1 × Bicyclo[2.2.1]heptane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−107.50	−107.20	−0.30	70VAR/BEL
Liquid Phase				
$\Delta_fH°$ =	−150.20	−146.10	−4.10	71KOZ/TIM

7,7-Dimethylbicyclo[2.2.1]heptane C_9H_{16}

(2 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) + (1 × C–(C)$_4$) +
(2 × –CH_3 corr (quaternary)) +
(1 × Bicyclo[2.2.1]heptane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−115.41		
Liquid Phase				
$\Delta_fH°$ =		−153.08		
Solid Phase				
$\Delta_fH°$ =	−148.20	−162.30	14.10	75KOZ/BYC

Bicyclo[3.3.1]nonane C_9H_{16}
(7 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × Bicyclo[3.3.1]nonane rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−127.50	−127.50	0.00	77PAR/STE
Solid Phase				
$\Delta_fH°$ =	−178.20	−178.20	0.00	77PAR/STE

Cyclopentylcyclohexane $C_{11}H_{20}$
(9 × C–(H)$_2$(C)$_2$) + (2 × C–(H)(C)$_3$) +
(1 × Cyclopentane (sub) rsc) + (1 × Cyclohexane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−168.85		
C_p^o =		195.48		

TABLE 14. Cyclic CH-03 (47) – Continued

Cyclopentylcyclohexane (Continued) $C_{11}H_{20}$
$(9\times C\text{-}(H)_2(C)_2)+(2\times C\text{-}(H)(C)_3)+(1\times \text{Cyclopentane (sub) rsc})+(1\times \text{Cyclohexane (sub) rsc})$

	Literature	Calculated	Residual	Reference
Liquid Phase				
Δ_fH° =	−230.20	−219.58	−10.62	61KOZ/SKU
C_p° =		267.01		
S° =		325.39		
Δ_fS° =		−1043.46		
Δ_fG° =		91.53		
$\ln K_f$ =		−36.92		

Cyclopentylcycloheptane $C_{12}H_{22}$
$(10\times C\text{-}(H)_2(C)_2)+(2\times C\text{-}(H)(C)_3)+(1\times \text{Cyclopentane (sub) rsc})+(1\times \text{Cycloheptane rsc})$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =		−162.75		
C_p° =		204.05		
Liquid Phase				
Δ_fH° =	−226.30	−219.75	−6.55	61KOZ/SKU
C_p° =		291.45		
S° =		348.56		
Δ_fS° =		−1156.60		
Δ_fG° =		125.09		
$\ln K_f$ =		−50.46		

Dicyclopentylmethane $C_{11}H_{20}$
$(9\times C\text{-}(H)_2(C)_2)+(2\times C\text{-}(H)(C)_3)+(2\times \text{Cyclopentane (sub) rsc})$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =		−148.91		
C_p° =		190.43		
Liquid Phase				
Δ_fH° =	−205.10	−193.93	−11.17	61KOZ/SKU
C_p° =		269.90		
S° =		356.94		
Δ_fS° =		−1011.91		
Δ_fG° =		107.77		
$\ln K_f$ =		−43.47		

TABLE 14. Cyclic CH-03 (47) – Continued

Heptylcyclohexane $C_{13}H_{26}$
$(1\times C\text{-}(H)_3(C))+(11\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)(C)_3)+(1\times \text{Cyclohexane (sub) rsc})$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =	−289.20	−270.75	−18.45	78FUC/PEA
C_p° =		274.78		
Liquid Phase				
Δ_fH° =	−353.00	−337.47	−15.53	40MOO/REN
C_p° =		366.27		
S° =		440.69		
Δ_fS° =		−1331.35		
Δ_fG° =		59.47		
$\ln K_f$ =		−23.99		

Bicyclohexyl $C_{12}H_{22}$
$(10\times C\text{-}(H)_2(C)_2)+(2\times C\text{-}(H)(C)_3)+(2\times \text{Cyclohexane (sub) rsc})$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =	−215.70	−209.42	−6.28	78MON/ROS
C_p° =		223.42		
Liquid Phase				
Δ_fH° =	−273.70	−270.96	−2.74	76GOO/LEE
C_p° =		294.54		
S° =		326.22		
Δ_fS° =		−1178.94		
Δ_fG° =		80.54		
$\ln K_f$ =		−32.49		

Bicycloheptyl $C_{14}H_{26}$
$(12\times C\text{-}(H)_2(C)_2)+(2\times C\text{-}(H)(C)_3)+(2\times \text{Cycloheptane rsc})$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =		−197.22		
C_p° =		240.56		
Liquid Phase				
Δ_fH° =	−285.00	−271.30	−13.70	61KOZ/SKU
C_p° =		343.42		
S° =		372.56		
Δ_fS° =		−1405.22		
Δ_fG° =		147.67		
$\ln K_f$ =		−59.57		

TABLE 14. Cyclic CH-03 (47) — Continued

cis-Diphenylcyclopropane $C_{15}H_{14}$

($10 \times C_B-(H)(C_B)_2$) + ($2 \times C_B-(C)(C_B)_2$) + ($1 \times C-(H)_2(C)_2$) + ($2 \times C-(H)(C)_2(C_B)$) + (1 × cyclopropane(sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		261.66		
Liquid Phase				
$\Delta_f H°$ =	178.80	179.13	−0.33	61KOZ/LUK

trans-Diphenylcyclopropane $C_{15}H_{14}$

($10 \times C_B-(H)(C_B)_2$) + ($2 \times C_B-(C)(C_B)_2$) + ($1 \times C-(H)_2(C)_2$) + ($2 \times C-(H)(C)_2(C_B)$) + (1 × cyclopropane(sub) rsc)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		261.66		
Liquid Phase				
$\Delta_f H°$ =	166.20	179.13	−12.93	61KOZ/LUK

trans, trans-1,4-Diphenyl-1,3-butadiene $C_{16}H_{14}$

($2 \times C_d-(H)(C_d)$) + ($2 \times C_d-(H)(C_B)$) + ($2 \times C_B-(C_d)(C_B)_2$) + ($10 \times C_B-(H)(C_B)_2$)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		299.56		
$C_p°$ =		238.50		
Liquid Phase				
$\Delta_f H°$ =		208.56		
$C_p°$ =		372.36		
$S°$ =		323.82		
$\Delta_f S°$ =		−682.02		
$\Delta_f G°$ =		411.90		
$\ln K_f$ =		−166.16		
Solid Phase				
$\Delta_f H°$ =	178.80	175.96	2.84	53COO/HOI2
$C_p°$ =		303.90		
$S°$ =		294.50		
$\Delta_f S°$ =		−711.34		
$\Delta_f G°$ =		388.05		
$\ln K_f$ =		−156.53		

TABLE 14. Cyclic CH-03 (47) — Continued

9,9′-Bianthracene $C_{28}H_{18}$

($18 \times C_B-(H)(C_B)_2$) + ($2 \times C_B-(C_B)(C_{BF})_2$) + ($8 \times C_{BF}-(C_{BF})(C_B)_2$)

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	454.30	454.30	0.00	58HOY/PEP
Solid Phase				
$\Delta_f H°$ =	326.20	326.20	0.00	51MAG/HAR

9,9′-Biphenanthrene $C_{28}H_{18}$

($18 \times C_B-(H)(C_B)_2$) + ($2 \times C_B-(C_B)_2(C_{BF})$) + ($8 \times C_{BF}-(C_{BF})(C_B)_2$)

	Literature	Calculated	Residual	Reference
Solid Phase				
$\Delta_f H°$ =	212.80	212.80	0.00	51MAG/HAR

Hexaphenylethane $C_{38}H_{30}$

($6 \times C_B-(C)(C_B)_2$) + ($30 \times C_B-(H)(C_B)_2$) + ($2 \times C-(C)(C_B)_3$)

	Literature	Calculated	Residual	Reference
Solid Phase				
$\Delta_f H°$ =	511.80	511.80	0.00	36BEN/CUT2

1,1,4,4-Tetraphenylbutane $C_{28}H_{26}$

($20 \times C_B-(H)(C_B)_2$) + ($2 \times C-(H)_2(C)_2$) + ($4 \times C_B-(C)(C_B)_2$) + ($2 \times C-(H)(C)(C_B)_2$)

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_f H°$ =		145.44		
$C_p°$ =		577.84		
$S°$ =		620.40		
$\Delta_f S°$ =		−1237.74		
$\Delta_f G°$ =		514.47		
$\ln K_f$ =		−207.53		
Solid Phase				
$\Delta_f H°$ =	163.30	160.18	3.12	53COO/HOI
$C_p°$ =		440.50		

TABLE 14. Cyclic CH-03 (47) — Continued

1,2′-Dinaphthylmethane $C_{21}H_{16}$
$(1\times C\text{-}(H)_2(C_B)_2)+(2\times C_B\text{-}(C)(C_B)_2)+(4\times C_{BF}\text{-}(C_{BF})(C_B)_2)+(14\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =		274.59		
Liquid Phase				
Δ_fH° =		189.38		
C_p° =		408.71		
S° =		394.99		
Δ_fS° =		−770.12		
Δ_fG° =		418.99		
$\ln K_f$ =		−169.02		
Solid Phase				
Δ_fH° =	162.00	154.18	7.82	78GOO
C_p° =		313.56		
S° =		306.35		
Δ_fS° =		−858.76		
Δ_fG° =		410.22		
$\ln K_f$ =		−165.48		

TABLE 15. Alcohols (69)

Methanol; Methyl alcohol CH_4O
$(1\times C\text{-}(H)_3(C))+(1\times O\text{-}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =	−201.10	201.59	0.49	32ROS
C_p° =	43.89	43.89	0.00	69STU/WES
S° =	239.70	239.69	0.01	69STU/WES
Δ_fS° =		−129.72		
Δ_fG° =		−162.91		
$\ln K_f$ =		65.72		
Liquid Phase				
Δ_fH° =	−238.50	−239.11	0.61	85MAJ/SVO
C_p° =	81.13	81.12	0.01	71CAR/WES
S° =	127.19	127.19	0.00	71CAR/WES
Δ_fS° =		−242.21		
Δ_fG° =		−166.89		
$\ln K_f$ =		67.32		

Ethanol; Ethyl alcohol C_2H_6O
$(1\times C\text{-}(H)_3(C))+(1\times O\text{-}(H)(C))+(1\times C\text{-}(H)_2(O)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =	−235.30	−234.49	−0.81	32ROS
C_p° =	65.44	64.22	1.22	69STU/WES
S° =	282.59	283.12	−0.53	69STU/WES
Δ_fS° =		−222.60		
Δ_fG° =		−168.12		
$\ln K_f$ =		67.82		
Liquid Phase				
Δ_fH° =	−277.60	−274.91	−2.69	85MAJ/SVO
C_p° =	112.50	114.76	−2.26	77HAI/SUG
S° =	159.86	159.78	0.08	77HAI/SUG
Δ_fS° =		−345.93		
Δ_fG° =		−171.77		
$\ln K_f$ =		69.29		

2-Propenol; Allyl alcohol C_3H_6O
$(1\times C_d\text{-}(H)_2)+(1\times C_d\text{-}(H)(C))+(1\times C\text{-}(H)_2(O)(C_d))+(1\times O\text{-}(H)(C))$, $\sigma = 1$

	Literature	Calculated	Residual	Reference
Gas Phase				
Δ_fH° =	−124.50	−124.18	−0.32	38DOL/GRE
C_p° =	76.02	76.02	0.00	69STU/WES
S° =	307.57	307.56	0.01	69STU/WES
Δ_fS° =		−203.89		
Δ_fG° =		−63.39		
$\ln K_f$ =		25.57		

TABLE 15. Alcohols (69) – Continued

2-Propenol; Allyl alcohol (Continued) C_3H_6O

$(1\times C_d\text{–}(H)_2)+(1\times C_d\text{–}(H)(C))+(1\times C\text{–}(H)_2(O)(C_d))+(1\times O\text{–}(H)(C))$, $\sigma = 1$

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	−171.10	−167.32	−3.78	49GEL/SKI
$C_p°$ =	138.91	138.91	0.00	1881REI

Propanol; n-Propyl alcohol C_3H_8O

$(1\times C\text{–}(H)_3(C))+(1\times C\text{–}(H)_2(C)_2)+(1\times O\text{–}(H)(C))+(1\times C\text{–}(H)_2(O)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−255.10	−255.12	0.02	61SNE/SKI
$C_p°$ =	87.11	87.11	0.00	69STU/WES
$S°$ =	324.80	322.28	2.52	69STU/WES
$\Delta_fS°$ =		−319.75		
$\Delta_fG°$ =		−159.79		
$\ln K_f$ =		64.46		
Liquid Phase				
$\Delta_fH°$ =	−302.60	−300.64	−1.96	61SNE/SKI
$C_p°$ =	143.80	145.18	−1.38	68COU/LEE
$S°$ =	192.80	192.16	0.64	68COU/LEE
$\Delta_fS°$ =		−449.87		
$\Delta_fG°$ =		−166.51		
$\ln K_f$ =		67.17		

Butanol; n-Butyl alcohol $C_4H_{10}O$

$(1\times C\text{–}(H)_3(C))+(2\times C\text{–}(H)_2(C)_2)+(1\times C\text{–}(H)_2(O)(C))+(1\times O\text{–}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−275.01	−275.75	0.74	66WAD2
$C_p°$ =	110.00	110.00	0.00	69STU/WES
$S°$ =	363.17	361.44	1.73	69STU/WES
$\Delta_fS°$ =		−416.90		
$\Delta_fG°$ =		−151.45		
$\ln K_f$ =		61.09		
Liquid Phase				
$\Delta_fH°$ =	−327.20	−326.37	−0.83	69MOS/DEK
$C_p°$ =	177.16	175.60	1.56	65COU/HAL
$S°$ =	225.70	224.54	1.16	65COU/HAL
$\Delta_fS°$ =		−553.80		
$\Delta_fG°$ =		−161.26		
$\ln K_f$ =		65.05		

TABLE 15. Alcohols (69) – Continued

Pentanol; n-Pentyl alcohol $C_5H_{12}O$

$(1\times C\text{–}(H)_3(C))+(3\times C\text{–}(H)_2(C)_2)+(1\times C\text{–}(H)_2(O)(C))+(1\times O\text{–}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−294.70	−296.38	1.68	66WAD2
$C_p°$ =	132.88	132.89	−0.01	69STU/WES
$S°$ =	402.54	400.60	1.94	69STU/WES
$\Delta_fS°$ =		−514.05		
$\Delta_fG°$ =		−143.12		
$\ln K_f$ =		57.73		
Liquid Phase				
$\Delta_fH°$ =	−351.60	−352.10	0.50	75MOS/DEK
$C_p°$ =	208.14	206.02	2.12	68COU/LEE
$S°$ =	258.90	256.92	1.98	68COU/LEE
$\Delta_fS°$ =		−657.73		
$\Delta_fG°$ =		−156.00		
$\ln K_f$ =		62.93		

Hexanol; n-Hexyl alcohol $C_6H_{14}O$

$(1\times C\text{–}(H)_3(C))+(4\times C\text{–}(H)_2(C)_2)+(1\times C\text{–}(H)_2(O)(C))+(1\times O\text{–}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−315.90	−317.01	1.11	66WAD2
$C_p°$ =	155.77	155.78	−0.01	69STU/WES
$S°$ =	441.50	439.76	1.74	69STU/WES
$\Delta_fS°$ =		−611.20		
$\Delta_fG°$ =		−134.78		
$\ln K_f$ =		54.37		
Liquid Phase				
$\Delta_fH°$ =	−377.50	−377.83	0.33	75MOS/DEK
$C_p°$ =	242.50	236.44	6.06	89VES/BAR
$S°$ =	287.40	289.30	−1.90	29KEL
$\Delta_fS°$ =		−761.66		
$\Delta_fG°$ =		−150.74		
$\ln K_f$ =		60.81		

Heptanol; n-Heptyl alcohol $C_7H_{16}O$

$(1\times C\text{–}(H)_3(C))+(5\times C\text{–}(H)_2(C)_2)+(1\times C\text{–}(H)_2(O)(C))+(1\times O\text{–}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−336.50	−337.64	1.14	77MAN/SEL
$C_p°$ =	178.66	178.67	−0.01	69STU/WES
$S°$ =	480.45	478.92	1.53	69STU/WES
$\Delta_fS°$ =		−708.35		
$\Delta_fG°$ =		−126.44		
$\ln K_f$ =		51.01		

TABLE 15. Alcohols (69) – Continued

Heptanol; n-Heptyl alcohol (Continued) $C_7H_{16}O$

$(1\times C\text{-}(H)_3(C)) + (5\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(O)(C)) + (1\times O\text{-}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	−403.30	−403.56	0.26	75MOS/DEK
$C_p°$ =	270.80	266.86	3.94	89VES/BAR
$S°$ =	325.90	321.68	4.22	56PAR/KEN
$\Delta_fS°$ =		−865.59		
$\Delta_fG°$ =		−145.48		
$\ln K_f$ =		58.69		

Octanol; n-Octyl alcohol $C_8H_{18}O$

$(1\times C\text{-}(H)_3(C)) + (6\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(O)(C)) + (1\times O\text{-}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−355.60	−358.27	2.67	77MAN/SEL
$C_p°$ =	201.54	201.56	−0.02	69STU/WES
$S°$ =	519.40	518.08	1.32	69STU/WES
$\Delta_fS°$ =		−805.50		
$\Delta_fG°$ =		−118.11		
$\ln K_f$ =		47.64		
Liquid Phase				
$\Delta_fH°$ =	−426.50	−429.29	2.79	75MOS/DEK
$C_p°$ =	304.00	297.28	6.72	89VES/BAR
$S°$ =		354.06		
$\Delta_fS°$ =		−969.52		
$\Delta_fG°$ =		−140.23		
$\ln K_f$ =		56.57		

Nonanol; n-Nonyl alcohol $C_9H_{20}O$

$(1\times C\text{-}(H)_3(C)) + (7\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(O)(C)) + (1\times O\text{-}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−375.50	−378.90	3.40	77MAN/SEL
$C_p°$ =	224.43	224.45	−0.02	69STU/WES
$S°$ =	558.35	557.24	1.11	69STU/WES
$\Delta_fS°$ =		−902.66		
$\Delta_fG°$ =		−109.77		
$\ln K_f$ =		44.28		
Liquid Phase				
$\Delta_fH°$ =	−453.60	−455.02	1.42	75MOS/DEK
$C_p°$ =		327.70		
$S°$ =		386.44		
$\Delta_fS°$ =		−1073.45		
$\Delta_fG°$ =		−134.97		
$\ln K_f$ =		54.45		

TABLE 15. Alcohols (69) – Continued

Decanol; n-Decyl alcohol $C_{10}H_{22}O$

$(1\times C\text{-}(H)_3(C)) + (8\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(O)(C)) + (1\times O\text{-}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−396.60	−399.53	2.93	79SVE
$C_p°$ =	247.32	247.34	−0.02	69STU/WES
$S°$ =	597.31	596.40	0.91	69STU/WES
$\Delta_fS°$ =		−999.81		
$\Delta_fG°$ =		−101.44		
$\ln K_f$ =		40.92		
Liquid Phase				
$\Delta_fH°$ =	−478.10	−480.75	2.65	75MOS/DEK
$C_p°$ =		358.12		
$S°$ =		418.82		
$\Delta_fS°$ =		−1177.38		
$\Delta_fG°$ =		−129.71		
$\ln K_f$ =		52.33		

Undecanol $C_{11}H_{24}O$

$(1\times C\text{-}(H)_3(C)) + (9\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(O)(C)) + (1\times O\text{-}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−422.20	−420.16	−2.04	69STU/WES
$C_p°$ =	270.20	270.23	−0.03	69STU/WES
$S°$ =	636.30	635.56	0.74	69STU/WES
$\Delta_fS°$ =		−1096.96		
$\Delta_fG°$ =		−93.10		
$\ln K_f$ =		37.56		
Liquid Phase				
$\Delta_fH°$ =	−504.80	−506.48	1.68	75MOS/DEK
$C_p°$ =	407.00	388.54	18.46	90ZAB/RUZ
$S°$ =		451.20		
$\Delta_fS°$ =		−1281.31		
$\Delta_fG°$ =		−124.46		
$\ln K_f$ =		50.20		

Dodecanol; n-Dodecyl alcohol $C_{12}H_{26}O$

$(1\times C\text{-}(H)_3(C)) + (10\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(O)(C)) + (1\times O\text{-}(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−436.60	−440.79	4.19	79SVE
$C_p°$ =	293.09	293.12	−0.03	69STU/WES
$S°$ =	675.21	674.72	0.49	69STU/WES
$\Delta_fS°$ =		−1194.11		
$\Delta_fG°$ =		−84.77		
$\ln K_f$ =		34.19		

TABLE 15. Alcohols (69) – Continued

Dodecanol; *n*-Dodecyl alcohol (Continued $C_{12}H_{26}O$
(1×C–(H)$_3$(C)) + (10×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_f H°$ =	−528.50	−532.21	3.71	75MOS/DEK
$C_p°$ =	438.30	418.96	19.34	90ZAB/RUZ
$S°$ =		483.58		
$\Delta_f S°$ =		−1385.24		
$\Delta_f G°$ =		−119.20		
lnK_f =		48.08		

Tridecanol; *n*-Tridecyl alcohol $C_{13}H_{28}O$
(1×C–(H)$_3$(C)) + (11×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−461.42		
$C_p°$ =	315.85	316.01	−0.16	69STU/WES
$S°$ =	711.82	713.88	−2.06	69STU/WES
$\Delta_f S°$ =		−1291.26		
$\Delta_f G°$ =		−76.43		
lnK_f =		30.83		
Liquid Phase				
$\Delta_f H°$ =		−557.94		
$C_p°$ =		449.38		
$S°$ =		515.96		
$\Delta_f S°$ =		−1489.18		
$\Delta_f G°$ =		−113.94		
lnK_f =		45.96		
Solid Phase				
$\Delta_f H°$ =	−599.40	−602.91	3.51	75MOS/DEK
$C_p°$ =	378.00	359.74	18.26	74MOS/MOU
$S°$ =		363.15		
$\Delta_f S°$ =		−1641.99		
$\Delta_f G°$ =		−113.35		
lnK_f =		45.73		

Tetradecanol; *n*-Tetradecyl alcohol $C_{14}H_{30}O$
(1×C–(H)$_3$(C)) + (12×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−474.80	−482.05	7.25	91STE/CHI
$C_p°$ =	338.74	338.90	−0.16	69STU/WES
$S°$ =	751.78	753.04	−1.26	69STU/WES
$\Delta_f S°$ =		−1388.41		
$\Delta_f G°$ =		−68.10		
lnK_f =		27.47		

TABLE 15. Alcohols (69) – Continued

Tetradecanol; *n*-Tetradecyl alcohol (Continued) $C_{14}H_{30}O$
(1×C–(H)$_3$(C)) + (12×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_f H°$ =	−579.70	−583.67	3.97	91STE/CHI
$C_p°$ =		479.80		
$S°$ =		548.34		
$\Delta_f S°$ =		−1593.11		
$\Delta_f G°$ =		−108.69		
lnK_f =		43.84		
Solid Phase				
$\Delta_f H°$ =	−628.18	−632.32	4.14	91STE/CHI
$C_p°$ =	388.00	381.66	6.34	74MOS/MOU
$C_p°$ =	426.32	381.66	44.66	91STE/CHI
$S°$ =		386.16		
$\Delta_f S°$ =		−1755.29		
$\Delta_f G°$ =		−108.98		
lnK_f =		43.96		

Pentadecanol; *n*-Pentadecyl alcohol $C_{15}H_{32}O$
(1×C–(H)$_3$(C)) + (13×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−502.68		
$C_p°$ =	361.58	361.79	−0.21	69STU/WES
$S°$ =	790.73	792.20	−1.47	69STU/WES
$\Delta_f S°$ =		−1485.56		
$\Delta_f G°$ =		−59.76		
lnK_f =		24.11		
Liquid Phase				
$\Delta_f H°$ =		−609.40		
$C_p°$ =		510.22		
$S°$ =		580.72		
$\Delta_f S°$ =		−1697.04		
$\Delta_f G°$ =		−103.43		
lnK_f =		41.72		
Solid Phase				
$\Delta_f H°$ =	−658.20	−661.73	3.53	75MOS/DEK
$C_p°$ =	400.00	403.58	−3.58	74MOS/MOU
$S°$ =		409.17		
$\Delta_f S°$ =		−1868.59		
$\Delta_f G°$ =		−104.61		
lnK_f =		42.20		

TABLE 15. Alcohols (69) – Continued

Hexadecanol; *n*-Hexadecyl alcohol; Cetyl alcohol $C_{16}H_{34}O$
(1×C–(H)$_3$(C)) + (14×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C)), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =	–517.00	–523.31	6.31	65DAV/KYB
$C_p°$ =	384.47	384.68	–0.21	69STU/WES
$S°$ =	829.69	831.36	–1.67	69STU/WES
$\Delta_f S°$ =		–1582.71		
$\Delta_f G°$ =		–51.42		
$\ln K_f$ =		20.74		
Liquid Phase				
$\Delta_f H°$ =		–635.13		
$C_p°$ =		540.64		
$S°$ =		613.10		
$\Delta_f S°$ =		–1800.97		
$\Delta_f G°$ =		–98.17		
$\ln K_f$ =		39.60		
Solid Phase				
$\Delta_f H°$ =	–686.30	–691.14	4.84	75MOS/DEK
$C_p°$ =	422.00	425.50	–3.50	74MOS/MOU
$S°$ =		432.18		
$\Delta_f S°$ =		–1981.89		
$\Delta_f G°$ =		–100.24		
$\ln K_f$ =		40.44		

Heptadecanol; *n*-Heptadecyl alcohol $C_{17}H_{36}O$
(1×C–(H)$_3$(C)) + (15×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C)), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =		–543.94		
$C_p°$ =	407.35	407.57	–0.22	69STU/WES
$S°$ =	868.64	870.52	–1.88	69STU/WES
$\Delta_f S°$ =		–1679.86		
$\Delta_f G°$ =		–43.09		
$\ln K_f$ =		17.38		
Liquid Phase				
$\Delta_f H°$ =		–660.86		
$C_p°$ =		571.06		
$S°$ =		645.48		
$\Delta_f S°$ =		–1904.90		
$\Delta_f G°$ =		–92.91		
$\ln K_f$ =		37.48		
Solid Phase				
$\Delta_f H°$ =		–720.55		
$C_p°$ =		447.42		
$S°$ =		455.19		
$\Delta_f S°$ =		–2095.19		
$\Delta_f G°$ =		–95.87		
$\ln K_f$ =		38.67		

TABLE 15. Alcohols (69) – Continued

Octadecanol; *n*-Octadecyl alcohol $C_{18}H_{38}O$
(1×C–(H)$_3$(C)) + (16×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C)), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =		–564.57		
$C_p°$ =	430.20	430.46	–0.26	69STU/WES
$S°$ =	907.59	909.68	–2.09	69STU/WES
$\Delta_f S°$ =		–1777.01		
$\Delta_f G°$ =		–34.75		
$\ln K_f$ =		14.02		
Liquid Phase				
$\Delta_f H°$ =		–686.59		
$C_p°$ =		601.48		
$S°$ =		677.86		
$\Delta_f S°$ =		–2008.83		
$\Delta_f G°$ =		–87.66		
$\ln K_f$ =		35.36		
Solid Phase				
$\Delta_f H°$ =		–749.96		
$C_p°$ =		469.34		
$S°$ =		478.20		
$\Delta_f S°$ =		–2208.49		
$\Delta_f G°$ =		–91.50		
$\ln K_f$ =		36.91		

Nonadecanol; *n*-Nonadecyl alcohol $C_{19}H_{40}O$
(1×C–(H)$_3$(C)) + (17×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C)), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_f H°$ =		–585.20		
$C_p°$ =	453.08	453.35	–0.27	69STU/WES
$S°$ =	946.55	948.84	–2.29	69STU/WES
$\Delta_f S°$ =		–1874.17		
$\Delta_f G°$ =		–26.42		
$\ln K_f$ =		10.66		
Liquid Phase				
$\Delta_f H°$ =		–712.32		
$C_p°$ =		631.90		
$S°$ =		710.24		
$\Delta_f S°$ =		–2112.76		
$\Delta_f G°$ =		–82.40		
$\ln K_f$ =		33.24		
Solid Phase				
$\Delta_f H°$ =		–779.37		
$C_p°$ =		491.26		
$S°$ =		501.21		
$\Delta_f S°$ =		–2321.79		
$\Delta_f G°$ =		–87.13		
$\ln K_f$ =		35.15		

TABLE 15. Alcohols (69) – Continued

Eicosanol; *n*-Eicosanyl alcohol $C_{20}H_{42}O$

(1×C–(H)$_3$(C)) + (18×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C)), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−605.83		
$C_p°$ =	475.97	476.24	−0.27	69STU/WES
$S°$ =	985.50	988.00	−2.50	69STU/WES
$\Delta_fS°$ =		−1971.32		
$\Delta_fG°$ =		−18.08		
$\ln K_f$ =		7.29		
Liquid Phase				
$\Delta_fH°$ =		−738.05		
$C_p°$ =		662.32		
$S°$ =		742.62		
$\Delta_fS°$ =		−2216.69		
$\Delta_fG°$ =		−77.14		
$\ln K_f$ =		31.12		
Solid Phase				
$\Delta_fH°$ =		−808.78		
$C_p°$ =		513.18		
$S°$ =		524.22		
$\Delta_fS°$ =		−2435.09		
$\Delta_fG°$ =		−82.76		
$\ln K_f$ =		33.38		

2-Methyl-1-propanol; Isobutyl alcohol $C_4H_{10}O$

(2×C–(H)$_3$(C)) + (1×C–(H)(C)$_3$) + (2×–CH$_3$ corr (tertiary)) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C))

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−283.80	−282.44	−1.36	66WAD2
$C_p°$ =		110.03		
Liquid Phase				
$\Delta_fH°$ =	−334.70	−331.65	−3.05	60SKI/SNE
$C_p°$ =	181.00	172.62	8.38	60SKI/SNE
$S°$ =	214.51	219.19	−4.68	68COU/LEE
$\Delta_fS°$ =		−559.15		
$\Delta_fG°$ =		−164.94		
$\ln K_f$ =		66.54		

2-Methyl-1-butanol $C_5H_{12}O$

(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_3$) + (1×–CH$_3$ corr (tertiary)) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C))

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−301.20	−300.81	−0.39	85MAJ/SVO
$C_p°$ =		132.92		
Liquid Phase				
$\Delta_fH°$ =	−356.60	−355.20	−1.40	65CHA/ROS
$C_p°$ =		203.04		
$S°$ =		251.57		
$\Delta_fS°$ =		−663.08		
$\Delta_fG°$ =		−157.50		
$\ln K_f$ =		63.54		

3-Methyl-1-butanol; Isoamyl alcohol $C_5H_{12}O$

(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_3$) + (2×–CH$_3$ corr (tertiary)) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C))

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−300.80	−303.07	2.27	85MAJ/SVO
$C_p°$ =		132.92		
Liquid Phase				
$\Delta_fH°$ =	−356.40	−357.38	0.98	65CHA/ROS
$C_p°$ =	209.50	203.04	6.46	45ZHD
$S°$ =		251.57		
$\Delta_fS°$ =		−663.08		
$\Delta_fG°$ =		−159.68		
$\ln K_f$ =		64.42		

Benzenemethanol; Benzyl alcohol; Phenylcarbinol C_7H_8O

(5×C$_B$–(H)(C$_B$)$_2$) + (1×C$_B$–(C)(C$_B$)$_2$) + (1×O–(H)(C)) + (1×C–(H)$_2$(O)(C$_B$))

	Literature	– Calculated	= Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−100.42	−100.40	−0.02	26MAT
Liquid Phase				
$\Delta_fH°$ =	−160.71	−160.71	0.00	54PAR/MAN
$C_p°$ =	215.94	214.62	1.32	75NIC/WAD

TABLE 15. Alcohols (69) – Continued

2-Ethyl-1-hexanol $C_8H_{18}O$
(2×C–(H)₃(C))+(4×C–(H)₂(C)₂)+(1×C–(H)(C)₃)+(1×C–(H)₂(O)(C))+(1×O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =		−360.44		
$C_p°$ =		201.59		
Liquid Phase				
$\Delta_f H°$ =	−432.80	−430.21	−2.59	60TJE
$C_p°$ =		294.30		
$S°$ =		348.71		
$\Delta_f S°$ =		−974.87		
$\Delta_f G°$ =		−139.55		
$\ln K_f$ =		56.29		

2-Propanol; Isopropyl alcohol C_3H_8O
(2×C–(H)₃(C))+(1×C–(H)(O)(C)₂ (alcohols,peroxides))+(1×O–(H)(C))+(2×–CH₃ corr (tertiary)), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−272.80	−274.47	1.67	66WAD2
$C_p°$ =	88.74	89.58	−0.84	69STU/WES
$S°$ =	309.91	309.06	0.85	69STU/WES
$\Delta_f S°$ =		−332.97		
$\Delta_f G°$ =		−175.20		
$\ln K_f$ =		70.67		
Liquid Phase				
$\Delta_f H°$ =	−318.10	−318.68	0.58	61SNE/SKI
$C_p°$ =	154.43	167.43	−13.00	63AND/COU2
$S°$ =	180.58	180.66	−0.08	63AND/COU2
$\Delta_f S°$ =		−461.37		
$\Delta_f G°$ =		−181.12		
$\ln K_f$ =		73.06		

2-Butanol; sec-Butyl alcohol $C_4H_{10}O$
(2×C–(H)₃(C))+(1×C–(H)₂(C)₂)+(1×C–(H)(O)(C)₂ (alcohols,peroxides))+(1×O–(H)(C))+(1×–CH₃ corr (tertiary)), σ = 9, η = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−292.70	−292.84	0.14	91STE/CHI
$C_p°$ =	113.30	112.47	0.83	69STU/WES
$S°$ =	359.03	359.74	−0.71	69STU/WES
$\Delta_f S°$ =		−418.59		
$\Delta_f G°$ =		−168.04		
$\ln K_f$ =		67.78		

2-Butanol; sec-Butyl alcohol $C_4H_{10}O$
(2×C–(H)₃(C))+(1×C–(H)₂(C)₂)+(1×C–(H)(O)(C)₂ (alcohols,peroxides))+(1×O–(H)(C))+(1×–CH₃ corr (tertiary)), σ = 9, η = 2

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_f H°$ =	−342.60	−342.23	−0.37	91STE/CHI
$C_p°$ =	197.40	197.85	−0.45	71AND/CON
$S°$ =	213.10	213.04	0.06	71AND/CON
$\Delta_f S°$ =		−565.30		
$\Delta_f G°$ =		−173.69		
$\ln K_f$ =		70.06		

2-Pentanol $C_5H_{12}O$
(2×C–(H)₃(C))+(2×C–(H)₂(C)₂)+(1×C–(H)(O)(C)₂ (alcohols,peroxides))+(1×O–(H)(C))+(1×–CH₃ corr (tertiary)), σ = 9, η = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−312.00	−313.47	1.47	85MAJ/SVO
$C_p°$ =		135.36		
$S°$ =		398.90		
$\Delta_f S°$ =		−515.75		
$\Delta_f G°$ =		−159.98		
$\ln K_f$ =		64.42		
Liquid Phase				
$\Delta_f H°$ =	−366.20	−367.96	1.76	74SAC/PES
$C_p°$ =		228.27		
$S°$ =		245.42		
$\Delta_f S°$ =		−669.23		
$\Delta_f G°$ =		−168.43		
$\ln K_f$ =		67.94		

3-Pentanol $C_5H_{12}O$
(2×C–(H)₃(C))+(2×C–(H)₂(C)₂)+(1×C–(H)(O)(C)₂ (alcohols,peroxides))+(1×O–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_f H°$ =	−314.60	−311.21	−3.39	85MAJ/SVO
$C_p°$ =		135.36		
$S°$ =		402.28		
$\Delta_f S°$ =		−512.37		
$\Delta_f G°$ =		−158.45		
$\ln K_f$ =		63.92		
Liquid Phase				
$\Delta_f H°$ =	−368.60	−365.78	−2.82	74SAC/PES
$C_p°$ =	240.00	228.27	11.73	76CON/GIN
$S°$ =		245.42		
$\Delta_f S°$ =		−669.23		
$\Delta_f G°$ =		−166.25		
$\ln K_f$ =		67.06		

TABLE 15. Alcohols (69) – Continued

2-Hexanol $C_6H_{14}O$

(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+
(1×C–(H)(O)(C)$_2$ (alcohols,peroxides))+(1×O–(H)(C))+
(1×–CH$_3$ corr (tertiary)), σ = 9, η = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−329.90	−334.10	4.20	85MAJ/SVO
$C_p°$ =		158.25		
$S°$ =		438.06		
$\Delta_fS°$ =		−612.90		
$\Delta_fG°$ =		−151.36		
$\ln K_f$ =		61.06		
Liquid Phase				
$\Delta_fH°$ =	−388.40	−393.69	5.29	74SAC/PES
$C_p°$ =		258.69		
$S°$ =		277.80		
$\Delta_fS°$ =		−773.16		
$\Delta_fG°$ =		−163.17		
$\ln K_f$ =		65.82		

3-Hexanol $C_6H_{14}O$

(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(1×O–(H)(C))+
(1×C–(H)(O)(C)$_2$ (alcohols,peroxides)), σ = 9, η = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−331.84		
$C_p°$ =		158.25		
$S°$(J/mol·K) =		438.06		
$\Delta_fS°$(J/mol·K) =		−612.90		
$\Delta_fG°$ =		−151.36		
$\ln K_f$ =		61.06		
Liquid Phase				
$\Delta_fH°$ =	−392.40	−391.51	−0.89	85MAJ/SVO
$C_p°$ =	286.00	258.69	27.31	76CON/GIN
$S°$ =		277.80		
$\Delta_fS°$ =		−773.16		
$\Delta_fG°$ =		−160.99		
$\ln K_f$ =		64.94		

4-Methyl-2-pentanol $C_6H_{14}O$

(3×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+
(1×C–(H)(O)(C)$_2$ (alcohols,peroxides))+(1×O–(H)(C))+
(1×C–(H)(C)$_3$)+(3×–CH$_3$ corr (tertiary)), σ = 27, η = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−340.79		
$C_p°$ =		158.28		
$S°$(J/mol·K) =		424.33		
$\Delta_fS°$(J/mol·K) =		−626.63		
$\Delta_fG°$(J/mol·K) =		−153.96		
$\ln K_f$ =		62.11		

TABLE 15. Alcohols (69) – Continued

4-Methyl-2-pentanol (Continued) $C_6H_{14}O$

(3×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+
(1×C–(H)(O)(C)$_2$ (alcohols,peroxides))+(1×O–(H)(C))+
(1×C–(H)(C)$_3$)+(3×–CH$_3$ corr (tertiary)), σ = 27, η = 2

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	−394.70	−398.97	4.27	74SAC/PES
$C_p°$ =		255.71		
$S°$ =		272.45		
$\Delta_fS°$ =		−778.51		
$\Delta_fG°$ =		−166.86		
$\ln K_f$ =		67.31		

2-Methyl-3-pentanol $C_6H_{14}O$

(3×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+
(1×O–(H)(C))+(1×C–(H)(O)(C)$_2$ (alcohols,peroxides))+
(2×–CH$_3$ corr (tertiary)), σ = 27, η = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−338.53		
$C_p°$ =		158.28		
$S°$ =		424.33		
$\Delta_fS°$ =		−626.63		
$\Delta_fG°$ =		−151.70		
$\ln K_f$ =		61.20		
Liquid Phase				
$\Delta_fH°$ =	−396.40	−396.79	0.39	74SAC/PES
$C_p°$ =		255.71		
$S°$ =		272.45		
$\Delta_fS°$ =		−778.51		
$\Delta_fG°$ =		−164.68		
$\ln K_f$ =		66.43		

2-Methyl-2-propanol; tert-Butyl alcohol $C_4H_{10}O$

(3×C–(H)$_3$(C))+(1×C–(O)(C)$_3$ (alcohols,peroxides))+
(1×O–(H)(C))+(3×–CH$_3$ corr (quaternary)), σ = 81

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−312.60	−313.29	0.69	66WAD2
$C_p°$ =	113.39	111.08	2.31	69STU/WES
$S°$ =	326.27	322.32	3.95	69STU/WES
$\Delta_fS°$ =		−456.01		
$\Delta_fG°$ =		−177.33		
$\ln K_f$ =		71.53		

TABLE 15. Alcohols (69) – Continued

2-Methyl-2-propanol; tert-Butyl alcohol (Continued) $C_4H_{10}O$
(3 × C–(H)$_3$(C)) + (1 × C–(O)(C)$_3$ (alcohols,peroxides)) + (1 × O–(H)(C)) + (3 × –CH$_3$ corr (quaternary)), σ = 81

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	−359.20	−358.63	−0.57	60SKI/SNE
$C_p°$ =	219.66	219.66	0.00	63OET
$S°$ =	171.31	171.31	0.00	63OET
$\Delta_fS°$ =		−607.03		
$\Delta_fG°$ =		−177.65		
$\ln K_f$ =		71.66		
Solid Phase				
$\Delta_fH°$ =	−365.90	−365.18	−0.72	63OET
$C_p°$ =	146.11	146.12	−0.01	63OET
$S°$ =	170.87	183.92	−13.05	63OET
$\Delta_fS°$ =		−594.42		
$\Delta_fG°$ =		−187.95		
$\ln K_f$ =		75.82		

2-Methyl-2-butanol $C_5H_{12}O$
(3 × C–(H)$_3$(C)) + (1 × C–(H)$_2$(C)$_2$) + (1 × C–(O)(C)$_3$ (alcohols,peroxides)) + (1 × O–(H)(C)) + (2 × –CH$_3$ corr (quaternary)), σ = 27

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−329.40	−329.36	−0.04	85MAJ/SVO
$C_p°$ =	131.67	133.97	−2.30	69STU/WES
$S°$ =	366.85	370.62	−3.77	69STU/WES
$\Delta_fS°$ =		−544.03		
$\Delta_fG°$ =		−167.16		
$\ln K_f$ =		67.43		
Liquid Phase				
$\Delta_fH°$ =	−379.50	−379.97	0.47	65CHA/ROS
$C_p°$ =	247.30	250.08	−2.78	83DAP/DEL
$S°$ =		203.69		
$\Delta_fS°$ =		−710.96		
$\Delta_fG°$ =		−168.00		
$\ln K_f$ =		67.77		

Triphenylmethanol; Triphenylcarbinol $C_{19}H_{16}O$
(15 × C$_B$–(H)(C$_B$)$_2$) + (3 × C$_B$–(C)(C$_B$)$_2$) + (1 × O–(H)(C)) + (1 × C–(O)(C$_B$)$_3$)

	Literature	Calculated	Residual	Reference
Solid Phase				
$\Delta_fH°$ =	−2.51	0.45	−2.96	54PAR/MAN
$C_p°$ =	318.80	318.91	−0.11	31SMI/AND

TABLE 15. Alcohols (69) – Continued

1,2-Ethanediol; Ethylene glycol $C_2H_6O_2$
(2 × C–(H)$_2$(O)(C)) + (2 × O–(H)(C)), σ = 2

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−387.50	−384.46	−3.04	29PAR/KEL
$C_p°$ =	97.07	76.98	20.09	69STU/WES
$S°$ =	323.55	324.10	−0.55	69STU/WES
$\Delta_fS°$ =		−284.14		
$\Delta_fG°$ =		−299.74		
$\ln K_f$ =		120.91		
Liquid Phase				
$\Delta_fH°$ =	−455.30	−454.60	−0.70	29PAR/KEL
$C_p°$ =	149.30	156.56	−7.26	79STE/TAM
$S°$ =	166.90	152.96	13.94	25PAR/KEL
$\Delta_fS°$ =		−455.28		
$\Delta_fG°$ =		−318.86		
$\ln K_f$ =		128.63		

1,2-Propanediol; Propylene glycol $C_3H_8O_2$
(1 × C–(H)$_3$(C)) + (2 × O–(H)(C)) + (1 × C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (1 × C–(H)$_2$(O)(C)) + (1 × –CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−421.30	−422.18	0.88	72GAR/HUS
$C_p°$ =		102.34		
Liquid Phase				
$\Delta_fH°$ =	−485.70	−496.19	10.49	72GAR/HUS
$C_p°$ =	188.10	209.23	−21.13	85WIL/CHA
$S°$ =		173.84		
$\Delta_fS°$ =		−570.71		
$\Delta_fG°$ =		−326.03		
$\ln K_f$ =		131.52		

1,3-Propanediol; Trimethylene glycol $C_3H_8O_2$
(1 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(O)(C)) + (2 × O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−392.10	−405.09	12.99	72GAR/HUS
$C_p°$ =		99.87		
Liquid Phase				
$\Delta_fH°$ =	−480.80	−480.33	−0.47	89KNA/SAB
$C_p°$ =		186.98		
$S°$ =		185.34		
$\Delta_fS°$ =		−559.21		
$\Delta_fG°$ =		−313.60		
$\ln K_f$ =		126.51		

TABLE 15. Alcohols (69) — Continued

1,2,3-Propanetriol; Glycerol $C_3H_8O_3$

(2×C–(H)$_2$(O)(C)) + (1×C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (3×O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−577.90	−569.89	−8.01	88BAS/NIL
$C_p°$ =		115.10		
Liquid Phase				
$\Delta_fH°$ =	−669.60	−673.70	4.10	88BAS/NIL
$C_p°$ =	219.00	251.03	−32.03	88BAS/NIL
$S°$ =	206.30	167.02	39.28	85WIL/CHA
$\Delta_fS°$ =		−680.05		
$\Delta_fG°$ =		−470.94		
$\ln K_f$ =		189.98		

1,2-Butanediol $C_4H_{10}O_2$

(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (2×O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−440.55		
$C_p°$ =		125.23		
Liquid Phase				
$\Delta_fH°$ =	−523.60	−519.74	−3.86	37MOU/DOD
$C_p°$ =		239.65		
$S°$ =		206.22		
$\Delta_fS°$ =		−674.64		
$\Delta_fG°$ =		−318.60		
$\ln K_f$ =		128.52		

1,3-Butanediol $C_4H_{10}O_2$

(1×C–(H)$_3$(C)) + (1×–CH$_3$ corr (tertiary)) + (1×C–(H)$_2$(C)$_2$) + (2×O–(H)(C)) + (1×C–(H)$_2$(O)(C)) + (1×C–(H)(O)(C)$_2$ (alcohols,peroxides))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−433.20	−442.81	9.61	72GAR/HUS
$C_p°$ =		125.23		
Liquid Phase				
$\Delta_fH°$ =	−501.00	−521.92	20.92	72GAR/HUS
$C_p°$ =		239.65		
$S°$ =		206.22		
$\Delta_fS°$ =		−674.64		
$\Delta_fG°$ =		−320.78		
$\ln K_f$ =		129.40		

TABLE 15. Alcohols (69) — Continued

1,4-Butanediol $C_4H_{10}O_2$

(2×O–(H)(C)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(O)(C))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−426.70	−425.72	−0.98	72GAR/HUS
$C_p°$ =		122.76		
Liquid Phase				
$\Delta_fH°$ =	−505.30	−506.06	0.76	89KNA/SAB
$C_p°$ =	200.10	217.40	−17.30	84VAS/PET
$S°$ =	223.40	217.72	5.68	79NIS/BAB
$\Delta_fS°$ =		−663.14		
$\Delta_fG°$ =		−308.35		
$\ln K_f$ =		124.38		

2,3-Butanediol $C_4H_{10}O_2$

(2×C–(H)$_3$(C)) + (2×C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (2×O–(H)(C)) + (2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−482.30	−459.90	−22.40	46KNO/SCH
$C_p°$ =		127.70		
Liquid Phase				
$\Delta_fH°$ =	−541.50	−537.78	−3.72	37MOU/DOD
$C_p°$ =	213.00	261.90	−48.90	36KHO/KAL
$S°$ =		194.72		
$\Delta_fS°$ =		−686.14		
$\Delta_fG°$ =		−333.21		
$\ln K_f$ =		134.41		

2-Methyl-1,2-propanediol $C_4H_{10}O_2$

(2×O–(H)(C)) + (2×C–(H)$_3$(C)) + (2×–CH$_3$ corr (quaternary)) + (1×C–(O)(C)$_3$ (alcohols,peroxides)) + (1×C–(H)$_2$(O)(C))

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =		−458.70		
$C_p°$ =		123.84		
Liquid Phase				
$\Delta_fH°$ =	−539.70	−533.93	−5.77	37MOU/DOD
$C_p°$ =		261.46		
$S°$ =		164.49		
$\Delta_fS°$ =		−716.37		
$\Delta_fG°$ =		−320.34		
$\ln K_f$ =		129.22		

TABLE 15. Alcohols (69) – *Continued*

1,2,3,4-Butanetetrol; Erythritol $C_4H_{10}O_4$
(4×O–(H)(C)) + (2×C–(H)₂(O)(C)) + (2×C–(H)(O)(C)₂ (alcohols,peroxides))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−775.20	−755.32	−19.88	50NIT/SEK
$C_p°$ =		153.22		
Liquid phase				
$\Delta_f H°$ =	−887.00	−892.80	5.80	52PAR/MAN
$C_p°$ =		345.50		
$S°$ =		181.08		
$\Delta_f S°$ =		−904.82		
$\Delta_f G°$ =		−623.03		
$\ln K_f$ =		251.33		
Solid phase				
$\Delta_f H°$ =	−910.40	−922.80	12.40	46PAR/WES
$C_p°$ =	170.70	170.38	0.32	32SPA/THO
$S°$ =	177.80	177.84	−0.04	26PAR/AND
$\Delta_f S°$ =		−908.06		
$\Delta_f G°$ =		−652.06		
$\ln K_f$ =		263.04		

1,5-Pentanediol $C_5H_{12}O_2$
(2×O–(H)(C)) + (3×C–(H)₂(C)₂) + (2×C–(H)₂(O)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−448.99	−446.35	−2.64	72GAR/HUS
$C_p°$ =		145.65		
Liquid phase				
$\Delta_f H°$ =	−531.49	−531.79	0.30	72GAR/HUS
$C_p°$ =		247.82		
$S°$ =		250.10		
$\Delta_f S°$ =		−767.07		
$\Delta_f G°$ =		−303.09		
$\ln K_f$ =		122.26		

2,2′-Bis(hydroxymethyl)-1,3-propanediol; Pentaerythritol $C_5H_{12}O_4$
(4×O–(H)(C)) + (1×C–(C)₄) + (4×C–(H)₂(O)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−776.70	−749.72	−26.98	54BRA/CLE
$C_p°$ =		170.49		

TABLE 15. Alcohols (69) – *Continued*

2,2′-Bis(hydroxymethyl)-1,3-propanediol; Pentaerythritol (Continued) $C_5H_{12}O_4$
(4×O–(H)(C)) + (1×C–(C)₄) + (4×C–(H)₂(O)(C))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		−891.21		
$C_p°$ =		323.36		
$S°$ =		207.27		
$\Delta_f S°$ =		−1014.94		
$\Delta_f G°$ =		−588.61		
$\ln K_f$ =		237.44		
Solid phase				
$\Delta_f H°$ =	−920.60	−918.17	−2.43	54MED/THO
$C_p°$ =	190.41	121.05	69.36	59WES
$S°$ =	198.07	180.21	17.86	59WES
$\Delta_f S°$ =		−1042.00		
$\Delta_f G°$ =		−607.50		
$\ln K_f$ =		245.06		

1,6-Hexanediol $C_6H_{14}O_2$
(4×C–(H)₂(C)₂) + (2×C–(H)₂(O)(C)) + (2×O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−459.40	−466.98	7.58	91STE/CHI
$C_p°$ =		168.54		
Liquid phase				
$\Delta_f H°$ =	−562.30	−557.52	−4.78	91STE/CHI
$C_p°$ =		278.24		
$S°$ =		282.48		
$\Delta_f S°$ =		−871.00		
$\Delta_f G°$ =		−297.83		
$\ln K_f$ =		120.14		
Solid phase				
$\Delta_f H°$ =	−583.86	−582.96	−0.90	91STE/CHI
$C_p°$ =	203.60	190.02	13.21	91STE/CHI
$S°$ =		198.74		
$\Delta_f S°$ =		−954.74		
$\Delta_f G°$ =		−298.30		
$\ln K_f$ =		120.33		

1,10-Decanediol $C_{10}H_{22}O_2$
(8×C–(H)₂(C)₂) + (2×O–(H)(C)) + (2×C–(H)₂(O)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−549.50		
$C_p°$ =		260.10		

TABLE 15. Alcohols (69) — Continued

1,10-Decanediol (Continued) $C_{10}H_{22}O_2$

(8×C–(H)$_2$(C)$_2$)+(2×O–(H)(C))+(2×C–(H)$_2$(O)(C))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−660.44		
$C_p°$ =		399.92		
$S°$ =		412.00		
$\Delta_fS°$ =		−1286.72		
$\Delta_fG°$ =		−276.80		
$\ln K_f$ =		111.66		
Solid phase				
$\Delta_fH°$ =	−693.50	−700.60	7.10	62PAR/MOS
$C_p°$ =		277.70		
$S°$ =		290.78		
$\Delta_fS°$ =		−1407.94		
$\Delta_fG°$ =		−280.82		
$\ln K_f$ =		113.28		

Cyclopentanol; Cyclopentyl alcohol $C_5H_{10}O$

(1×O–(H)(C))+(1×C–(H)(O)(C)$_2$ (alcohols,peroxides))+(4×C–(H)$_2$(C)$_2$)+(1×Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−242.60	−248.40	5.80	62SEL/SUN
$C_p°$ =		101.81		
Liquid phase				
$\Delta_fH°$ =	−300.00	−298.43	−1.57	62SEL/SUN
$C_p°$ =	184.10	192.83	−8.73	56PAR/KEN
$S°$ =	206.30	200.23	6.07	56PAR/KEN
$\Delta_fS°$ =		−583.85		
$\Delta_fG°$ =		−124.36		
$\ln K_f$ =		50.16		

Cyclohexanol; Cyclohexyl alcohol $C_6H_{12}O$

(1×O–(H)(C))+(1×C–(H)(O)(C)$_2$ (alcohols,peroxides))+(5×C–(H)$_2$(C)$_2$)+(1×Cyclohexane (sub) rsc), σ = 1

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−286.20	−288.97	2.77	66WAD2
$C_p°$ =	127.24	129.75	−2.51	69STU/WES
$S°$ =	360.04	358.22	1.82	69STU/WES
$\Delta_fS°$ =		−562.17		
$\Delta_fG°$ =		−121.36		
$\ln K_f$ =		48.96		

TABLE 15. Alcohols (69) — Continued

Cyclohexanol; Cyclohexyl alcohol (Continued) $C_6H_{12}O$

(1×O–(H)(C))+(1×C–(H)(O)(C)$_2$ (alcohols,peroxides))+(5×C–(H)$_2$(C)$_2$)+(1×Cyclohexane (sub) rsc), σ = 1

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−348.60	−349.81	1.21	62RAB/TEL
$C_p°$ =	213.59	220.36	−6.77	68ADA/SUG
$S°$ =	203.87	201.06	2.81	68ADA/SUG
$\Delta_fS°$ =		−719.33		
$\Delta_fG°$ =		−135.34		
$\ln K_f$ =		54.60		

Cycloheptanol; Cycloheptyl alcohol $C_7H_{14}O$

(1×O–(H)(C))+(1×C–(H)(O)(C)$_2$ (alcohols,peroxides))+(6×C–(H)$_2$(C)$_2$)+(1×Cycloheptane rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−282.87		
$C_p°$ =		138.32		
Liquid phase				
$\Delta_fH°$ =		−349.98		
$C_p°$ =	250.20	244.80	5.40	72ADA/SUG
$S°$ =	241.63	224.23	17.40	72ADA/SUG
$\Delta_fS°$ =		−832.47		
$\Delta_fG°$ =		−101.78		
$\ln K_f$ =		41.06		

1-Adamantanol $C_{10}H_{16}O$

(3×C–(H)(C)$_3$)+(6×C–(H)$_2$(C)$_2$)+(1×Adamantane rsc)+(1×C–(O)(C)$_3$ (alcohols,peroxides))+(1×O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−310.90	−306.26	−4.64	78ARO/STE
Solid phase				
$\Delta_fH°$ =	−397.50	−403.13	5.63	78ARO/STE

2-Adamantanol $C_{10}H_{16}O$

(4×C–(H)(C)$_3$)+(5×C–(H)$_2$(C)$_2$)+(1×Adamantane rsc)+(1×C–(H)$_2$(O)(C))+(1×O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−299.20	−306.20	7.00	78ARO/STE
Solid phase				
$\Delta_fH°$ =	−387.90	−400.45	12.55	78ARO/STE

TABLE 15. Alcohols (69) – Continued

Phenol C_6H_6O

$(5\times C_B{-}(H)(C_B)_2)+(1\times C_B{-}(O)C_B)_2+(1\times O{-}(H)(C_B))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−96.40	−96.00	−0.40	60AND/BID
$C_p°$ =	103.55	102.07	1.48	69STU/WES
$S°$ =	315.60	313.57	2.03	69STU/WES
$\Delta_fS°$ =		−215.11		
$\Delta_fG°$ =		−31.87		
$\ln K_f$ =		12.85		
Liquid phase				
$\Delta_fH°$ =	−153.86	−156.56	2.70	63AND/COU
$C_p°$ =		197.75		
$S°$ =		177.65		
$\Delta_fS°$ =		−351.02		
$\Delta_fG°$ =		−51.90		
$\ln K_f$ =		20.94		
Solid phase				
$\Delta_fH°$ =	−165.10	−165.60	0.50	60AND/BID
$C_p°$ =	127.44	129.61	−2.17	63AND/COU
$S°$ =	144.01	143.96	0.05	63AND/COU
$\Delta_fS°$ =		−384.71		
$\Delta_fG°$ =		−50.90		
$\ln K_f$ =		20.53		

2-Methylphenol; o-Cresol C_7H_8O

$(1\times C{-}(H)_3(C))+(1\times O{-}(H)(C_B))+(4\times C_B{-}(H)(C_B)_2)+(1\times C_B{-}(C)(C_B)_2)+(1\times$ *ortho* corr$)+(1\times C_B{-}(O)(C_B)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−128.60	−127.17	−1.43	60AND/BID
$C_p°$ =	130.33	130.34	−0.01	69STU/WES
$S°$ =	357.61	351.10	6.51	69STU/WES
$\Delta_fS°$ =		−313.89		
$\Delta_fG°$ =		−33.58		
$\ln K_f$ =		13.55		
Liquid phase				
$\Delta_fH°$ =		−189.91		
$C_p°$ =		225.15		
$S°$ =		212.58		
$\Delta_fS°$ =		−452.41		
$\Delta_fG°$ =		−55.03		
$\ln K_f$ =		22.20		
Solid phase				
$\Delta_fH°$ =	−204.60	−199.97	−4.63	60AND/BID
$C_p°$ =	154.56	153.67	0.89	67AND/COU
$S°$ =	165.44	172.40	−6.96	67AND/COU
$\Delta_fS°$ =		−492.59		
$\Delta_fG°$ =		−53.11		
$\ln K_f$ =		21.42		

TABLE 15. Alcohols (69) – Continued

3-Methylphenol; m-Cresol C_7H_8O

$(1\times C{-}(H)_3(C))+(1\times O{-}(H)(C_B))+(4\times C_B{-}(H)(C_B)_2)+(1\times C_B{-}(C)(C_B)_2)+(1\times$ *meta* corr$)+(1\times C_B{-}(O)C_B)_2$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−132.30	−129.06	−3.24	60AND/BID
$C_p°$ =	122.47	124.65	−2.18	69STU/WES
$S°$ =	356.77	353.60	3.17	69STU/WES
$\Delta_fS°$ =		−311.39		
$\Delta_fG°$ =		−36.22		
$\ln K_f$ =		14.61		
Liquid phase				
$\Delta_fH°$ =	−194.00	−193.17	−0.83	60AND/BID
$C_p°$ =	224.93	221.65	3.28	67AND/COU
$S°$ =	212.59	212.58	0.01	67AND/COU
$\Delta_fS°$ =		−452.41		
$\Delta_fG°$ =		−58.29		
$\ln K_f$ =		23.51		

4-Methylphenol; p-Cresol C_7H_8O

$(1\times C{-}(H)_3(C))+(1\times O{-}(H)(C_B))+(4\times C_B{-}(H)(C_B)_2)+(1\times C_B{-}(C)(C_B)_2)+(1\times C_B{-}(O)C_B)_2$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−125.40	−128.43	3.03	60AND/BID
$C_p°$ =	124.47	123.94	0.53	69STU/WES
$S°$ =	347.65	347.83	−0.18	69STU/WES
$\Delta_fS°$ =		−317.15		
$\Delta_fG°$ =		−33.87		
$\ln K_f$ =		13.66		
Liquid phase				
$\Delta_fH°$ =		−193.17		
$C_p°$ =	221.04	221.65	0.61	75NIC/WAD
$S°$ =		212.58		
$\Delta_fS°$ =		−452.41		
$\Delta_fG°$ =		−58.29		
$\ln K_f$ =		23.51		
Solid phase				
$\Delta_fH°$ =	−199.28	−204.97	5.69	60AND/BID
$C_p°$ =	150.25	153.67	−3.42	67AND/COU
$S°$ =	167.32	172.40	−5.08	67AND/COU
$\Delta_fS°$ =		−492.59		
$\Delta_fG°$ =		−58.11		
$\ln K_f$ =		23.44		

TABLE 15. Alcohols (69) – Continued

2-Ethylphenol $C_8H_{10}O$
$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times O-(H)(C_B))+(1\times C_B-(O)(C_B)_2)+(1\times$ *ortho* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−145.18	−148.51	3.33	63BID/HAN
$C_p°$ =		155.95		
Liquid phase				
$\Delta_fH°$ =	−208.78	−214.72	5.94	63BID/HAN
$C_p°$ =		248.05		
$S°$ =		259.98		
$\Delta_fS°$ =		−541.32		
$\Delta_fG°$ =		−53.33		
$\ln K_f$ =		21.51		

3-Ethylphenol $C_8H_{10}O$
$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times O-(H)(C_B))+(1\times C_B-(O)(C_B)_2)+(1\times$ *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−146.11	−150.40	4.29	63BID/HAN
$C_p°$ =		150.26		
Liquid phase				
$\Delta_fH°$ =	−214.30	−217.98	3.68	63BID/HAN
$C_p°$ =		244.55		
$S°$ =		259.98		
$\Delta_fS°$ =		−541.32		
$\Delta_fG°$ =		−56.59		
$\ln K_f$ =		22.83		

4-Ethylphenol $C_8H_{10}O$
$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times O-(H)(C_B))+(1\times C_B-(O)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−144.10	−149.77	5.67	63BID/HAN
$C_p°$ =		149.55		
Liquid phase				
$\Delta_fH°$ =		−217.98		
$C_p°$ =		244.55		
$S°$ =		259.98		
$\Delta_fS°$ =		−541.32		
$\Delta_fG°$ =		−56.59		
$\ln K_f$ =		22.83		

TABLE 15. Alcohols (69) – Continued

4-Ethylphenol (Continued) $C_8H_{10}O$
$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times O-(H)(C_B))+(1\times C_B-(O)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−224.39	−227.07	2.68	63BID/HAN
$C_p°$ =	206.90	203.05	3.85	75NIC/WAD
$S°$ =		199.30		
$\Delta_fS°$ =		−602.00		
$\Delta_fG°$ =		−47.58		
$\ln K_f$ =		19.20		

2,3-Dimethylphenol $C_8H_{10}O$
$(2\times C-(H)_3(C))+(2\times C_B-(C)(C_B)_2)+(3\times C_B-(H)(C_B)_2)+(1\times O-(H)(C_B))+(1\times C_B-(O)(C_B)_2)+(2\times$ *ortho* corr$)+(1\times$ *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−157.19	−158.97	1.78	60AND/BID
$C_p°$ =		159.32		
Liquid phase				
$\Delta_fH°$ =		−223.26		
$C_p°$ =		252.55		
$S°$ =		247.51		
$\Delta_fS°$ =		−553.79		
$\Delta_fG°$ =		−58.15		
$\ln K_f$ =		23.46		
Solid phase				
$\Delta_fH°$ =	−241.21	−232.34	−8.87	60AND/BID
$C_p°$ =		177.73		
$S°$ =		200.84		
$\Delta_fS°$ =		−600.46		
$\Delta_fG°$ =		−53.31		
$\ln K_f$ =		21.51		

2,4-Dimethylphenol $C_8H_{10}O$
$(2\times C-(H)_3(C))+(2\times C_B-(C)(C_B)_2)+(3\times C_B-(H)(C_B)_2)+(1\times O-(H)(C_B))+(1\times C_B-(O)(C_B)_2)+(1\times$ *ortho* corr$)+(1\times$ *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−162.88	−160.23	−2.65	60AND/BID
$C_p°$ =		152.92		
Liquid phase				
$\Delta_fH°$ =	−228.78	−226.52	−2.26	60AND/BID
$C_p°$ =		249.05		
$S°$ =		247.51		
$\Delta_fS°$ =		−553.79		
$\Delta_fG°$ =		−61.41		
$\ln K_f$ =		24.77		

TABLE 15. Alcohols (69) – *Continued*

2,5-Dimethylphenol $C_8H_{10}O$

(2×C–(H)$_3$(C)) + (2×C$_B$–(C)(C$_B$)$_2$) + (1×O–(H)(C$_B$)) + (1×C$_B$–(O)(C$_B$)$_2$) + (3×C$_B$–(H)(C$_B$)$_2$) + (1×*ortho* corr) + (1×*meta* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	–161.59	–160.23	–1.36	60AND/BID
$C_p°$ =		152.92		
Liquid phase				
$\Delta_fH°$ =		–226.52		
$C_p°$ =		249.05		
$S°$ =		247.51		
$\Delta_fS°$ =		–553.79		
$\Delta_fG°$ =		–61.41		
$\ln K_f$ =		24.77		
Solid phase				
$\Delta_fH°$ =	–246.60	–237.34	–9.26	60AND/BID
$C_p°$ =		177.73		
$S°$ =		200.84		
$\Delta_fS°$ =		–600.46		
$\Delta_fG°$ =		–58.31		
$\ln K_f$ =		23.52		

2,6-Dimethylphenol $C_8H_{10}O$

(2×C–(H)$_3$(C)) + (2×C$_B$–(C)(C$_B$)$_2$) + (3×C$_B$–(H)(C$_B$)$_2$) + (1×O–(H)(C$_B$)) + (1×C$_B$–(O)(C$_B$)$_2$) + (2×*ortho* corr) + (1×*meta* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	–161.80	–158.97	–2.83	60AND/BID
$C_p°$ =		159.32		
Liquid phase				
$\Delta_fH°$ =		–223.26		
$C_p°$ =		252.55		
$S°$ =		247.51		
$\Delta_fS°$ =		–553.79		
$\Delta_fG°$ =		–58.15		
$\ln K_f$ =		23.46		
Solid phase				
$\Delta_fH°$ =	–237.40	–232.34	–5.06	60AND/BID
$C_p°$ =		177.73		
$S°$ =		200.84		
$\Delta_fS°$ =		–600.46		
$\Delta_fG°$ =		–53.31		
$\ln K_f$ =		21.51		

TABLE 15. Alcohols (69) – *Continued*

3,4-Dimethylphenol $C_8H_{10}O$

(2×C–(H)$_3$(C)) + (2×C$_B$–(C)(C$_B$)$_2$) + (3×C$_B$–(H)(C$_B$)$_2$) + (1×O–(H)(C$_B$)) + (1×C$_B$–(O)(C$_B$)$_2$) + (1×*ortho* corr) + (1×*meta* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	–156.57	–160.23	3.66	60AND/BID
$C_p°$ =		152.92		
Liquid phase				
$\Delta_fH°$ =		–226.52		
$C_p°$ =		249.05		
$S°$ =		247.51		
$\Delta_fS°$ =		–553.79		
$\Delta_fG°$ =		–61.41		
$\ln K_f$ =		24.77		
Solid phase				
$\Delta_fH°$ =	–242.30	–237.34	–4.96	60AND/BID
$C_p°$ =		177.73		
$S°$ =		200.84		
$\Delta_fS°$ =		–600.46		
$\Delta_fG°$ =		–58.31		
$\ln K_f$ =		23.52		

3,5-Dimethylphenol $C_8H_{10}O$

(2×C–(H)$_3$(C)) + (2×C$_B$–(C)(C$_B$)$_2$) + (3×C$_B$–(H)(C$_B$)$_2$) + (1×O–(H)(C$_B$)) + (1×C$_B$–(O)(C$_B$)$_2$) + (3×*meta* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	–161.59	–162.75	1.16	60AND/BID
$C_p°$ =		147.94		
Liquid phase				
$\Delta_fH°$ =		–229.78		
$C_p°$ =		245.55		
$S°$ =		247.51		
$\Delta_fS°$ =		–553.79		
$\Delta_fG°$ =		–64.67		
$\ln K_f$ =		26.09		
Solid phase				
$\Delta_fH°$ =	–244.39	–238.34	–6.05	60AND/BID
$C_p°$ =		177.73		
$S°$ =		200.84		
$\Delta_fS°$ =		–600.46		
$\Delta_fG°$ =		–59.31		
$\ln K_f$ =		23.93		

TABLE 15. Alcohols (69) — Continued

1,2-Benzenediol; Catechol $C_6H_6O_2$

$(2\times O-(H)(C_B))+(2\times C_B-(O)C_B)_2+(4\times C_B-(H)(C_B)_2)+(1\times OH-OH$ *ortho* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−267.50	−268.66	1.16	84RIB/RIB
$C_p°$ =		128.88		
Liquid phase				
$\Delta_fH°$ =		−358.82		
$C_p°$ =		262.92		
$S°$ =		182.08		
$\Delta_fS°$ =		−449.12		
$\Delta_fG°$ =		−224.92		
$\ln K_f$ =		90.73		
Solid phase				
$\Delta_fH°$ =	−354.10	−354.38	0.28	84RIB/RIB
$C_p°$ =	140.58	138.44	2.14	50UEB/ORT
$S°$ =		151.42		
$\Delta_fS°$ =		−479.78		
$\Delta_fG°$ =		−211.33		
$\ln K_f$ =		85.25		

1,3-Benzenediol; Resorcinol $C_6H_6O_2$

$(2\times O-(H)(C_B))+(2\times C_B-(O)C_B)_2+(4\times C_B-(H)(C_B)_2)+(1\times OH-OH$ *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−274.70	−274.86	0.16	68DES/WIL
$C_p°$ =		123.19		
Liquid phase				
$\Delta_fH°$ =		−362.08		
$C_p°$ =		259.42		
$S°$ =		182.08		
$\Delta_fS°$ =		−346.59		
$\Delta_fG°$ =		−258.74		
$\ln K_f$ =		104.38		
Solid phase				
$\Delta_fH°$ =	−368.00	−368.38	0.38	68DES/WIL
$C_p°$ =	139.33	138.44	0.89	50UEB/ORT
$S°$ =		151.42		
$\Delta_fS°$ =		−377.25		
$\Delta_fG°$ =		−255.90		
$\ln K_f$ =		103.23		

TABLE 15. Alcohols (69) — Continued

1,4-Benzenediol; Hydroquinone $C_6H_6O_2$

$(2\times O-(H)(C_B))+(2\times C_B-(O)C_B)_2+(4\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−265.30	−274.86	9.56	56MAG
$C_p°$ =		122.48		
Liquid phase				
$\Delta_fH°$ =		−362.08		
$C_p°$ =		259.42		
$S°$ =		182.08		
$\Delta_fS°$ =		−449.12		
$\Delta_fG°$ =		−228.18		
$\ln K_f$ =		92.04		
Solid phase				
$\Delta_fH°$ =	−364.50	−370.38	5.88	56PIL/SUT
$C_p°$ =	136.40	138.44	−2.04	50UEB/ORT
$S°$ =		151.42		
$\Delta_fS°$ =		−479.78		
$\Delta_fG°$ =		−227.33		
$\ln K_f$ =		91.71		

1-Naphthol $C_{10}H_8O$

$(7\times C_B-(H)(C_B)_2)+(1\times O-(H)(C_B))+(1\times C_B-(O)C_B)_2+(2\times C_{BF}-(C_{BF})(C_B)_2)+(1\times$ naphthalene 1 sub)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−30.80	−28.18	−2.62	88RIB/RIB
$C_p°$ =		143.68		
Liquid phase				
$\Delta_fH°$ =		−108.58		
$C_p°$ =		262.15		
$S°$ =		224.31		
$\Delta_fS°$ =		−457.90		
$\Delta_fG°$ =		27.94		
$\ln K_f$ =		−11.27		
Solid phase				
$\Delta_fH°$ =	−122.00	−124.34	2.34	88RIB/RIB
$C_p°$ =		174.47		
$S°$ =		177.46		
$\Delta_fS°$ =		−504.75		
$\Delta_fG°$ =		26.15		
$\ln K_f$ =		−10.55		

TABLE 15. Alcohols (69) — Continued

2-Naphthol $C_{10}H_8O$

$(7\times C_B-(H)(C_B)_2)+(1\times O-(H)(C_B))+(1\times C_B-(O)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(1\times \text{naphthalene 1 sub})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−29.90	−28.18	−1.72	88RIB/RIB
$C_p°$ =		143.68		
Liquid phase				
$\Delta_fH°$ =		−108.58		
$C_p°$ =		262.15		
$S°$ =		224.31		
$\Delta_fS°$ =		−457.90		
$\Delta_fG°$ =		27.94		
$\ln K_f$ =		−11.27		
Solid phase				
$\Delta_fH°$ =	−124.20	−124.34	0.14	88RIB/RIB
$C_p°$ =		174.47		
$S°$ =		177.46		
$\Delta_fS°$ =		−504.75		
$\Delta_fG°$ =		26.15		
$\ln K_f$ =		−10.55		

2,3-Naphthalenediol; 2,3-Dihydroxynaphthalene $C_{10}H_8O_2$

$(6\times C_B-(H)(C_B)_2)+(2\times O-(H)(C_B))+(2\times C_B-(O)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(1\times \text{naphthalene 2 sub})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−192.80	−207.04	14.24	88RIB/RIB
$C_p°$ =		166.18		
Liquid phase				
$\Delta_fH°$ =		−314.10		
$C_p°$ =		323.82		
$S°$ =		228.74		
$\Delta_fS°$ =		−555.99		
$\Delta_fG°$ =		−148.33		
$\ln K_f$ =		59.84		
Solid phase				
$\Delta_fH°$ =	−316.40	−329.12	12.72	76COL/ROU
$C_p°$ =		183.30		
$S°$ =		184.92		
$\Delta_fS°$ =		−599.81		
$\Delta_fG°$ =		−150.29		
$\ln K_f$ =		60.62		

TABLE 15. Alcohols (69) — Continued

2,2-Bis(4-hydroxyphenyl)-propane $C_{15}H_{16}O_2$

$(2\times C-(H)_3(C))+(2\times C_B-(C)(C_B)_2)+(2\times C_B-(O)(C_B)_2)+(8\times C_B-(H)(C_B)_2)+(2\times -CH_3 \text{ corr (quaternary)})+(1\times C-(C)_2(C_B)_2)+(2\times O-(H)(C_B))$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−368.60	−365.83	−2.77	48HUB/KNO

1,2-Naphthalenediol $C_{10}H_8O_2$

$(6\times C_B-(H)(C_B)_2)+(2\times O-(H)(C_B))+(2\times C_B-(O)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(1\times \text{naphthalene 2 sub})+(1\times OH-OH(\textit{ortho} \text{ corr}))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−200.50	−200.04	−0.43	88RIB/RIB
$C_p°$ =		166.18		
Liquid phase				
$\Delta_fH°$ =		−314.10		
$C_p°$ =		323.82		
$S°$ =		228.74		
$\Delta_fS°$ =		−555.99		
$\Delta_fG°$ =		−148.33		
$\ln K_f$ =		59.84		
Solid phase				
$\Delta_fH°$ =	−309.80	−313.12	3.32	88RIB/RIB
$C_p°$ =		183.30		
$S°$ =		184.92		
$\Delta_fS°$ =		−599.81		
$\Delta_fG°$ =		−134.29		
$\ln K_f$ =		54.17		

1,3-Naphthalenediol $C_{10}H_8O_2$

$(6\times C_B-(H)(C_B)_2)+(2\times O-(H)(C_B))+(2\times C_B-(O)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(1\times \text{naphthalene 2 sub})+(1\times OH-OH(\textit{meta} \text{ corr}))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−211.20	−207.04	−4.16	88RIB/RIB
$C_p°$ =		166.18		
Liquid phase				
$\Delta_fH°$ =		−314.10		
$C_p°$ =		323.82		
$S°$ =		228.74		
$\Delta_fS°$ =		−555.99		
$\Delta_fG°$ =		−148.33		
$\ln K_f$ =		59.84		

TABLE 15. Alcohols (69) — Continued

1,3-Naphthalenediol (Continued) $C_{10}H_8O_2$
$(6\times C_B\text{–}(H)(C_B)_2)+(2\times O\text{–}(H)(C_B))+(2\times C_B\text{–}(O)(C_B)_2)+(2\times C_{BF}\text{–}(C_{BF})(C_B)_2)+(1\times \text{naphthalene 2 sub})+(1\times \text{OH–OH}(\textit{meta}\ \text{corr})$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−327.20	−327.12	−0.08	88RIB/RIB
$C_p°$ =		183.30		
$S°$ =		184.92		
$\Delta_fS°$ =		−599.81		
$\Delta_fG°$ =		−148.29		
$\ln K_f$ =		59.82		

1,4-Naphthalenediol $C_{10}H_8O_2$
$(6\times C_B\text{–}(H)(C_B)_2)+(2\times O\text{–}(H)(C_B))+(2\times C_B\text{–}(O)(C_B)_2)+(2\times C_{BF}\text{–}(C_{BF})(C_B)_2)+(1\times \text{naphthalene 2 sub})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−197.00	−207.04	10.04	88RIB/RIB
$C_p°$ =		166.18		
Liquid phase				
$\Delta_fH°$ =		−314.10		
$C_p°$ =		323.82		
$S°$ =		228.74		
$\Delta_fS°$ =		−555.99		
$\Delta_fG°$ =		−148.33		
$\ln K_f$ =		59.84		
Solid phase				
$\Delta_fH°$ =	−317.40	−329.12	11.72	88RIB/RIB
$C_p°$ =		183.30		
$S°$ =		184.92		
$\Delta_fS°$ =		−599.81		
$\Delta_fG°$ =		−150.29		
$\ln K_f$ =		60.62		

TABLE 16. Ethers (53)

Methoxymethane; Dimethyl ether C_2H_6O
$(2\times C\text{–}(H)_3(C))+(1\times O\text{–}(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−184.10	−185.94	1.84	64PIL/PEL
$C_p°$ =	65.81	70.00	−4.19	69STU/WES
$S°$ =	267.06	259.94	7.12	69STU/WES
$\Delta_fS°$ =		−245.78		
$\Delta_fG°$ =		−112.66		
$\ln K_f$ =		45.45		

Ethoxyethane; Diethyl ether $C_4H_{10}O$
$(2\times C\text{–}(H)_3(C))+(1\times O\text{–}(C)_2)+(2\times C\text{–}(H)_2(O)(C))$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−252.10	−251.74	−0.36	63PIL/SKI
$C_p°$ =	112.51	110.66	1.85	69STU/WES
$S°$ =	342.67	346.80	−4.13	69STU/WES
$\Delta_fS°$ =		−431.54		
$\Delta_fG°$ =		−123.08		
$\ln K_f$ =		49.65		
Liquid phase				
$\Delta_fH°$ =	−279.40	−277.65	−1.75	71COU/LEE
$C_p°$ =	172.51	164.51	8.00	71COU/LEE
$S°$ =	253.50	258.56	−5.06	71COU/LEE
$\Delta_fS°$ =		−519.78		
$\Delta_fG°$ =		−122.68		
$\ln K_f$ =		49.49		

Propoxypropane; Di-*n*-propyl ether $C_6H_{14}O$
$(2\times C\text{–}(H)_3(C))+(1\times O\text{–}(C)_2)+(2\times C\text{–}(H)_2(C)_2)+(2\times C\text{–}(H)_2(O)(C))$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−293.10	−293.00	−0.10	80MAJ/WAG
$C_p°$ =	158.28	156.44	1.84	69STU/WES
$S°$ =	422.50	425.12	−2.62	69STU/WES
$\Delta_fS°$ =		−625.84		
$\Delta_fG°$ =		−106.41		
$\ln K_f$ =		42.92		
Liquid phase				
$\Delta_fH°$ =	−328.82	−329.11	0.29	65COL/PEL
$C_p°$ =	221.58	225.35	−3.77	75AND/COU
$S°$ =	323.88	323.32	0.56	75AND/COU
$\Delta_fS°$ =		−727.64		
$\Delta_fG°$ =		−112.16		
$\ln K_f$ =		45.25		

TABLE 16. Ethers (53) – Continued

Butoxybutane; Di-n-butyl ether $C_8H_{18}O$
(2×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(O)(C))+(1×O–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−332.90	−334.26	1.36	80MAJ/WAG
$C_p°$ =	204.01	202.22	1.79	69STU/WES
$S°$ =	500.41	503.44	−3.03	69STU/WES
$\Delta_fS°$ =		−820.14		
$\Delta_fG°$ =		−89.73		
$\ln K_f$ =		36.20		
Liquid phase				
$\Delta_fH°$ =	−377.90	−380.57	2.67	65COL/PEL
$C_p°$ =		286.19		
$S°$ =		388.08		
$\Delta_fS°$ =		−935.50		
$\Delta_fG°$ =		−101.65		
$\ln K_f$ =		41.01		

Methoxyethane; Methyl ethyl ether C_3H_8O
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(O)(C))+(1×O–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−216.40	−218.84	2.44	64PIL/PEL
$C_p°$ =	89.75	90.33	−0.58	69STU/WES
$S°$ =	310.62	309.13	1.49	69STU/WES
$\Delta_fS°$ =		−332.89		
$\Delta_fG°$ =		−119.59		
$\ln K_f$ =		48.24		

Methoxypropane; Methyl propyl ether $C_4H_{10}O$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(O)(C))+(1×O–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−237.70	−239.47	1.77	64PIL/PEL
$C_p°$ =	112.51	113.22	−0.71	69STU/WES
$S°$ =	349.45	348.29	1.16	69STU/WES
$\Delta_fS°$ =		−430.05		
$\Delta_fG°$ =		−111.25		
$\ln K_f$ =		44.88		
Liquid phase				
$\Delta_fH°$ =	−265.89	−267.58	1.69	80MAJ/WAG
$C_p°$ =	161.90	161.29	0.61	75AND/MAR
$S°$ =	253.70	258.35	−4.65	75AND/MAR
$\Delta_fS°$ =		−519.99		
$\Delta_fG°$ =		−112.55		
$\ln K_f$ =		45.40		

TABLE 16. Ethers (53) – Continued

Methoxybutane; Methyl butyl ether $C_5H_{12}O$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(O)(C))+(1×O–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−258.10	−260.10	2.00	75FEN/HAR
$C_p°$ =		136.11		
$S°$ =		387.45		
$\Delta_fS°$ =		−527.20		
$\Delta_fG°$ =		−102.92		
$\ln K_f$ =		41.52		
Liquid phase				
$\Delta_fH°$ =	−290.60	−293.31	2.71	75FEN/HAR
$C_p°$ =	192.72	191.71	1.01	75AND/MAR
$S°$ =	295.30	290.73	4.57	75AND/MAR
$\Delta_fS°$ =		−623.92		
$\Delta_fG°$ =		−107.29		
$\ln K_f$ =		43.28		

Methoxydecane; Methyl decyl ether $C_{11}H_{24}O$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(O)(C))+(1×O–(C)$_2$)+(8×C–(H)$_2$(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−381.12	−383.88	2.76	75FEN/HAR
$C_p°$ =		273.45		
$S°$ =		622.41		
$\Delta_fS°$ =		−1110.10		
$\Delta_fG°$ =		−52.90		
$\ln K_f$ =		21.34		
Liquid phase				
$\Delta_fH°$ =	−443.42	−447.69	4.27	75FEN/HAR
$C_p°$ =	370.80	374.23	−3.43	75AND/MAR
$S°$ =	490.50	485.01	5.49	75AND/MAR
$\Delta_fS°$ =		−1247.50		
$\Delta_fG°$ =		−75.75		
$\ln K_f$ =		30.56		

2-Methoxypropane; Methyl isopropyl ether $C_4H_{10}O$
(3×C–(H)$_3$(C))+(1×O–(C)$_2$)+(1×C–(H)(O)(C)$_2$ (ethers,esters))+(2×–CH$_3$ corr (tertiary)), σ = 27

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−252.00	−252.18	0.18	64PIL/PEL
$C_p°$ =	111.09	113.51	−2.42	69STU/WES
$S°$ =	338.32	331.09	7.23	69STU/WES
$\Delta_fS°$ =		−447.25		
$\Delta_fG°$ =		−118.83		
$\ln K_f$ =		47.94		

TABLE 16. Ethers (53) — Continued

2-Methoxypropane; Methyl isopropyl ether (Continued) $C_4H_{10}O$
(3×C-(H)$_3$(C))+(1×O-(C)$_2$)+
(1×C-(H)(O)(C)$_2$ (ethers,esters))+
(2×-CH$_3$ corr (tertiary)), σ = 27

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−278.70	−279.02	0.32	80MAJ/WAG
$C_p°$ =	161.92	159.27	2.65	75AND/MAR
$S°$ =	253.72	251.37	2.35	75AND/MAR
$\Delta_fS°$ =		−526.97		
$\Delta_fG°$ =		−121.90		
$\ln K_f$ =		49.18		

2-Methoxy-(2-methyl)propane; Methyl tert-butyl ether $C_5H_{12}O$
(4×C-(H)$_3$(C))+(1×C-(O)(C)$_3$ (ethers,esters))+(1×O-(C)$_2$)+
(3×-CH$_3$ corr (quaternary)), σ = 243

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−283.50	−274.64	−8.86	80MAJ/WAG
$C_p°$ =	134.18	136.06	−1.88	69STU/WES
$S°$ =	352.96	351.02	1.94	69STU/WES
$\Delta_fS°$ =		−563.63		
$\Delta_fG°$ =		−106.59		
$\ln K_f$ =		43.00		
Liquid phase				
$\Delta_fH°$ =	−313.60	−313.65	0.05	75FEN/HAR
$C_p°$ =	187.50	190.65	−3.15	75AND/MAR
$S°$ =	265.30	265.30	0.00	75AND/MAR
$\Delta_fS°$ =		−649.35		
$\Delta_fG°$ =		−120.05		
$\ln K_f$ =		48.43		

Ethoxypropane; Ethyl propyl ether $C_5H_{12}O$
(2×C-(H)$_3$(C))+(1×C-(H)$_2$(C)$_2$)+(2×C-(H)$_2$(O)(C))+
(1×O-(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−272.21	−272.37	0.16	75FEN/HAR
$C_p°$ =		133.55		
$S°$ =		391.72		
$\Delta_fS°$ =		−522.93		
$\Delta_fG°$ =		−116.46		
$\ln K_f$ =		46.98		
Liquid phase				
$\Delta_fH°$ =	−303.59	−303.38	−0.21	75FEN/HAR
$C_p°$ =	197.20	194.93	2.27	75AND/MAR
$S°$ =	295.00	290.94	4.06	75AND/MAR
$\Delta_fS°$ =		−623.71		
$\Delta_fG°$ =		−117.42		
$\ln K_f$ =		47.37		

TABLE 16. Ethers (53) — Continued

2-Propoxy-2-propane; Diisopropyl ether $C_6H_{14}O$
(4×C-(H)$_3$(C))+(2×C-(H)(O)(C)$_2$ (ethers,esters))+
(1×O-(C)$_2$)+(4×-CH$_3$ corr (tertiary)), σ = 162

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−319.40	−318.42	−0.98	80MAJ/WAG
$C_p°$ =	158.28	157.02	1.26	69STU/WES
$S°$ =	390.24	390.71	−0.47	69STU/WES
$\Delta_fS°$ =		−660.25		
$\Delta_fG°$ =		−121.57		
$\ln K_f$ =		49.04		
Liquid phase				
$\Delta_fH°$ =	−351.50	−351.99	0.49	65COL/PEL
$C_p°$ =	216.10	221.31	−5.21	74AND/COU
$S°$ =	304.60	309.36	−4.76	74AND/COU
$\Delta_fS°$ =		−741.60		
$\Delta_fG°$ =		−130.88		
$\ln K_f$ =		52.80		

2-Butoxy-2-butane; Di-sec-butyl ether $C_8H_{18}O$
(4×C-(H)$_3$(C))+(2×C-(H)$_2$(C)$_2$)+
(2×C-(H)(O)(C)$_2$ (ethers,esters))+(1×O-(C)$_2$)+
(2×-CH$_3$ corr (tertiary)), σ = 162

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−360.70	−355.16	−5.54	80MAJ/SVO
$C_p°$ =	204.01	202.80	1.21	69STU/WES
$S°$ =	462.62	469.03	−6.41	69STU/WES
$\Delta_fS°$ =		−854.55		
$\Delta_fG°$ =		−100.38		
$\ln K_f$ =		40.49		
Liquid phase				
$\Delta_fH°$ =	−401.50	−399.09	−2.41	65COL/PEL
$C_p°$ =		282.15		
$S°$ =		374.12		
$\Delta_fS°$ =		−949.46		
$\Delta_fG°$ =		−116.01		
$\ln K_f$ =		46.80		

TABLE 16. Ethers (53) – *Continued*

2-Propoxy-2-(2-methyl)propane; Isopropyl tert-butyl ether $C_7H_{16}O$

$(5\times C-(H)_3(C))+(1\times C-(O)(C)_3$ (ethers,esters)$)+$
$(1\times C-(H)(O)(C)_2$ (ethers,esters)$)+(1\times O-(C)_2)+$
$(2\times -CH_3$ corr (tertiary)$)+$
$(3\times -CH_3$ corr (quaternary)$)$, $\sigma = 729$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−357.73	−340.88	−16.85	70COX/PIL
C_p° =	181.17	179.57	1.60	69STU/WES
S° =	417.94	416.40	1.54	69STU/WES
$\Delta_f S^\circ$ =		−770.87		
$\Delta_f G^\circ$ =		−111.05		
$\ln K_f$ =		44.80		
Liquid phase				
$\Delta_f H^\circ$ =	−392.88	−386.62	−6.26	61SMU/BON
C_p° =		252.69		
S° =		323.29		
$\Delta_f S^\circ$ =		−863.98		
$\Delta_f G^\circ$ =		−129.02		
$\ln K_f$ =		52.05		

(2-Methyl)propoxy-2-(2-methyl)propane; Di-tert-butyl ether $C_8H_{18}O$

$(6\times C-(H)_3(C))+(1\times O-(C)_2)+(2\times C-(O)(C)_3$ (ethers,esters)$)+$
$(6\times -CH_3$ corr (quaternary)$)$, $\sigma = 13122$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−362.00	−363.34	1.34	75FEN/HAR
C_p° =	204.01	202.12	1.89	69STU/WES
S° =	427.27	430.57	−3.30	69STU/WES
$\Delta_f S^\circ$ =		−893.01		
$\Delta_f G^\circ$ =		−97.09		
$\ln K_f$ =		39.17		
Liquid phase				
$\Delta_f H^\circ$ =	−399.61	−421.25	21.64	75FEN/HAR
C_p° =	276.10	284.07	−7.97	75FEN/HAR
S° =		337.22		
$\Delta_f S^\circ$ =		−986.36		
$\Delta_f G^\circ$ =		−127.17		
$\ln K_f$ =		51.30		

1,1′-Oxybisethene; Ethenoxyethene; Divinyl ether C_4H_6O

$(2\times C_d-(H)_2)+(1\times O-(C_d)_2)+(2\times C_d-(O)(H))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−14.02	−14.01	−0.01	63PIL/SKI
Liquid phase				
$\Delta_f H^\circ$ =	−39.80	−31.72	−8.08	63PIL/SKI

Ethoxyethene; Ethyl vinyl ether C_4H_8O

$(1\times C-(H)_3(C))+(1\times C_d-(H)_2)+(1\times C-(H)_2(O)(C))+$
$(1\times O-(C)(C_d))+(1\times C_d-(O)(H))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−140.16	−141.85	1.69	63PIL/SKI
Liquid phase				
$\Delta_f H^\circ$ =	−166.65	−164.33	−2.32	70COX/PIL
C_p° =		174.30		

Butoxyethene; *n*-Butyl vinyl ether $C_6H_{12}O$

$(1\times C_d-(H)_2)+(1\times C_d-(O)(H))+(1\times O-(C)(C_d))+$
$(1\times C-(H)_2(O)(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−184.50	−183.11	−1.39	81TRO/NED
Liquid phase				
$\Delta_f H^\circ$ =	−218.80	−215.79	−3.01	81TRO/NED
C_p° =	231.79	235.14	−3.35	47SCH/ZOS

Dimethoxymethane $C_3H_8O_2$

$(2\times C-(H)_3(C))+(2\times O-(C)_2)+(1\times C-(H)_2(O)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−348.20	−349.58	1.38	69PIL/FLE
Liquid phase				
$\Delta_f H^\circ$ =	−378.20	−379.77	1.57	70BIR/SKI
C_p° =	161.42	161.42	0.00	64MCE/KIL
S° =	244.01	244.01	0.00	64MCE/KIL
$\Delta_f S^\circ$ =		−500.54		
$\Delta_f G^\circ$ =		−230.53		
$\ln K_f$ =		93.00		

Trimethoxymethane $C_4H_{10}O_3$

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

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−545.00	−545.01	0.01	71PIN/TUO
Liquid phase				
$\Delta_f H^\circ$ =	−583.10	−583.06	−0.04	71PIN/TUO
C_p° =		203.96		

TABLE 16. Ethers (53) — Continued

1,1-Dimethoxyethane $C_4H_{10}O_2$
(3×C–(H)$_3$(C)) + (2×O–(C)$_2$) + (1×C–(H)(O)$_2$(C)) + (1×–CH_3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−389.70	−389.66	−0.04	69PIL/FLE
Liquid phase				
$\Delta_f H°$ =	−420.00	−418.09	−1.91	70BIR/SKI
C_p° =		170.36		

2,2-Dimethoxypropane $C_5H_{12}O_2$
(4×C–(H)$_3$(C)) + (2×O–(C)$_2$) + (1×C–(O)$_2$(C)$_2$) + (2×–CH_3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−424.31	−429.96	5.65	79WIB/SQU
Liquid phase				
$\Delta_f H°$ =	−459.48	−457.76	−1.72	79WIB/SQU

Diethoxymethane; 3,5-Dioxaheptane $C_5H_{12}O_2$
(2×C–(H)$_3$(C)) + (2×O–(C)$_2$) + (2×C–(H)$_2$(O)(C)) + (1×C–(H)$_2$(O)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−414.80	−415.38	0.58	69MAN
Liquid phase				
$\Delta_f H°$ =	−450.41	−451.37	0.96	69MAN
C_p° =		228.70		
$S°$ =		309.19		
$\Delta_f S°$ =		−707.98		
$\Delta_f G°$ =		−240.29		
$\ln K_f$ =		96.93		

1,1,1-Trimethoxyethane $C_5H_{12}O_3$
(4×C–(H)$_3$(C)) + (3×O–(C)$_2$) + (1×C–(O)$_3$(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−587.70	−587.69	−0.01	74HIN/KLU
Liquid phase				
$\Delta_f H°$ =	−626.90	−622.47	−4.43	74HIN/KLU

TABLE 16. Ethers (53) — Continued

Tetramethoxymethane; Tetramethyl orthocarbonate $C_5H_{12}O_4$
(4×C–(H)$_3$(C)) + (4×O–(C)$_2$) + (1×C–(O)$_4$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−727.18	−727.18	0.00	79WIB/SQU
Liquid phase				
$\Delta_f H°$ =	−767.10	−767.10	0.00	79WIB/SQU

1,1-Diethoxyethane $C_6H_{14}O_2$
(3×C–(H)$_3$(C)) + (1×C–(H)(O)$_2$(C)) + (2×O–(C)$_2$) + (2×C–(H)$_2$(O)(C)) + (1×–CH_3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−453.59	−455.46	1.87	68PIH/HEI
Liquid phase				
$\Delta_f H°$ =	−491.41	−489.69	−1.72	68PIH/HEI
C_p° =		237.64		

1,2-Diethoxyethane $C_6H_{14}O_2$
(2×C–(H)$_3$(C)) + (4×C–(H)$_2$(O)(C)) + (2×O–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−408.19	−418.96	10.77	70KUZ/WAD
C_p° =		169.86		
Liquid phase				
$\Delta_f H°$ =	−450.41	−460.08	9.67	69MAN
C_p° =		256.06		
$S°$ =		350.52		
$\Delta_f S°$ =		−802.96		
$\Delta_f G°$ =		−220.68		
$\ln K_f$ =		89.02		

3,5,7-Trioxanonane $C_6H_{14}O_3$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(O)(C)) + (3×O–(C)$_2$) + (2×C–(H)$_2$(O)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−581.10	−579.02	−2.08	69MAN

TABLE 16. Ethers (53) – Continued

3,5,7-Trioxanonane (Continued) $C_6H_{14}O_3$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(O)(C)) + (3×O–(C)$_2$) + (2×C–(H)$_2$(O)$_2$)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−625.80	−625.09	−0.71	69MAN
$C_p°$ =		292.89		
$S°$ =		359.82		
$\Delta_f S°$ =		−896.18		
$\Delta_f G°$ =		−357.89		
$\ln K_f$ =		144.37		

1,3-Diethoxypropane $C_7H_{16}O_2$
(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (4×C–(H)$_2$(O)(C)) + (2×O–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−436.18	−439.59	3.41	72MAN
$C_p°$ =		192.75		
Liquid phase				
$\Delta_f H°$ =	−482.08	−485.81	3.73	72MAN
$C_p°$ =		286.48		
$S°$ =		382.90		
$\Delta_f S°$ =		−906.89		
$\Delta_f G°$ =		−215.42		
$\ln K_f$ =		86.90		

2,2-Diethoxypropane $C_7H_{16}O_2$
(4×C–(H)$_3$(C)) + (2×C–(H)$_2$(O)(C)) + (1×C–(O)$_2$(C)$_2$) + (2×O–(C)$_2$) + (2×–CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−506.60	−500.36	−6.24	62STE/DOR
Liquid phase				
$\Delta_f H°$ =	−538.50	−533.78	−4.72	62STE/DOR

3,5,7,9-Tetraoxaundecane $C_7H_{16}O_4$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(O)(C)) + (4×O–(C)$_2$) + (3×C–(H)$_2$(O)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−741.00	−742.66	1.66	69MAN

TABLE 16. Ethers (53) – Continued

3,5,7,9-Tetraoxaundecane (Continued) $C_7H_{16}O_4$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(O)(C)) + (4×O–(C)$_2$) + (3×C–(H)$_2$(O)$_2$)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−794.60	−798.81	4.21	69MAN
$C_p°$ =		357.08		
$S°$ =		410.45		
$\Delta_f S°$ =		−1084.38		
$\Delta_f G°$ =		−475.50		
$\ln K_f$ =		191.81		

2-Methoxyethanol $C_3H_8O_2$
(1×C–(H)$_3$(C)) + (1×O–(C)$_2$) + (1×O–(H)(C)) + (2×C–(H)$_2$(O)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−368.81		
$C_p°$ =		103.09		
Liquid phase				
$\Delta_f H°$ =		−421.54		
$C_p°$ =	174.90	172.67	2.23	73KUS/SUU
$S°$ =		219.15		
$\Delta_f S°$ =		−525.40		
$\Delta_f G°$ =		−264.89		
$\ln K_f$ =		106.86		

2-Ethoxyethanol $C_4H_{10}O_2$
(1×C–(H)$_3$(C)) + (3×C–(H)$_2$(O)(C)) + (1×O–(C)$_2$) + (1×O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−401.71		
$C_p°$ =		123.42		
Liquid phase				
$\Delta_f H°$ =		−457.34		
$C_p°$ =	210.80	206.31	4.49	73KUS/SUU
$S°$ =		251.74		
$\Delta_f S°$ =		−629.12		
$\Delta_f G°$ =		−269.77		
$\ln K_f$ =		108.82		

TABLE 16. Ethers (53) — Continued

Diethylene glycol $C_4H_{10}O_3$
(2×O–(H)(C))+(4×C–(H)$_2$(O)(C))+(1×O–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−571.20	−551.68	−19.52	37GAL/HIB
$C_p°$ =		136.18		
Liquid phase				
$\Delta_fH°$ =	−628.50	−637.03	8.53	37MOU/DOD
$C_p°$ =	243.90	248.11	−4.21	82ZAR
$S°$ =		244.92		
$\Delta_fS°$ =		−738.46		
$\Delta_fG°$ =		−416.86		
$\ln K_f$ =		168.16		

2-Propoxyethanol $C_5H_{12}O_2$
(1×O–(H)(C))+(3×C–(H)$_2$(O)(C))+(1×C–(H)$_2$(C)$_2$)+
(1×C–(H)$_3$(C))+(1×O–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−422.34		
$C_p°$ =		146.31		
Liquid phase				
$\Delta_fH°$ =		−483.07		
$C_p°$ =	241.60	236.73	4.87	73KUS/SUU
$S°$ =		284.12		
$\Delta_fS°$ =		−733.05		
$\Delta_fG°$ =		−264.51		
$\ln K_f$ =		106.70		

2-Isopropoxyethanol $C_5H_{12}O_2$
(1×O–(H)(C))+(2×C–(H)$_2$(O)(C))+(1×O–(C)$_2$)+
(2×C–(H)$_3$(C))+ (1×C–(H)(O)(C)$_2$ (alcohols,peroxides))+
(2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−441.69		
$C_p°$ =		148.78		
Liquid phase				
$\Delta_fH°$ =		−501.11		
$C_p°$ =	238.80	258.98	−20.18	73KUS/SUU
$S°$ =		272.62		
$\Delta_fS°$ =		−744.55		
$\Delta_fG°$ =		−279.12		
$\ln K_f$ =		112.60		

TABLE 16. Ethers (53) — Continued

Triethyleneglycol $C_6H_{14}O_4$
(2×O–(H)(C))+(6×C–(H)$_2$(O)(C))+(2×O–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−725.00	−718.90	−6.10	37GAL/HIB
$C_p°$ =		195.38		
Liquid phase				
$\Delta_fH°$ =	−804.20	−819.46	15.26	37MOU/DOD
$C_p°$ =	333.70	339.66	−5.96	82ZAR
$S°$ =		336.88		
$\Delta_fS°$ =		−1021.64		
$\Delta_fG°$ =		−514.86		
$\ln K_f$ =		207.69		

Tetraethyleneglycol $C_8H_{18}O_5$
(2×O–(H)(C))+(8×C–(H)$_2$(O)(C))+(3×O–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−883.00	−886.12	3.12	37GAL/HIB
$C_p°$ =		254.58		
Liquid phase				
$\Delta_fH°$ =	−981.70	−1001.89	20.19	37MOU/DOD
$C_p°$ =	428.80	431.21	−2.41	82ZAR
$S°$ =		428.84		
$\Delta_fS°$ =		−1304.83		
$\Delta_fG°$ =		−612.86		
$\ln K_f$ =		247.22		

Oxirane; Ethylene oxide C_2H_4O
(2×C–(H)$_2$(O)(C))+(1×O–(C)$_2$)+
(1×ethylene oxide rsc), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−52.60	−52.60	0.00	65PEL/PIL
$C_p°$ =	48.28	48.28	0.00	69STU/WES
$S°$ =	242.42	242.43	−0.01	69STU/WES
$\Delta_fS°$ =		−132.72		
$\Delta_fG°$ =		−13.03		
$\ln K_f$ =		5.26		
Liquid phase				
$\Delta_fH°$ =	−77.61	−77.61	0.00	49GIA/GOR
$C_p°$ =		67.65		
$S°$ =		172.46		
$\Delta_fS°$ =		−202.68		
$\Delta_fG°$ =		−19.41		
$\ln K_f$ =		7.83		

TABLE 16. Ethers (53) – Continued

2-Methyloxirane; Propylene oxide C_3H_6O

(1 × C–(H)$_3$(C)) + (1 × C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (1 × C–(H)$_2$(O)(C)) + (1 × O–(C)$_2$) + (1 × ethylene oxide rsc) + (1 × –CH$_3$ corr (tertiary)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−94.70	−90.32	−4.38	61POP
$C_p°$ =	72.34	73.64	−1.30	69STU/WES
$S°$ =	286.73	279.90	6.83	69STU/WES
$\Delta_fS°$ =		−231.56		
$\Delta_fG°$ =		−21.28		
$\ln K_f$ =		8.58		
Liquid phase				
$\Delta_fH°$ =	−122.60	−119.20	−3.40	62SIN/HIL
$C_p°$ =	120.37	120.32	0.05	64OET
$S°$ =	196.27	193.34	2.93	64OET
$\Delta_fS°$ =		−318.11		
$\Delta_fG°$ =		−26.58		
$\ln K_f$ =		10.72		

Oxetane; Trimethylene oxide C_3H_6O

(1 × C–(H)$_2$(C)$_2$) + (1 × O–(C)$_2$) + (2 × C–(H)$_2$(O)(C)) + (1 × trimethylene oxide)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−80.50	−80.50	0.00	65PEL/PIL
Liquid phase				
$C_p°$ =	99.60	99.59	0.01	76CON/GIN

1,3-Dioxolane $C_3H_6O_2$

(2 × O–(C)$_2$) + (2 × C–(H)$_2$(O)(C)) + (1 × C–(H)$_2$(O)$_2$) + (1 × 1,3-dioxolane rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−301.80	−301.80	0.00	59FLE/MOR
Liquid phase				
$\Delta_fH°$ =	−337.40	−337.40	0.00	69PIH/HEI
$C_p°$ =	118.00	118.00	0.00	76CON/GIN

TABLE 16. Ethers (53) – Continued

Furan C_4H_4O

(4 × C$_B$–(H)(C$_B$)$_2$) + (1 × O–(C$_B$)$_2$) + (1 × Furan rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−34.60	−34.60	0.00	52GUT/SCO
Liquid phase				
$\Delta_fH°$ =	−62.60	−62.60	0.00	52GUT/SCO

Oxolane; Tetrahydrofuran C_4H_8O

(1 × O–(C)$_2$) + (2 × C–(H)$_2$(O)(C)) + (2 × C–(H)$_2$(C)$_2$) + (1 × tetrahydrofuran rsc), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−184.20	−184.20	0.00	65PEL/PIL
$C_p°$ =	76.25	76.25	0.00	86CHA/HAL
$S°$ =	302.41	302.41	0.00	86CHA/HAL
$\Delta_fS°$ =		−345.36		
$\Delta_fG°$ =		−81.16		
$\ln K_f$ =		32.74		
Liquid phase				
$\Delta_fH°$ =	−216.19	−216.19	0.00	57SKU/STR
$C_p°$ =	123.90	123.90	0.00	85WIL/CHA
$S°$ =	203.90	203.90	0.00	85WIL/CHA
$\Delta_fS°$ =		−444.02		
$\Delta_fG°$ =		−84.01		
$\ln K_f$ =		33.89		

1,3-Dioxane $C_4H_8O_2$

(2 × O–(C)$_2$) + (1 × C–(H)$_2$(O)$_2$) + (2 × C–(H)$_2$(O)(C)) + (1 × C–(H)$_2$(C)$_2$) + (1 × 1,3-dioxane rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−340.60	−340.59	−0.01	82BYS/MAN
Liquid phase				
$\Delta_fH°$ =	−377.50	−377.48	−0.02	82BYS/MAN
$C_p°$ =	143.90	143.90	0.00	82BYS/MAN

TABLE 16. Ethers (53) — Continued

1,4-Dioxane $C_4H_8O_2$

(2×O–(C)$_2$)+(4×C–(H)$_2$(O)(C))+(1×1,4-dioxane rsc), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−315.30	−315.29	−0.01	82BYS/MAN
$C_p°$ =	94.06	94.06	0.00	69STU/WES
$S°$ =	299.78	299.78	0.00	69STU/WES
$\Delta_fS°$ =		−450.51		
$\Delta_fG°$ =		−180.97		
$\ln K_f$ =		73.00		
Liquid phase				
$\Delta_fH°$ =	−355.10	−355.10	0.00	82BYS/MAN
$C_p°$ =	153.60	153.60	0.00	85WIL/CHA
$S°$ =	270.20	270.20	0.00	85WIL/CHA
$\Delta_fS°$ =		−480.09		
$\Delta_fG°$ =		−212.02		
$\ln K_f$ =		85.53		

Oxane; Tetrahydropyran $C_5H_{10}O$

(1×O–(C)$_2$)+(2×C–(H)$_2$(O)(C))+(3×C–(H)$_2$(C)$_2$)+(1×tetrahydropyran rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−223.40	−223.40	0.00	65PEL/PIL
Liquid phase				
$\Delta_fH°$ =	−258.30	−258.30	0.00	58CAS/FLE2
$C_p°$ =	140.60	140.59	0.01	76CON/GIN

1,3-Dioxepane $C_5H_{10}O_2$

(2×O–(C)$_2$)+(1×C–(H)$_2$(O)$_2$)+(2×C–(H)$_2$(O)(C))+(2×C–(H)$_2$(C)$_2$)+(1×1,3-dioxepane rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−346.60	−346.60	0.00	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−387.60	−387.60	0.00	57SKU/STR
$C_p°$ =	167.40	167.38	0.02	76CON/GIN

Methoxybenzene; Methyl phenyl ether; Anisole C_7H_8O

(1×C–(H)$_3$(C))+(1×O–(C)(C$_B$))+(1×C$_B$–(O)(C$_B$)$_2$)+(5×C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−67.90	−70.51	2.61	75FEN/HAR

TABLE 16. Ethers (53) — Continued

Methoxybenzene; Methyl phenyl ether; Anisole (Continued) C_7H_8O

(1×C–(H)$_3$(C))+(1×O–(C)(C$_B$))+(1×C$_B$–(O)(C$_B$)$_2$)+(5×C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−114.80	−117.27	2.47	75FEN/HAR
$C_p°$ =	199.00	197.69	1.31	75FEN/HAR

Ethoxybenzene; Ethyl phenyl ether; Phenetole $C_8H_{10}O$

(1×C–(H)$_3$(C))+(1×C–(H)$_2$(O)(C))+(1×O–(C)(C$_B$))+(1×C$_B$–(O)(C$_B$)$_2$)+(5×C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−101.60	−103.41	1.81	75FEN/HAR
Liquid phase				
$\Delta_fH°$ =	−152.60	−153.07	0.47	75FEN/HAR
$C_p°$ =	228.50	231.33	−2.83	75FEN/HAR

1-Methoxy-3-methylbenzene; Methyl *tolyl* ether $C_8H_{10}O$

(2×C–(H)$_3$(C))+(1×O–(C)(C$_B$))+(1×C$_B$–(O)(C$_B$)$_2$)+(1×C$_B$–(C)(C$_B$)$_2$)+(4×C$_B$–(H)(C$_B$)$_2$)+(1×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−104.10	−103.57	−0.53	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−155.60	−153.88	−1.72	41BAD
$C_p°$ =		221.59		

1,2-Dimethoxybenzene $C_8H_{10}O_2$

(2×C–(H)$_3$(C))+(2×O–(C)(C$_B$))+(2×C$_B$–(O)(C$_B$)$_2$)+(4×C$_B$–(H)(C$_B$)$_2$)+(1×*ortho* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−223.38	−222.62	−0.76	58CAS/FLE3
Liquid phase				
$\Delta_fH°$ =	−290.30	−280.24	−10.06	58CAS/FLE3
$C_p°$ =		262.80		

TABLE 16. Ethers (53) – Continued

1,1′-Oxybisbenzene; Diphenyl ether; Diphenyl oxide $C_{12}H_{10}O$
$(10 \times C_B-(H)(C_B)_2) + (2 \times C_B-(O)(C_B)_2) + (1 \times O-(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	52.00	50.94	1.06	72MOR2
Liquid phase				
$\Delta_f H°$ =	−14.90	−14.89	−0.01	51FUR/GIN
$S°$ =		290.83		
$\Delta_f S°$ =		−533.43		
$\Delta_f G°$ =		144.15		
$\ln K_f$ =		−58.15		
Solid phase				
$\Delta_f H°$ =	−32.10	−28.90	−3.20	51FUR/GIN
$C_p°$ =	216.56	216.62	−0.06	51FUR/GIN
$S°$ =	233.93	233.82	0.11	51FUR/GIN
$\Delta_f S°$ =		−590.44		
$\Delta_f G°$ =		147.14		
$\ln K_f$ =		−59.35		

TABLE 17. Aldehydes (16)

Methanal; Formaldehyde CH_2O
$(1 \times CO-(H)_2$, Formaldehyde), $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−108.60	−108.60	0.00	70FLE/PIL
$C_p°$ =	35.40	35.40	0.00	69STU/WES
$S°$ =	218.78	218.78	0.00	69STU/WES
$\Delta_f S°$ =		−20.06		
$\Delta_f G°$ =		−102.62		
$\ln K_f$ =		41.40		

Ethanal; Acetaldehyde C_2H_4O
$(1 \times C-(H)_3(C)) + (1 \times CO-(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−166.10	−166.65	0.55	38DOL/GRE
$C_p°$ =	54.64	54.73	−0.09	69STU/WES
$S°$ =	264.22	265.22	−1.00	69STU/WES
$\Delta_f S°$ =		−109.93		
$\Delta_f G°$ =		−133.87		
$\ln K_f$ =		54.00		
Liquid phase				
$\Delta_f H°$ =	−191.80	−190.03	−1.77	49COL/DEV
$C_p°$ =	89.05	101.58	−12.53	88LEB/VAS
$S°$ =	117.30	176.85	−59.55	88LEB/VAS
$\Delta_f S°$ =		−198.29		
$\Delta_f G°$ =		−130.91		
$\ln K_f$ =		52.81		

Ethanedial; Glyoxal $C_2H_2O_2$
$(2 \times CO-(H)(CO))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−211.96	−211.96	0.00	70FLE/PIL

Propanal; Propionaldehyde C_3H_6O
$(1 \times C-(H)_3(C)) + (1 \times C-(H)_2(CO)(C)) + (1 \times CO-(H)(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−189.40	−188.49	−0.91	67BUC/COX
$C_p°$ =	78.66	79.42	−0.76	69STU/WES
$S°$ =	304.72	304.80	−0.08	69STU/WES
$\Delta_f S°$ =		−206.66		
$\Delta_f G°$ =		−126.87		
$\ln K_f$ =		51.18		

TABLE 17. Aldehydes (16) — Continued

Propanal; Propionaldehyde (Continued) C_3H_6O
(1×C–(H)$_3$(C))+(1×C–(H)$_2$(CO)(C))+(1×CO–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−215.30	−214.17	−1.13	67BUC/COX
$C_p°$ =	159.10	130.87	28.23	77KOR/VAS
$S°$ =	212.90	216.72	−3.82	77KOR/VAS
$\Delta_fS°$ =		−294.73		
$\Delta_fG°$ =		−126.29		
$\ln K_f$ =		50.95		

trans-2-Butenal; Crotonaldehyde C_4H_6O
(1×C–(H)$_3$(C))+(1×C$_d$–(H)(C))+(1×C$_d$–(H)(CO))+(1×CO–(H)(C$_d$))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−100.60	−100.60	0.00	38DOL/GRE
Liquid phase				
$\Delta_fH°$ =	−144.10	−143.00	−1.10	60TJE

Butanal; Butyraldehyde C_4H_8O
(1×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−204.70	−209.12	4.42	79SUN/SVE
$C_p°$ =	102.59	102.31	0.28	69STU/WES
$S°$ =	344.93	343.96	0.97	69STU/WES
$\Delta_fS°$ =		−303.81		
$\Delta_fG°$ =		−118.54		
$\ln K_f$ =		47.82		
Liquid phase				
$\Delta_fH°$ =	−239.40	−239.90	0.50	79SUN/SVE
$C_p°$ =	164.70	161.29	3.41	89VAS/LEB
$S°$ =	242.70	249.10	−6.40	89VAS/LEB
$\Delta_fS°$ =		−398.67		
$\Delta_fG°$ =		−121.04		
$\ln K_f$ =		48.83		

TABLE 17. Aldehydes (16) — Continued

Pentanal; Pentaldehyde $C_5H_{10}O$
(1×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−228.50	−229.75	1.25	70CON
$C_p°$ =	125.35	125.20	0.15	69STU/WES
$S°$ =	382.96	383.12	−0.16	69STU/WES
$\Delta_fS°$ =		−400.96		
$\Delta_fG°$ =		−110.20		
$\ln K_f$ =		44.46		
Liquid phase				
$\Delta_fH°$ =	−267.30	−265.63	−1.67	70CON
$C_p°$ =	174.39	191.71	−17.32	84VAS/PET
$S°$ =	273.59	281.48	−7.89	84VAS/PET
$\Delta_fS°$ =		−502.60		
$\Delta_fG°$ =		−115.78		
$\ln K_f$ =		46.71		

Hexanal; Hexaldehyde $C_6H_{12}O$
(1×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−250.38		
$C_p°$ =	148.24	148.09	0.15	69STU/WES
$S°$ =	422.88	422.28	0.60	69STU/WES
$\Delta_fS°$ =		−498.11		
$\Delta_fG°$ =		−101.87		
$\ln K_f$ =		41.09		
Liquid phase				
$\Delta_fH°$ =		−291.36		
$C_p°$ =	210.40	222.13	−11.73	91VAS/BYK
$S°$ =	280.30	313.86	−33.56	91VAS/BYK
$\Delta_fS°$ =		−606.53		
$\Delta_fG°$ =		−110.52		
$\ln K_f$ =		44.58		

Heptanal; Heptaldehyde $C_7H_{14}O$
(1×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−263.80	−271.01	7.21	70COX/PIL
$C_p°$ =	171.08	170.98	0.10	69STU/WES
$S°$ =	461.66	461.44	0.22	69STU/WES
$\Delta_fS°$ =		−595.26		
$\Delta_fG°$ =		−93.53		
$\ln K_f$ =		37.73		

TABLE 17. Aldehydese (16) – Continued

Heptanal; Heptaldehyde (Continued) $C_7H_{14}O$
(1×C–(H)$_3$(C)) + (4×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−311.50	−317.09	5.59	60NIC
$C_p°$ =	230.15	252.55	−22.40	84VAS/PET
$S°$ =	335.43	346.24	−10.81	84VAS/PET
$\Delta_fS°$ =		−710.46		
$\Delta_fG°$ =		−105.27		
$\ln K_f$ =		42.46		

Octanal; Octaldehyde $C_8H_{16}O$
(1×C–(H)$_3$(C)) + (5×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−291.64		
$C_p°$ =	193.97	193.87	0.10	69STU/WES
$S°$ =	500.66	500.60	0.06	69STU/WES
$\Delta_fS°$ =		−692.41		
$\Delta_fG°$ =		−85.20		
$\ln K_f$ =		34.37		
Liquid phase				
$\Delta_fH°$ =		−342.82		
$C_p°$ =	259.58	282.97	−23.39	84VAS/PET
$S°$ =	365.45	378.62	−13.17	84VAS/PET
$\Delta_fS°$ =		−814.39		
$\Delta_fG°$ =		−100.01		
$\ln K_f$ =		40.34		

Nonanal; Nonaldehyde $C_9H_{18}O$
(1×C–(H)$_3$(C)) + (6×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−312.27		
$C_p°$ =	216.81	216.76	0.05	69STU/WES
$S°$ =	539.61	539.76	−0.15	69STU/WES
$\Delta_fS°$ =		−789.56		
$\Delta_fG°$ =		−76.86		
$\ln K_f$ =		31.01		
Liquid phase				
$\Delta_fH°$ =		−368.55		
$C_p°$ =	290.26	313.39	−23.13	84VAS/PET
$S°$ =	396.92	411.00	−14.08	84VAS/PET
$\Delta_fS°$ =		−918.32		
$\Delta_fG°$ =		−94.75		
$\ln K_f$ =		38.22		

TABLE 17. Aldehydes (16) – Continued

Decanal; Decaldehyde $C_{10}H_{20}O$
(1×C–(H)$_3$(C)) + (7×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(H)(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−332.90		
$C_p°$ =	239.70	239.65	0.05	69STU/WES
$S°$ =	578.56	578.92	−0.36	69STU/WES
$\Delta_fS°$ =		−886.72		
$\Delta_fG°$ =		−68.53		
$\ln K_f$ =		27.64		
Liquid phase				
$\Delta_fH°$ =		−394.28		
$C_p°$ =	319.67	343.81	−24.14	84VAS/PET
$S°$ =	429.46	443.38	−13.92	84VAS/PET
$\Delta_fS°$ =		−1022.25		
$\Delta_fG°$ =		−89.50		
$\ln K_f$ =		36.10		

2-Methylpropanal; Isobutyraldehyde C_4H_8O
(2×C–(H)$_3$(C)) + (1×C–(H)(CO)(C)$_2$) + (1×CO–(H)(C)) + (2×–CH_3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−215.80	−213.68	−2.12	75CON
Liquid phase				
$\Delta_fH°$ =	−247.30	−245.89	−1.41	75CON
$C_p°$ =		155.47		
$S°$ =		235.63		
$\Delta_fS°$ =		−412.14		
$\Delta_fG°$ =		−123.01		
$\ln K_f$ =		49.62		

2-Ethylhexanal $C_8H_{16}O$
(2×C–(H)$_3$(C)) + (4×C–(H)$_2$(C)$_2$) + (1×C–(H)(CO)(C)$_2$) + (1×CO–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−299.62	−291.68	−7.94	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−348.50	−344.45	−4.05	60TJE
$C_p°$ =		277.15		
$S°$ =		365.15		
$\Delta_fS°$ =		−827.86		
$\Delta_fG°$ =		−97.62		
$\ln K_f$ =		39.38		

TABLE 17. Aldehydes (16) – Continued

Furfural $C_5H_4O_2$

$(3\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(CO)(C_B)_2)+(1\times O\text{–}(C_B)_2)+(1\times CO\text{–}(H)(C_B))+(1\times \text{Furan rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−151.04	−154.26	3.22	75KUD/KUD
Liquid phase				
$\Delta_fH°$ =	−201.60	−198.38	−3.22	29LAN/BAY

Benzaldehyde C_7H_6O

$(5\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(CO)(C_B)_2)+(1\times CO\text{–}(H)(C_B))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−36.80	−36.80	0.00	75AMB/CON
Liquid phase				
$\Delta_fH°$ =	−86.82	−86.82	0.00	75AMB/CON
C_p° =	172.00	172.01	−0.01	75AMB/CON

TABLE 18. Ketones (42)

Propanone; Acetone; Dimethyl ketone C_3H_6O

$(2\times C\text{–}(H)_3(CO))+(1\times CO\text{–}(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−217.50	−217.19	−0.31	65BUC/HER
C_p° =	74.89	74.89	0.00	69STU/WES
$S°$ =	294.93	294.92	0.01	69STU/WES
$\Delta_fS°$ =		−216.54		
$\Delta_fG°$ =		−152.63		
$\ln K_f$ =		61.57		
Liquid phase				
$\Delta_fH°$ =	−248.10	−247.98	−0.12	57PEN/KOB
C_p° =	124.68	125.93	−1.25	29KEL3
$S°$ =	200.41	200.41	0.00	29KEL3
$\Delta_fS°$ =		−311.04		
$\Delta_fG°$ =		−155.24		
$\ln K_f$ =		62.62		

Butanone; Methyl ethyl ketone C_4H_8O

$(2\times C\text{–}(H)_3(C))+(1\times CO\text{–}(C)_2)+(1\times C\text{–}(H)_2(CO)(C))$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−238.90	−239.03	0.13	79SUN/SVE
C_p° =	102.88	99.58	3.30	69STU/WES
$S°$ =	338.11	340.26	−2.15	69STU/WES
$\Delta_fS°$ =		−307.50		
$\Delta_fG°$ =		−147.35		
$\ln K_f$ =		59.44		
Liquid phase				
$\Delta_fH°$ =	−273.20	−272.12	−1.08	79SUN/SVE
C_p° =	158.70	155.22	3.48	68AND/COU
$S°$ =	239.00	240.28	−1.28	68AND/COU
$\Delta_fS°$ =		−407.49		
$\Delta_fG°$ =		−150.63		
$\ln K_f$ =		60.76		

2-Pentanone; Methyl propyl ketone $C_5H_{10}O$

$(2\times C\text{–}(H)_3(C))+(1\times C\text{–}(H)_2(C)_2)+(1\times C\text{–}(H)_2(CO)(C))+(1\times CO\text{–}(C)_2)$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−259.05	−259.66	0.61	70HAR/HEA
C_p° =	120.96	122.47	−1.51	69STU/WES
$S°$ =	376.18	373.66	2.52	69STU/WES
$\Delta_fS°$ =		−410.42		
$\Delta_fG°$ =		−137.29		
$\ln K_f$ =		55.38		

TABLE 18. Ketones (42) – Continued

2-Pentanone; Methyl propyl ketone (Continued) $C_5H_{10}O$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−297.29	−297.85	0.56	70HAR/HEA
$C_p°$ =	184.20	185.64	−1.44	68AND/COU
$S°$ =	274.10	272.66	1.44	68AND/COU
$\Delta_fS°$ =		−511.42		
$\Delta_fG°$ =		−145.37		
$\ln K_f$ =		58.64		

3-Pentanone; Diethyl ketone $C_5H_{10}O$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(CO)(C))+(1×CO–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−257.95	−260.87	2.92	70HAR/HEA
$C_p°$ =		124.27		
$S°$ =	370.00	374.08	−4.08	65BUC/HER
$\Delta_fS°$ =		410.00		
$\Delta_fG°$ =		−138.63		
$\ln K_f$ =		55.92		
Liquid phase				
$\Delta_fH°$ =	−296.51	−296.26	−0.25	70HAR/HEA
$C_p°$ =	190.90	184.51	6.39	68AND/COU
$S°$ =	266.00	280.15	−14.15	68AND/COU
$\Delta_fS°$ =		−503.93		
$\Delta_fG°$ =		−146.01		
$\ln K_f$ =		58.90		

2-Hexanone; Methyl butyl ketone $C_6H_{12}O$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−279.79	−280.29	0.50	70HAR/HEA
$C_p°$ =		145.36		
$S°$ =		412.82		
$\Delta_fS°$ =		−507.57		
$\Delta_fG°$ =		−128.96		
$\ln K_f$ =		52.02		
Liquid phase				
$\Delta_fH°$ =	−322.01	−323.58	1.57	70HAR/HEA
$C_p°$ =	213.38	216.06	−2.68	70AND/COU
$S°$ =	308.11	305.04	3.07	70AND/COU
$\Delta_fS°$ =		−615.35		
$\Delta_fG°$ =		−140.11		
$\ln K_f$ =		56.52		

TABLE 18. Ketones (42) – Continued

3-Hexanone; Ethyl propyl ketone $C_6H_{12}O$
(2×C–(H)$_3$(C))+(1×CO–(C)$_2$)+(2×C–(H)$_2$(CO)(C))+(1×C–(H)$_2$(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−278.25	−281.50	3.25	70HAR/HEA
$C_p°$ =		147.16		
$S°$ =		413.24		
$\Delta_fS°$ =		−507.15		
$\Delta_fG°$ =		−130.29		
$\ln K_f$ =		52.56		
Liquid phase				
$\Delta_fH°$ =	−320.13	−321.99	1.86	70HAR/HEA
$C_p°$ =	216.90	214.93	1.97	70AND/COU
$S°$ =	305.31	312.53	−7.22	70AND/COU
$\Delta_fS°$ =		−607.86		
$\Delta_fG°$ =		−140.76		
$\ln K_f$ =		56.78		

2-Octanone; Methyl hexyl ketone $C_8H_{16}O$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)$_2$)+(4×C–(H)$_2$(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−321.55		
$C_p°$ =		191.14		
$S°$ =		491.14		
$\Delta_fS°$ =		−701.87		
$\Delta_fG°$ =		−112.29		
$\ln K_f$ =		45.30		
Liquid phase				
$\Delta_fH°$ =		−375.04		
$C_p°$ =	273.26	276.90	−3.64	65OET
$S°$ =	373.84	369.80	4.04	65OET
$\Delta_fS°$ =		−823.21		
$\Delta_fG°$ =		−129.60		
$\ln K_f$ =		52.28		

5-Nonanone; Di-*n*-butyl ketone $C_9H_{18}O$
(2×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(CO)(C))+(1×CO–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−344.94	−343.39	−1.55	70HAR/HEA
$C_p°$ =		215.83		
$S°$ =		530.72		
$\Delta_fS°$ =		−798.60		
$\Delta_fG°$ =		−105.29		
$\ln K_f$ =		42.47		

TABLE 18. Ketones (42) – Continued

5-Nonanone; Di-*n*-butyl ketone (Continued) $C_9H_{18}O$
(2×C–(H)$_3$(C)) + (4×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(CO)(C)) + (1×CO–(C)$_2$), σ = 18

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_fH°$ =	–398.24	–399.18	0.94	70HAR/HEA
$C_p°$ =	303.59	306.19	–2.60	70AND/COU
$S°$ =	401.41	409.67	–8.26	70AND/COU
$\Delta_fS°$ =		–919.65		
$\Delta_fG°$ =		–124.99		
$\ln K_f$ =		50.42		

6-Undecanone; Di-*n*-pentyl ketone $C_{11}H_{22}O$
(2×C–(H)$_3$(C)) + (6×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(CO)(C)) + (1×CO–(C)$_2$), σ = 18

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	–387.41	–384.65	–2.76	70HAR/HEA
$C_p°$ =		261.61		
$S°$ =		609.04		
$\Delta_fS°$ =		–992.90		
$\Delta_fG°$ =		–88.62		
$\ln K_f$ =		35.75		
Liquid phase				
$\Delta_fH°$ =	–448.13	–450.64	2.51	70HAR/HEA
$C_p°$ =		367.03		
$S°$ =		474.43		
$\Delta_fS°$ =		–1127.51		
$\Delta_fG°$ =		–114.47		
$\ln K_f$ =		46.18		

2-Tetradecanone; Methyl *n*-dodecyl ketone $C_{14}H_{28}O$
(2×C–(H)$_3$(C)) + (1×CO–(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (10×C–(H)$_2$(C)$_2$), σ = 18

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		–445.33		
$C_p°$ =		328.48		
$S°$ =		726.10		
$\Delta_fS°$ =		–1284.78		
$\Delta_fG°$ =		–62.27		
$\ln K_f$ =		25.12		
Liquid phase				
$\Delta_fH°$ =		–529.42		
$C_p°$ =		459.42		
$S°$ =		564.08		
$\Delta_fS°$ =		–1446.80		
$\Delta_fG°$ =		–98.06		
$\ln K_f$ =		39.56		

TABLE 18. Ketones (42) – Continued

2-Tetradecanone; Methyl *n*-dodecyl ketone (Continued) $C_{14}H_{28}O$
(2×C–(H)$_3$(C)) + (1×CO–(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (10×C–(H)$_2$(C)$_2$), σ = 18

	Literature	– Calculated	= Residual	Reference
Solid phase				
$\Delta_fH°$ =		–573.43		
$C_p°$ =	415.20	409.91	5.29	79SUN/SVE

2-Pentadecanone; Methyl *n*-tridecyl ketone $C_{15}H_{30}O$
(2×C–(H)$_3$(C)) + (1×CO–(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (11×C–(H)$_2$(C)$_2$), σ = 18

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		–465.96		
$C_p°$ =		351.37		
$S°$ =		765.26		
$\Delta_fS°$ =		–1381.93		
$\Delta_fG°$ =		–53.94		
$\ln K_f$ =		21.76		
Liquid phase				
$\Delta_fH°$ =		–555.15		
$C_p°$ =		489.84		
$S°$ =		596.46		
$\Delta_fS°$ =		–1550.73		
$\Delta_fG°$ =		–92.80		
$\ln K_f$ =		37.44		
Solid phase				
$\Delta_fH°$ =		–602.84		
$C_p°$ =	426.77	431.83	–5.06	79SUN/SVE

3-Methyl-2-butanone; Methyl isopropyl ketone $C_5H_{10}O$
(3×C–(H)$_3$(C)) + (1×C–(H)(CO)(C)$_2$) + (1×CO–(C)$_2$) + (2×–CH$_3$ corr (tertiary))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	–262.57	–264.22	1.65	70HAR/HEA
Liquid phase				
$\Delta_fH°$ =	–299.47	–303.84	4.37	70HAR/HEA
$C_p°$ =		179.82		
$S°$ =		259.19		
$\Delta_fS°$ =		–524.89		
$\Delta_fG°$ =		–147.35		
$\ln K_f$ =		59.44		

TABLE 18. Ketones (42) – Continued

2-Methyl-3-pentanone; Ethyl isopropyl ketone $C_6H_{12}O$

(3 × C–(H)$_3$(C)) + (1 × C–(H)(CO)(C)$_2$) + (1 × CO–(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (2 × –CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−286.10	−286.06	−0.04	70SEL
Liquid phase				
$\Delta_f H°$ =	−325.90	−327.98	2.08	70SEL
$C_p°$ =		209.11		
$S°$ =		299.06		
$\Delta_f S°$ =		−621.33		
$\Delta_f G°$ =		−142.73		
$\ln K_f$ =		57.58		

3,3-Dimethyl-2-butanone; Methyl tert-butyl ketone $C_6H_{12}O$

(4 × C–(H)$_3$(C)) + (1 × CO–(C)$_2$) + (1 × C–(CO)(C)$_3$) + (3 × –CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−290.67	−291.46	0.79	70HAR/HEA
Liquid phase				
$\Delta_f H°$ =	−328.54	−330.22	1.68	70HAR/HEA
$C_p°$ =	206.90	206.88	0.02	70AND/COU
$S°$ =	282.42	281.03	1.39	70AND/COU
$\Delta_f S°$ =		−639.36		
$\Delta_f G°$ =		−139.60		
$\ln K_f$ =		56.31		

2,2-Dimethyl-3-pentanone; Ethyl tert-butyl ketone $C_7H_{14}O$

(4 × C–(H)$_3$(C)) + (1 × C–(CO)(C)$_3$) + (1 × CO–(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (3 × –CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−313.72	−313.30	−0.42	70SEL
Liquid phase				
$\Delta_f H°$ =	−356.10	−354.36	−1.74	70SEL
$C_p°$ =		236.17		
$S°$ =		320.90		
$\Delta_f S°$ =		−735.80		
$\Delta_f G°$ =		−134.98		
$\ln K_f$ =		54.45		

TABLE 18. Ketones (42) – Continued

2,4-Dimethyl-3-pentanone; Diisopropyl ketone $C_7H_{14}O$

(4 × C–(H)$_3$(C)) + (2 × C–(H)(CO)(C)$_2$) + (1 × CO–(C)$_2$) + (4 × –CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−311.10	−311.25	0.15	70SEL
Liquid phase				
$\Delta_f H°$ =	−352.92	−359.70	6.78	70SEL
$C_p°$ =	233.70	233.71	−0.01	70AND/COU
$S°$ =	318.00	317.97	0.03	70AND/COU
$\Delta_f S°$ =		−738.73		
$\Delta_f G°$ =		−139.45		
$\ln K_f$ =		56.25		

2,2,4-Trimethyl-3-pentanone; Isopropyl tert-butyl ketone $C_8H_{16}O$

(5 × C–(H)$_3$(C)) + (1 × C–(CO)(C)$_3$) + (1 × C–(H)(CO)(C)$_2$) + (1 × CO–(C)$_2$) + (2 × –CH$_3$ corr (tertiary)) + (3 × –CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−338.30	−338.49	0.19	70SEL
Liquid phase				
$\Delta_f H°$ =	−381.60	−386.08	4.48	70SEL
$C_p°$ =		260.77		
$S°$ =		339.81		
$\Delta_f S°$ =		−853.20		
$\Delta_f G°$ =		−131.70		
$\ln K_f$ =		53.13		

2,2,4,4-Tetramethyl-3-pentanone; Di-tert-butyl ketone $C_9H_{18}O$

(6 × C–(H)$_3$(C)) + (2 × C–(CO)(C)$_3$) + (1 × CO–(C)$_2$) + (6 × –CH$_3$ corr (*quat/quat*))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−345.81	−342.21	−3.60	70SEL
Liquid phase				
$\Delta_f H°$ =	−391.10	−389.96	−1.14	70SEL
$C_p°$ =		287.83		
$S°$ =		361.65		
$\Delta_f S°$ =		−967.67		
$\Delta_f G°$ =		−101.45		
$\ln K_f$ =		40.92		

TABLE 18. Ketones (42) — Continued

2,6-Dimethyl-4-heptanone $C_9H_{18}O$

(4 × C–(H)$_3$(C)) + (2 × C–(H)(C)$_3$) + (4 × –CH$_3$ corr (tertiary)) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−357.61	−356.77	−0.84	70SEL
$C_p°$ =		215.89		
Liquid phase				
$\Delta_f H°$ =	−408.50	−409.74	1.24	70SEL
$C_p°$ =		300.23		
$S°$ =		398.97		
$\Delta_f S°$ =		−930.35		
$\Delta_f G°$ =		−132.36		
$\ln K_f$ =		53.39		

2,2,6,6-Tetramethyl-4-heptanone $C_{11}H_{22}O$

(6 × C–(H)$_3$(C)) + (2 × C–(C)$_4$) + (6 × –CH$_3$ corr (quaternary)) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−421.20	−418.87	−2.33	71SEL
$C_p°$ =		260.25		
Liquid phase				
$\Delta_f H°$ =	−474.10	−477.06	2.96	71SEL
$C_p°$ =		350.91		
$S°$ =		416.05		
$\Delta_f S°$ =		−1185.89		
$\Delta_f G°$ =		−123.49		
$\ln K_f$ =		49.81		

Biacetyl; 2,3-Butanedione; Diacetyl $C_4H_6O_2$

(2 × C–(H)$_3$(C)) + (2 × CO–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−327.10	−327.10	0.00	54NIC/SZW
Liquid phase				
$\Delta_f H°$ =	−365.30	−365.30	−0.00	54NIC/SZW

2,4-Pentanedione $C_5H_8O_2$

(2 × C–(H)$_3$(C)) + (2 × CO–(C)$_2$) + (1 × C–(H)$_2$(CO)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−380.60	−380.60	0.00	70IRV/WAD

TABLE 18. Ketones (42) — Continued

2,4-Pentanedione (Continued) $C_5H_8O_2$

(2 × C–(H)$_3$(C)) + (2 × CO–(C)$_2$) + (1 × C–(H)$_2$(CO)$_2$)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−423.80	−423.80	0.00	57NIC
$C_p°$ =		194.46		

Cyclopentanone C_5H_8O

(2 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$) + (1 × cyclopentanone rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−194.76	−194.76	0.00	72WOL
Liquid phase				
$\Delta_f H°$ =	−237.40	−237.40	0.00	72WOL

Cyclohexanone $C_6H_{10}O$

(3 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$) + (1 × cyclohexanone rsc), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−227.74	−227.74	0.00	72WOL
$C_p°$ =	109.66	109.66	0.00	69STU/WES
$S°$ =	322.17	322.17	0.00	69STU/WES
$\Delta_f S°$ =		−467.65		
$\Delta_f G°$ =		−88.31		
$\ln K_f$ =		35.62		
Liquid phase				
$\Delta_f H°$ =	−272.63	−272.63	0.00	72WOL
$C_p°$ =	177.20	177.20	0.00	80NAK/SUG
$S°$ =	221.98	221.98	0.00	80NAK/SUG
$\Delta_f S°$ =		−567.84		
$\Delta_f G°$ =		−103.33		
$\ln K_f$ =		41.68		

Cycloheptanone $C_7H_{12}O$

(4 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$) + (1 × cycloheptanone rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−248.11	−248.11	0.00	72WOL
Liquid phase				
$\Delta_f H°$ =	−297.65	−297.65	0.00	72WOL

TABLE 18. Ketones (42) — Continued

Cyclooctanone $C_8H_{14}O$
(5 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$) + (1 × cyclooctanone rsc)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−272.17	−272.17	0.00	72WOL
Liquid phase $\Delta_fH°$ =	−320.68	−320.68	0.00	72WOL
Solid phase $\Delta_fH°$ =	−323.42	−323.42	0.00	72WOL

Cyclononanone $C_9H_{16}O$
(6 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$) + (1 × cyclononanone)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−279.70	−279.70	0.00	72WOL
Liquid phase $\Delta_fH°$ =	−332.85	−332.85	0.00	72WOL
Solid phase $\Delta_fH°$ =	−334.94	−334.93	−0.01	72WOL

Cyclodecanone $C_{10}H_{18}O$
(7 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$) + (1 × cyclodecanone)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−305.06	−305.06	0.00	72WOL
Liquid phase $\Delta_fH°$ =	−363.42	−363.42	0.00	72WOL

Cycloundecanone $C_{11}H_{20}O$
(8 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$) + (1 × cycloundecanone)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−322.00	−322.00	0.00	72WOL

TABLE 18. Ketones (42) — Continued

Cycloundecanone (Continued) $C_{11}H_{20}O$
(8 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$) + (1 × cycloundecanone)

	Literature	Calculated	Residual	Reference
Liquid phase $\Delta_fH°$ =	−386.35	−386.35	0.00	72WOL

Cyclododecanone $C_{12}H_{22}O$
(9 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)$_2$) + (1 × cyclododecanone)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−349.11	−349.11	0.00	72WOL
Liquid phase $\Delta_fH°$ =	−414.59	−414.59	0.00	72WOL
Solid phase $\Delta_fH°$ =	−431.33	−431.33	0.00	72WOL

Cyclopentadecanone $C_{15}H_{28}O$
(1 × CO–(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (12 × C–(H)$_2$(C)$_2$) + (1 × cyclopentadecanone rsc)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−414.50	−414.50	0.00	38WOL/WEG
Solid phase $\Delta_fH°$ =	−491.90	−491.90	0.00	33RUZ/SCH

Cycloheptadecanone $C_{17}H_{32}O$
(1 × CO–(C)$_2$) + (2 × C–(H)$_2$(CO)(C)) + (14 × C–(H)$_2$(C)$_2$) + (1 × cycloheptadecanone rsc)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−460.30	−460.30	0.00	38WOL/WEG
Solid phase $\Delta_fH°$ =	−536.00	−536.00	0.00	33RUZ/SCH

TABLE 18. Ketones (42) — Continued

Acetophenone; Methyl phenyl ketone C_8H_8O

$(1\times C\text{-}(H)_3(C)) + (1\times CO\text{-}(C)(C_B)) + (1\times C_B\text{-}(CO)(C_B)_2) + (5\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−106.53		
Liquid phase				
$\Delta_fH°$ =	−142.50	−141.53	−0.97	61COL/LAT
$C_p°$ =	227.60	227.62	−0.02	39PHI

1-Phenyl-1-propanone; Ethyl phenyl ketone $C_9H_{10}O$

$(1\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)_2(CO)(C)) + (1\times CO\text{-}(C)(C_B)) + (1\times C_B\text{-}(CO)(C_B)_2) + (5\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−128.37		
Liquid phase				
$\Delta_fH°$ =	−167.20	−165.67	−1.53	61COL/LAT
$C_p°$ =		256.91		

1-Phenyl-2-propanone; Methyl benzyl ketone $C_9H_{10}O$

$(1\times C\text{-}(H)_3(CO)) + (1\times CO\text{-}(C)_2) + (1\times C\text{-}(H)_2(CO)(C_B)) + (1\times C_B\text{-}(C)(C_B)_2) + (5\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−98.40	−98.44	0.04	54NIC/SZW
Liquid phase				
$\Delta_fH°$ =	−151.90	−152.08	0.18	54NIC/SZW

1-Phenyl-1-butanone; Propyl phenyl ketone $C_{10}H_{12}O$

$(1\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(CO)(C)) + (1\times CO\text{-}(C)(C_B)) + (1\times C_B\text{-}(CO)(C_B)_2) + (5\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−149.00		
Liquid phase				
$\Delta_fH°$ =	−188.90	−191.40	2.50	61COL/LAT
$C_p°$ =		287.33		

TABLE 18. Ketones (42) — Continued

Benzophenone; Diphenyl ketone $C_{13}H_{10}O$

$(10\times C_B\text{-}(H)(C_B)_2) + (2\times C_B\text{-}(CO)(C_B)_2) + (1\times CO\text{-}(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	60.30	59.10	1.20	83DEK/VAN
Liquid phase				
$\Delta_fH°$ =	−16.30	−16.40	0.10	83DEK/VAN
Solid phase				
$\Delta_fH°$ =	−34.40	−34.40	0.00	59COL/CAM
$C_p°$ =	224.81	224.85	−0.04	83DEK/VAN

4-Methylbenzophenone; Phenyl p-tolyl ketone $C_{14}H_{12}O$

$(1\times C\text{-}(H)_3(C)) + (9\times C_B\text{-}(H)(C_B)_2) + (2\times C_B\text{-}(CO)(C_B)_2) + (1\times CO\text{-}(C_B)_2) + (1\times C_B\text{-}(C)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		26.67		
Liquid phase				
$\Delta_fH°$ =		−53.01		
Solid phase				
$\Delta_fH°$ =	−77.80	−73.77	−4.03	59COL/CAM
$C_p°$ =		248.91		

4-Ethyl benzophenone $C_{15}H_{14}O$

$(9\times C_B\text{-}(H)(C_B)_2) + (2\times C_B\text{-}(CO)(C_B)_2) + (1\times C_B\text{-}(C)(C_B)_2) + (1\times CO\text{-}(C_B)_2) + (1\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)_2(C)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		5.33		
Liquid phase				
$\Delta_fH°$ =	−64.30	−77.82	13.52	59COL/CAM
Solid phase				
$\Delta_fH°$ =		−95.87		
$C_p°$ =		298.29		

TABLE 18. Ketones (42) – Continued

Diphenylethanedione; Benzil; Diphenyl diketone $C_{14}H_{10}O_2$
(10×C_B–(H)(C_B)$_2$)+(2×C_B–(CO)(C_B)$_2$)+(2×CO–(CO)(C_B))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	–55.50	–55.50	0.00	59AIH
Solid phase				
$\Delta_fH°$ =	–153.90	–153.90	0.00	62PAR/MOS

1,3-Diphenyl-1,3-propanedione; Dibenzoylmethane $C_{15}H_{12}O_2$
(10×C_B–(H)(C_B)$_2$)+(2×C_B–(CO)(C_B)$_2$)+(2×CO–(C)(C_B))+
(1×C–(H)$_2$(CO)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		–159.26		
Liquid phase				
$\Delta_fH°$ =		–210.89		
$C_p°$ =		397.84		
Solid phase				
$\Delta_fH°$ =	–224.90	–224.90	0.00	65KOZ/SHI

Cyclobutane-1,3-dione $C_4H_4O_2$
(2×C–(H)$_2$(CO)$_2$)+(2×CO–(C)$_2$)+
(1×cyclobutane-1,3-dione rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	–186.30	–186.30	0.00	78CHI/SHE
Solid phase				
$\Delta_fH°$ =	–260.00	–260.00	0.00	78CHI/SHE

TABLE 19. Acids (89)

Methanoic acid; Formic acid CH_2O_2
(1×O–(H)(CO))+(1×CO–(H)(O)), σ = 1

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	–378.70	–378.69	–0.01	70KON/WAD
$C_p°$ =	45.23	45.23	0.00	69STU/WES
$S°$ =	248.74	248.74	0.00	69STU/WES
$\Delta_fS°$ =		–92.61		
$\Delta_fG°$ =		–351.08		
$\ln K_f$ =		141.62		
Liquid phase				
$\Delta_fH°$ =	–425.50	–428.06	2.56	64LEB
$C_p°$ =	99.03	102.92	–3.89	41STO/FIS
$S°$ =	131.84	132.96	–1.12	41STO/FIS
$\Delta_fS°$ =		–208.39		
$\Delta_fG°$ =		–365.93		
$\ln K_f$ =		147.61		

Ethanoic acid; Acetic acid $C_2H_4O_2$
(1×C–(H)$_3$(C))+(1×CO–(C)(O))+(1×O–(H)(CO)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	–432.80	–433.80	1.00	70KON/WAD
$C_p°$ =	66.53	66.52	0.01	69STU/WES
$S°$ =	282.50	282.49	0.01	69STU/WES
$\Delta_fS°$ =		–195.18		
$\Delta_fG°$ =		–375.61		
$\ln K_f$ =		151.52		
Liquid phase				
$\Delta_fH°$ =	–484.50	–482.62	–1.88	64LEB
$C_p°$ =	123.10	119.28	3.82	82MAR/AND
$S°$ =	158.00	154.30	3.70	82MAR/AND
$\Delta_fS°$ =		–323.36		
$\Delta_fG°$ =		–386.21		
$\ln K_f$ =		155.79		

Propanoic acid; Propionic acid $C_3H_6O_2$
(1×C–(H)$_3$(C))+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(O))+
(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	–455.70	–455.64	–0.06	70KON/WAD
$C_p°$ =		91.21		
Liquid phase				
$\Delta_fH°$ =	–508.50	–506.76	–1.74	70KON/WAD
$C_p°$ =	152.80	148.57	4.23	82MAR/AND
$S°$ =	191.00	194.17	–3.17	82MAR/AND
$\Delta_fS°$ =		–419.81		
$\Delta_fG°$ =		–381.59		
$\ln K_f$ =		153.93		

TABLE 19. Acids (89) — Continued

L-2-Hydroxypropanoic acid; L-Lactic acid $C_3H_6O_3$
(1×C–(H)₃(C))+(1×C–(H)(O)(CO)(C))+(1×O–(H)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))+(1×–CH₃ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−468.76		
Liquid phase				
$\Delta_f H°$ =		−552.87		
$C_p°$ =		171.36		
$S°$ =		151.48		
$\Delta_f S°$ =		−565.02		
$\Delta_f G°$ =		−384.41		
$\ln K_f$ =		155.07		
Solid phase				
$\Delta_f H°$ =	−694.00	−698.88	4.88	59SAV/GUN
$C_p°$ =		127.83		
$S°$ =		147.30		
$\Delta_f S°$ =		−569.20		
$\Delta_f G°$ =		−529.17		
$\ln K_f$ =		213.47		

Butanoic acid; Butyric acid $C_4H_8O_2$
(1×C–(H)₃(C))+(1×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−475.80	−476.27	0.47	70KON/WAD
$C_p°$ =		114.10		
Liquid phase				
$\Delta_f H°$ =	−533.80	−532.49	−1.31	64LEB
$C_p°$ =	177.70	178.99	−1.29	82MAR/AND
$S°$ =	225.30	226.55	−1.25	82MAR/AND
$\Delta_f S°$ =		−523.74		
$\Delta_f G°$ =		−376.34		
$\ln K_f$ =		151.81		

Pentanoic acid; Valeric acid $C_5H_{10}O_2$
(1×C–(H)₃(C))+(2×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−496.30	−496.90	0.60	79KRU/OON
$C_p°$ =		136.99		

TABLE 19. Acids (89) — Continued

Pentanoic acid; Valeric acid (Continued) $C_5H_{10}O_2$
(1×C–(H)₃(C))+(2×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−558.70	−558.22	−0.48	65ADR/DEK
$C_p°$ =	210.33	209.41	0.92	65MCD/KIL
$S°$ =	259.83	258.93	0.90	65MCD/KIL
$\Delta_f S°$ =		−627.67		
$\Delta_f G°$ =		−371.08		
$\ln K_f$ =		149.69		

Hexanoic acid; Caproic acid $C_6H_{12}O_2$
(1×C–(H)₃(C))+(3×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−513.40	−517.53	4.13	79KRU/OON
$C_p°$ =		159.88		
Liquid phase				
$\Delta_f H°$ =	−585.60	−583.95	−1.65	64LEB
$C_p°$ =		239.83		
$S°$ =		291.31		
$\Delta_f S°$ =		−731.60		
$\Delta_f G°$ =		−365.82		
$\ln K_f$ =		147.57		

Heptanoic acid; Enanthylic acid $C_7H_{14}O_2$
(1×C–(H)₃(C))+(4×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−539.40	−538.16	−1.24	79KRU/OON
$C_p°$ =		182.77		
Liquid phase				
$\Delta_f H°$ =	−611.40	−609.68	−1.72	64LEB
$C_p°$ =	265.43	270.25	−4.82	82SCH/MIL
$S°$ =		323.69		
$\Delta_f S°$ =		−835.53		
$\Delta_f G°$ =		−360.57		
$\ln K_f$ =		145.45		

TABLE 19. Acids (89) — Continued

Octanoic acid; Caprylic acid $C_8H_{16}O_2$
(1×C–(H)$_3$(C)) + (5×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−553.90	−558.79	4.89	79KRU/OON
$C_p°$ =		205.66		
Liquid phase				
$\Delta_f H°$ =	−636.80	−635.41	−1.39	64LEB
$C_p°$ =	297.92	300.67	−2.75	82SCH/MIL2
$S°$ =		356.07		
$\Delta_f S°$ =		−939.46		
$\Delta_f G°$ =		−355.31		
$\ln K_f$ =		143.33		

Nonanoic acid; Pelargonic acid $C_9H_{18}O_2$
(1×C–(H)$_3$(C)) + (6×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−579.60	−579.42	−0.18	68BAC/NOV
$C_p°$ =		228.55		
Liquid phase				
$\Delta_f H°$ =	−661.80	−661.14	−0.66	64LEB
$C_p°$ =	326.37	331.09	−4.72	82SCH/MIL
$S°$ =		388.45		
$\Delta_f S°$ =		−1043.39		
$\Delta_f G°$ =		−350.05		
$\ln K_f$ =		141.21		

Decanoic acid; Capric acid $C_{10}H_{20}O_2$
(1×C–(H)$_3$(C)) + (7×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−594.90	−600.05	5.15	68BAC/NOV
$C_p°$ =		251.44		
Liquid phase				
$\Delta_f H°$ =	−684.30	−686.87	2.57	65ADR/DEK
$C_p°$ =		361.51		
$S°$ =		420.83		
$\Delta_f S°$ =		−1147.32		
$\Delta_f G°$ =		−344.80		
$\ln K_f$ =		139.09		

TABLE 19. Acids (89) — Continued

Decanoic acid; Capric acid (Continued) $C_{10}H_{20}O_2$
(1×C–(H)$_3$(C)) + (7×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	−713.70	−716.26	2.56	65ADR/DEK
$C_p°$ =		332.39		
$S°$ =		296.40		
$\Delta_f S°$ =		−1271.75		
$\Delta_f G°$ =		−337.09		
$\ln K_f$ =		135.98		

Undecanoic acid; Undecylic acid $C_{11}H_{22}O_2$
(1×C–(H)$_3$(C)) + (8×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−614.60	−620.68	6.08	68BAC/NOV
$C_p°$ =		274.33		
Liquid phase				
$\Delta_f H°$ =	−710.20	−712.60	2.40	65ADR/DEK
$C_p°$ =		391.93		
$S°$ =		453.21		
$\Delta_f S°$ =		−1251.25		
$\Delta_f G°$ =		−339.54		
$\ln K_f$ =		136.97		
Solid phase				
$\Delta_f H°$ =	−735.90	−745.67	9.77	65ADR/DEK
$C_p°$ =		354.31		
$S°$ =		319.41		
$\Delta_f S°$ =		−1385.05		
$\Delta_f G°$ =		−332.72		
$\ln K_f$ =		134.22		

Dodecanoic acid; Lauric acid $C_{12}H_{24}O_2$
(1×C–(H)$_3$(C)) + (9×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−642.00	−641.31	−0.69	68BAC/NOV
$C_p°$ =		297.22		
Liquid phase				
$\Delta_f H°$ =	−737.90	−738.33	0.43	65ADR/DEK
$C_p°$ =		422.35		
$S°$ =		485.59		
$\Delta_f S°$ =		−1355.18		
$\Delta_f G°$ =		−334.28		
$\ln K_f$ =		134.85		

TABLE 19. Acids (89) – Continued

Dodecanoic acid; Lauric acid (Continued) $C_{12}H_{24}O_2$
(1×C–(H)₃(C))+(9×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	−774.60	−775.08	0.48	65ADR/DEK
$C_p°$ =	404.28	376.23	28.05	82SCH/MIL2
$S°$ =		342.42		
$\Delta_f S°$ =		−1498.35		
$\Delta_f G°$ =		−328.35		
$\ln K_f$ =		132.45		

Tridecanoic acid; Tridecylic acid $C_{13}H_{26}O_2$
(1×C–(H)₃(C))+(10×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−660.20	−661.94	1.74	68BAC/NOV
$C_p°$ =		320.11		
Liquid phase				
$\Delta_f H°$ =	−763.50	−764.06	0.56	65ADR/DEK
$C_p°$ =		452.77		
$S°$ =		517.97		
$\Delta_f S°$ =		−1459.12		
$\Delta_f G°$ =		−329.02		
$\ln K_f$ =		132.73		
Solid phase				
$\Delta_f H°$ =	−806.60	−804.49	−2.11	65ADR/DEK
$C_p°$ =	387.61	398.15	−10.54	82SCH/MIL
$S°$ =		365.43		
$\Delta_f S°$ =		−1611.66		
$\Delta_f G°$ =		−323.97		
$\ln K_f$ =		130.69		

Tetradecanoic acid; Myristic acid $C_{14}H_{28}O_2$
(1×C–(H)₃(C))+(11×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−693.80	−682.57	−11.23	61DAV/MAL
$C_p°$ =		343.00		
Liquid phase				
$\Delta_f H°$ =	−788.80	−789.79	0.99	65ADR/DEK
$C_p°$ =		483.19		
$S°$ =		550.35		
$\Delta_f S°$ =		−1563.05		
$\Delta_f G°$ =		−323.77		
$\ln K_f$ =		130.61		

TABLE 19. Acids (89) – Continued

Tetradecanoic acid; Myristic acid (Continued) $C_{14}H_{28}O_2$
(1×C–(H)₃(C))+(11×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	−833.50	−833.90	0.40	65ADR/DEK
$C_p°$ =	432.00	420.07	11.93	82SCH/MIL2
$S°$ =		388.44		
$\Delta_f S°$ =		−1724.96		
$\Delta_f G°$ =		−319.60		
$\ln K_f$ =		128.93		

Pentadecanoic acid; Pentadecylic acid $C_{15}H_{30}O_2$
(1×C–(H)₃(C))+(12×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−699.00	−703.20	4.20	68BAC/NOV
$C_p°$ =		365.89		
Liquid phase				
$\Delta_f H°$ =	−811.70	−815.52	3.82	65ADR/DEK
$C_p°$ =		513.61		
$S°$ =		582.73		
$\Delta_f S°$ =		−1666.98		
$\Delta_f G°$ =		−318.51		
$\ln K_f$ =		128.48		
Solid phase				
$\Delta_f H°$ =	−861.70	−863.31	1.61	65ADR/DEK
$C_p°$ =	443.29	441.99	1.30	82SCH/MIL
$S°$ =		411.45		
$\Delta_f S°$ =		−1838.26		
$\Delta_f G°$ =		−315.23		
$\ln K_f$ =		127.16		

Hexadecanoic acid; Palmitic acid $C_{16}H_{32}O_2$
(1×C–(H)₃(C))+(13×C–(H)₂(C)₂)+(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−737.00	−723.83	−13.17	61DAV/MAL
$C_p°$ =		388.78		
Liquid phase				
$\Delta_f H°$ =	−838.10	−841.25	3.15	65ADR/DEK
$C_p°$ =		544.03		
$S°$ =		615.11		
$\Delta_f S°$ =		−1770.91		
$\Delta_f G°$ =		−313.25		
$\ln K_f$ =		126.36		

TABLE 19. Acids (89) – Continued

Hexadecanoic acid; Palmitic acid (Continued) $C_{16}H_{32}O_2$

(1×C–(H)$_3$(C)) + (13×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	−891.50	−892.72	1.22	65ADR/DEK
$C_p°$ =	463.36	463.91	−0.55	82SCH/MIL2
$S°$ =		434.46		
$\Delta_f S°$ =		−1951.56		
$\Delta_f G°$ =		−310.86		
$\ln K_f$ =		125.40		

Heptadecanoic acid; Margaric acid $C_{17}H_{34}O_2$

(1×C–(H)$_3$(C)) + (14×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−744.46		
$C_p°$ =		411.67		
Liquid phase				
$\Delta_f H°$ =	−865.60	−866.98	1.38	65ADR/DEK
$C_p°$ =		574.45		
$S°$ =		647.49		
$\Delta_f S°$ =		−1874.84		
$\Delta_f G°$ =		−308.00		
$\ln K_f$ =		124.24		
Solid phase				
$\Delta_f H°$ =	−924.40	−922.13	−2.27	65ADR/DEK
$C_p°$ =	475.72	485.83	−10.11	82SCH/MIL
$S°$ =		457.47		
$\Delta_f S°$ =		−2064.86		
$\Delta_f G°$ =		306.49		
$\ln K_f$ =		123.64		

Octadecanoic acid; Stearic acid $C_{18}H_{36}O_2$

(1×C–(H)$_3$(C)) + (15×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−781.20	−765.09	−16.11	61DAV/MAL
$C_p°$ =		434.56		
Liquid phase				
$\Delta_f H°$ =	−884.70	−892.71	8.01	65ADR/DEK
$C_p°$ =		604.87		
$S°$ =		679.87		
$\Delta_f S°$ =		−1978.77		
$\Delta_f G°$ =		−302.74		
$\ln K_f$ =		122.12		

TABLE 19. Acids (89) – Continued

Octadecanoic acid; Stearic acid (Continued) $C_{18}H_{36}O_2$

(1×C–(H)$_3$(C)) + (15×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	−948.00	−951.54	3.54	65ADR/DEK
$C_p°$ =	501.55	507.75	−6.20	82SCH/MIL2
$S°$ =		480.48		
$\Delta_f S°$ =		−2178.16		
$\Delta_f G°$ =		−302.12		
$\ln K_f$ =		121.87		

Nonadecanoic acid; Nonadecylic acid $C_{19}H_{38}O_2$

(1×C–(H)$_3$(C)) + (16×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−785.30	−785.72	0.42	68BAC/NOV
$C_p°$ =		457.45		
Liquid phase				
$\Delta_f H°$ =	−916.40	−918.44	2.04	65ADR/DEK
$C_p°$ =		635.29		
$S°$ =		712.25		
$\Delta_f S°$ =		−2082.70		
$\Delta_f G°$ =		−297.48		
$\ln K_f$ =		120.00		
Solid phase				
$\Delta_f H°$ =	−984.00	−980.95	−3.05	65ADR/DEK
$C_p°$ =	525.34	529.67	−4.33	82SCH/MIL
$S°$ =		503.49		
$\Delta_f S°$ =		−2291.46		
$\Delta_f G°$ =		−297.75		
$\ln K_f$ =		120.11		

Eicosanoic acid; Arachidic acid $C_{20}H_{40}O_2$

(1×C–(H)$_3$(C)) + (17×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−812.40	−806.35	−6.05	61DAV/MAL
$C_p°$ =		480.34		
Liquid phase				
$\Delta_f H°$ =	−940.00	−944.17	4.17	65ADR/DEK
$C_p°$ =		665.71		
$S°$ =		744.63		
$\Delta_f S°$ =		−2186.63		
$\Delta_f G°$ =		−292.23		
$\ln K_f$ =		117.88		

TABLE 19. Acids (89) — Continued

Eicosanoic acid; Arachidic acid (Continued) $C_{20}H_{40}O_2$

(1 × C–(H)$_3$(C)) + (17 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)(O)) + (1 × O–(H)(CO))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−1011.90	−1010.36	−1.54	65ADR/DEK
$C_p°$ =	545.14	551.59	−6.45	82SCH/MIL2
$\Delta_fS°$ =		−2404.76		
$\Delta_fG°$ =		−293.38		
$\ln K_f$ =		118.35		

2-Methylbutanoic acid $C_5H_{10}O_2$

(1 × O–(H)(CO)) + (1 × CO–(C)(O)) + (1 × C–(H)(CO)(C)$_2$) + (2 × C–(H)$_3$(C)) + (1 × C–(H)$_2$(C)$_2$) + (1 × –CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−499.20		
Liquid phase				
$\Delta_fH°$ =	−554.50	−562.03	7.53	54HAN/WAT
$C_p°$ =		203.59		
$S°$ =		245.46		
$\Delta_fS°$ =		−641.14		
$\Delta_fG°$ =		−370.87		
$\ln K_f$ =		149.61		

3-Methylbutanoic acid $C_5H_{10}O_2$

(2 × C–(H)$_3$(C)) + (1 × C–(H)(C)$_3$) + (1 × –CH$_3$ corr (tertiary)) + (1 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)(O)) + (1 × O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−504.10	−501.33	−2.77	79KRU/OON
$C_p°$ =		137.02		
Liquid phase				
$\Delta_fH°$ =	−561.60	−561.32	−0.28	54HAN/WAT
$C_p°$ =		206.43		
$S°$ =		253.58		
$\Delta_fS°$ =		−633.02		
$\Delta_fG°$ =		−372.59		
$\ln K_f$ =		150.30		

2,2-Dimethylpropanoic acid; Pivalic acid $C_5H_{10}O_2$

(1 × O–(H)(CO)) + (1 × CO–(C)(O)) + (1 × C–(CO)(C)$_3$) + (3 × C–(H)$_3$(C)) + (3 × –CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−491.30	−508.07	16.77	79KRU/OON
Liquid phase				
$\Delta_fH°$ =	−564.50	−564.86	0.36	54HAN/WAT
$C_p°$ =		200.23		
$S°$ =		234.92		
$\Delta_fS°$ =		−651.68		
$\Delta_fG°$ =		−370.56		
$\ln K_f$ =		149.48		
Solid phase				
$\Delta_fH°$ =		−565.00		
$C_p°$ =	177.82	177.83	−0.01	71KON/WAD

2-Propenoic acid; Acrylic acid $C_3H_4O_2$

(1 × O–(H)(CO)) + (1 × CO–(C$_d$)(O)) + (1 × C$_d$–(H)(CO)) + (1 × C$_d$–(H)$_2$), σ = 1

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−332.41		
$C_p°$ =	77.78	77.78	0.00	69STU/WES
$S°$ =	315.01	315.01	0.00	69STU/WES
$\Delta_fS°$ =		−168.39		
$\Delta_fG°$ =		−282.20		
$\ln K_f$ =		113.84		
Liquid phase				
$\Delta_fH°$ =	−383.88	−392.84	8.96	59SKI/SNE
$C_p°$ =		142.47		

Adamantane-1-carboxylic acid $C_{11}H_{16}O_2$

(3 × C–(H)(C)$_3$) + (6 × C–(H)$_2$(C)$_2$) + (1 × Adamantane rsc) + (1 × C–(CO)(C)$_3$) + (1 × CO–(C)(O)) + (1 × O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−501.04		
Solid phase				
$\Delta_fH°$ =	−643.08	−602.95	−40.13	73STE/CAR

TABLE 19. Acids (89) – Continued

Adamantane-2-carboxylic acid $C_{11}H_{16}O_2$

(4×C–(H)(C)$_3$)+(5×C–(H)$_2$(C)$_2$)+(1×Adamantane rsc)+(1×C–(H)(CO)(C)$_2$)+(1×CO–(C)(O))+(1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−505.76		
Solid phase				
$\Delta_f H°$ =	−627.18	−613.37	−13.81	73STE/CAR

(Z)-2-Butenedioic acid; Maleic acid $C_4H_4O_4$

(2×O–(H)(CO))+(2×CO–(C$_d$)(O))+(2×C$_d$–(H)(CO))+(1×*cis*(unsat) corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−679.40	−712.61	33.21	38WOL/WEG
$C_p°$ =		104.77		
Liquid phase				
$\Delta_f H°$ =		−823.91		
$C_p°$ =		228.20		
Solid phase				
$\Delta_f H°$ =	−789.40	−811.13	21.73	38HUF/FOX
$C_p°$ =	137.00	139.38	−2.38	85WIL/CHA
$S°$ =	160.80	164.42	−3.62	85WIL/CHA
$\Delta_f S°$ =		−529.77		
$\Delta_f G°$ =		−653.18		
$\ln K_f$ =		263.49		

(E)-2-Butenedioic acid; Fumaric acid $C_4H_4O_4$

(2×O–(H)(CO))+(2×CO–(C$_d$)(O))+(2×C$_d$–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−675.80	−717.46	41.66	38WOL/WEG
$C_p°$ =		112.80		
Liquid phase				
$\Delta_f H°$ =		−829.18		
$C_p°$ =		228.20		
Solid phase				
$\Delta_f H°$ =	−812.20	−816.86	4.66	38HUF/FOX
$C_p°$ =	142.00	139.38	2.62	85WIL/CHA
$S°$ =	168.00	164.42	3.58	85WIL/CHA
$\Delta_f S°$ =		−529.77		
$\Delta_f G°$ =		−658.91		
$\ln K_f$ =		265.80		

TABLE 19. Acids (89) – Continued

Ethanedioic acid; Oxalic acid $C_2H_2O_4$

(2×CO–(O)(CO))+(2×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−732.00	−756.10	24.10	53BRA/COT
Liquid phase				
$\Delta_f H°$ =		−817.88		
$C_p°$ =		156.90		
Solid phase				
$\Delta_f H°$ =	−829.70	−805.92	−23.78	64WIL/SHI

Propanedioic acid; Malonic acid $C_3H_4O_4$

(2×O–(H)(CO))+(2×CO–(C)(O))+(1×C–(H)$_2$(CO)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−813.80		
Liquid phase				
$\Delta_f H°$ =		−893.07		
$C_p°$ =		181.16		
Solid phase				
$\Delta_f H°$ =	−891.00	−890.60	−0.40	64WIL/SHI

Butanedioic acid; Succinic acid $C_4H_6O_4$

(2×O–(H)(CO))+(2×CO–(C)(O))+(2×C–(H)$_2$(CO)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−823.00	−826.76	3.76	60DAV/THO
$C_p°$ =		130.96		
Liquid phase				
$\Delta_f H°$ =		−918.30		
$C_p°$ =		224.18		
$S°$ =		221.74		
$\Delta_f S°$ =		−603.02		
$\Delta_f G°$ =		−738.51		
$\ln K_f$ =		297.91		
Solid phase				
$\Delta_f H°$ =	−940.40	−927.30	−13.10	72VAN/MAN
$C_p°$ =		223.00		
$S°$ =		157.28		
$\Delta_f S°$ =		−667.48		
$\Delta_f G°$ =		−728.29		
$\ln K_f$ =		293.79		

TABLE 19. Acids (89) — Continued

Pentanedioic acid; Glutaric acid $C_5H_8O_4$

(2×O–(H)(CO)) + (2×CO–(C)(O)) + (2×C–(H)$_2$(CO)(C)) + (1×C–(H)$_2$(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−847.39		
$C_p°$ =		153.85		
Liquid phase				
$\Delta_f H°$ =		−944.03		
$C_p°$ =		254.60		
$S°$ =		254.12		
$\Delta_f S°$ =		−706.95		
$\Delta_f G°$ =		−733.25		
$\ln K_f$ =		295.79		
Solid phase				
$\Delta_f H°$ =	−959.90	−956.71	−3.19	64WIL/SHI
$C_p°$ =		244.92		
$S°$ =		180.29		
$\Delta_f S°$ =		−780.78		
$\Delta_f G°$ =		−723.92		
$\ln K_f$ =		292.02		

Hexanedioic acid; Adipic acid $C_6H_{10}O_4$

(2×O–(H)(CO)) + (2×CO–(C)(O)) + (2×C–(H)$_2$(CO)(C)) + (2×C–(H)$_2$(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−865.00	−868.02	3.02	60DAV/THO
$C_p°$ =		176.74		
Liquid phase				
$\Delta_f H°$ =		−969.76		
$C_p°$ =		285.02		
$S°$ =		286.50		
$\Delta_f S°$ =		−810.88		
$\Delta_f G°$ =		−728.00		
$\ln K_f$ =		293.67		
Solid phase				
$\Delta_f H°$ =	−994.30	−986.12	−8.18	26VER/HAR
$C_p°$ =		266.84		
$S°$ =		203.30		
$\Delta_f S°$ =		−894.08		
$\Delta_f G°$ =		−719.55		
$\ln K_f$ =		290.26		

TABLE 19. Acids (89) — Continued

Heptanedioic acid; Pimelic acid $C_7H_{12}O_4$

(2×O–(H)(CO)) + (2×CO–(C)(O)) + (2×C–(H)$_2$(CO)(C)) + (3×C–(H)$_2$(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−888.65		
$C_p°$ =		199.63		
Liquid phase				
$\Delta_f H°$ =		−995.49		
$C_p°$ =		315.44		
$S°$ =		318.88		
$\Delta_f S°$ =		−914.81		
$\Delta_f G°$ =		−722.74		
$\ln K_f$ =		291.55		
Solid phase				
$\Delta_f H°$ =	−1009.80	−1015.53	5.73	26VER/HAR
$C_p°$ =		288.76		
$S°$ =		226.31		
$\Delta_f S°$ =		−1007.38		
$\Delta_f G°$ =		−715.18		
$\ln K_f$ =		288.50		

Octanedioic acid; Suberic acid $C_8H_{14}O_4$

(2×O–(H)(CO)) + (2×CO–(C)(O)) + (2×C–(H)$_2$(CO)(C)) + (4×C–(H)$_2$(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−894.90	−909.28	14.38	60DAV/THO
$C_p°$ =		222.52		
Liquid phase				
$\Delta_f H°$ =		−1021.22		
$C_p°$ =		345.86		
$S°$ =		351.26		
$\Delta_f S°$ =		−1018.74		
$\Delta_f G°$ =		−717.48		
$\ln K_f$ =		289.43		
Solid phase				
$\Delta_f H°$ =	−1038.00	−1044.94	6.94	26VER/HAR
$C_p°$ =		310.68		
$S°$ =		249.32		
$\Delta_f S°$ =		−1120.68		
$\Delta_f G°$ =		−710.81		
$\ln K_f$ =		286.74		

TABLE 19. Acids (89) – Continued

Nonanedioic acid; Azelaic acid $C_9H_{16}O_4$
(2×O–(H)(CO)) + (2×CO–(C)(O)) + (2×C–(H)$_2$(CO)(C)) + (5×C–(H)$_2$(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−929.91		
$C_p°$ =		245.41		
Liquid phase				
$\Delta_fH°$ =		−1046.95		
$C_p°$ =		376.28		
$S°$ =		383.64		
$\Delta_fS°$ =		−1122.67		
$\Delta_fG°$ =		−712.22		
$\ln K_f$ =		287.31		
Solid phase				
$\Delta_fH°$ =	−1054.30	−1074.35	20.05	26VER/HAR
$C_p°$ =		332.60		
$S°$ =		272.33		
$\Delta_fS°$ =		−1233.98		
$\Delta_fG°$ =		−706.44		
$\ln K_f$ =		284.97		

Decanedioic acid; Sebacic acid $C_{10}H_{18}O_4$
(2×O–(H)(CO)) + (2×CO–(C)(O)) + (2×C–(H)$_2$(CO)(C)) + (6×C–(H)$_2$(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−921.90	−950.54	28.64	60DAV/THO
$C_p°$ =		268.30		
Liquid phase				
$\Delta_fH°$ =		−1072.68		
$C_p°$ =		406.70		
$S°$ =		416.02		
$\Delta_fS°$ =		−1226.60		
$\Delta_fG°$ =		−706.97		
$\ln K_f$ =		285.19		
Solid phase				
$\Delta_fH°$ =	−1082.60	−1103.76	21.16	26VER/HAR
$C_p°$ =		354.52		
$S°$ =		295.34		
$\Delta_fS°$ =		−1347.29		
$\Delta_fG°$ =		−702.07		
$\ln K_f$ =		283.21		

TABLE 19. Acids (89) – Continued

Undecanedioic acid $C_{11}H_{20}O_4$
(2×O–(H)(CO)) + (2×CO–(C)(O)) + (2×C–(H)$_2$(CO)(C)) + (7×C–(H)$_2$(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−971.17		
$C_p°$ =		291.19		
Liquid phase				
$\Delta_fH°$ =		−1098.41		
$C_p°$ =		437.12		
$S°$ =		448.40		
$\Delta_fS°$ =		−1330.54		
$\Delta_fG°$ =		−701.71		
$\ln K_f$ =		283.07		
Solid phase				
$\Delta_fH°$ =	−1099.40	−1133.17	33.77	26VER/HAR
$C_p°$ =		376.44		
$S°$ =		318.35		
$\Delta_fS°$ =		−1460.59		
$\Delta_fG°$ =		−697.70		
$\ln K_f$ =		281.45		

Dodecanedioic acid $C_{12}H_{22}O_4$
(2×O–(H)(CO)) + (2×CO–(C)(O)) + (2×C–(H)$_2$(CO)(C)) + (8×C–(H)$_2$(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−976.90	−991.80	14.90	60DAV/THO
$C_p°$ =		314.08		
Liquid phase				
$\Delta_fH°$ =		−1124.14		
$C_p°$ =		467.54		
$S°$ =		480.78		
$\Delta_fS°$ =		−1434.47		
$\Delta_fG°$ =		−696.45		
$\ln K_f$ =		280.94		
Solid phase				
$\Delta_fH°$ =	−1130.00	−1162.58	32.58	26VER/HAR
$C_p°$ =		398.36		
$S°$ =		341.36		
$\Delta_fS°$ =		−1573.89		
$\Delta_fG°$ =		−693.33		
$\ln K_f$ =		279.68		

TABLE 19. Acids (89) – Continued

Tridecanedioic acid $C_{13}H_{24}O_4$
(2×O–(H)(CO))+(2×CO–(C)(O))+(2×C–(H)$_2$(CO)(C))+
(9×C–(H)$_2$(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−1012.43		
C_p° =		336.97		
Liquid phase				
Δ_fH° =		−1149.87		
C_p° =		497.96		
S° =		513.16		
Δ_fS° =		−1538.40		
Δ_fG° =		−691.20		
$\ln K_f$ =		278.82		
Solid phase				
Δ_fH° =	−1148.30	−1191.99	43.69	26VER/HAR
C_p° =		420.28		
S° =		364.37		
Δ_fS° =		−1687.19		
Δ_fG° =		−688.95		
$\ln K_f$ =		277.92		

Methylbutanedioic acid; Methylsuccinic acid $C_5H_8O_4$
(2×O–(H)(CO))+(2×CO–(C)(O))+(1×C–(H)$_2$(CO)(C))+
(1×C–(H)(CO)(C)$_2$)+(1×C–(H)$_3$(C))+
(1×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−849.69		
Liquid phase				
Δ_fH° =		−947.84		
C_p° =		248.78		
S° =		240.65		
Δ_fS° =		−720.42		
Δ_fG° =		−733.05		
$\ln K_f$ =		295.71		
Solid phase				
Δ_fH° =	−958.20	−958.31	0.11	33VER/HAR
C_p° =		188.02		

TABLE 19. Acids (89) – Continued

2,2-Dimethyl-1,4-butanedioic acid; 2,2-Dimethylsuccinic acid $C_6H_{10}O_4$
(2×O–(H)(CO))+(2×CO–(C)(O))+(1×C–(H)$_2$(CO)(C))+
(1×C–(CO)(C)$_3$)+(2×C–(H)$_3$(C))+
(2×–CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−874.63		
Liquid phase				
Δ_fH° =		−972.01		
C_p° =		275.84		
S° =		262.49		
Δ_fS° =		−834.89		
Δ_fG° =		−723.09		
$\ln K_f$ =		291.69		
Solid phase				
Δ_fH° =	−987.80	−977.56	−10.24	33VER/HAR
C_p° =		221.88		

meso-2,3-Dimethyl-1,4-butanedioic acid; meso-2,3-Dimethylsuccinic acid $C_6H_{10}O_4$
(2×O–(H)(CO))+(2×CO–(C)(O))+(2×C–(H)(CO)(C)$_2$)+
(2×C–(H)$_3$(C))+(2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−872.62		
Liquid phase				
Δ_fH° =		−977.38		
C_p° =		273.38		
S° =		259.56		
Δ_fS° =		−837.82		
Δ_fG° =		−727.58		
$\ln K_f$ =		293.50		
Solid phase				
Δ_fH° =	−977.50	−989.32	11.82	33VER/HAR
C_p° =		153.04		

racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethylsuccinic acid $C_6H_{10}O_4$
(2×O–(H)(CO))+(2×CO–(C)(O))+(2×C–(H)(CO)(C)$_2$)+
(2×C–(H)$_3$(C))+(2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−872.62		

TABLE 19. Acids (89) — Continued

racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethylsuccinic acid (Continued) $C_6H_{10}O_4$

(2×O–(H)(CO))+(2×CO–(C)(O))+(2×C–(H)(CO)(C)₂)+(2×C–(H)₃(C))+(2×–CH₃ corr (tertiary))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		−977.38		
$C_p°$ =		273.38		
$S°$ =		259.56		
$\Delta_f S°$ =		−837.82		
$\Delta_f G°$ =		−727.58		
$\ln K_f$ =		293.50		
Solid phase				
$\Delta_f H°$ =	−983.80	−989.32	5.52	33VER/HAR
$C_p°$ =		153.04		

Trimethylbutanedioic acid; Trimethylsuccinic acid $C_7H_{12}O_4$

(2×O–(H)(CO))+(2×CO–(C)(O))+(1×C–(H)(CO)(C)₂)+(1×C–(CO)(C)₃)+(3×C–(H)₃(C))+(1×–CH₃ corr (tertiary))+(2×–CH₃ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−897.56		
Liquid phase				
$\Delta_f H°$ =		−1001.55		
$C_p°$ =		300.44		
$S°$ =		281.40		
$\Delta_f S°$ =		−952.29		
$\Delta_f G°$ =		−717.62		
$\ln K_f$ =		289.48		
Solid phase				
$\Delta_f H°$ =	−1000.80	−1008.57	7.77	33VER/HAR
$C_p°$ =		186.90		

Tetramethylbutanedioic acid; Tetramethylsuccinic acid $C_8H_{14}O_4$

(2×O–(H)(CO))+(2×CO–(C)(O))+(2×C–(CO)(C)₃)+(4×C–(H)₃(C))+(4×–CH₃ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−922.50		
Liquid phase				
$\Delta_f H°$ =		−1025.72		
$C_p°$ =		327.50		
$S°$ =		303.24		
$\Delta_f S°$ =		−1066.76		
$\Delta_f G°$ =		−707.66		
$\ln K_f$ =		285.47		

TABLE 19. Acids (89) — Continued

Tetramethylbutanedioic acid; Tetramethylsuccinic acid (Continued) $C_8H_{14}O_4$

(2×O–(H)(CO))+(2×CO–(C)(O))+(2×C–(CO)(C)₃)+(4×C–(H)₃(C))+(4×–CH₃ corr (quaternary))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	−1012.40	−1027.82	15.42	33VER/HAR
$C_p°$ =		220.76		

Ethylbutanedioic acid; Ethylsuccinic acid $C_6H_{10}O_4$

(2×O–(H)(CO))+(2×CO–(C)(O))+(1×C–(H)(CO)(C)₂)+(1×C–(H)₂(CO)(C))+(1×C–(H)₂(C)₂)+(1×C–(H)₃(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−868.06		
Liquid phase				
$\Delta_f H°$ =		−971.39		
$C_p°$ =		279.20		
$S°$ =		273.03		
$\Delta_f S°$ =		−824.35		
$\Delta_f G°$ =		−725.61		
$\ln K_f$ =		292.71		
Solid phase				
$\Delta_f H°$ =	−989.20	−985.38	−3.82	33VER/HAR
$C_p°$ =		209.94		

2,2-Diethyl-1,4-butanedioic acid; 2,2-Diethylsuccinic acid $C_8H_{14}O_4$

(2×O–(H)(CO))+(2×CO–(C)(O))+(1×C–(H)₂(CO)(C))+(1×C–(CO)(C)₃)+(2×C–(H)₂(C)₂)+(2×C–(H)₃(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−906.77		
Liquid phase				
$\Delta_f H°$ =		−1014.69		
$C_p°$ =		336.68		
$S°$ =		327.25		
$\Delta_f S°$ =		−1042.75		
$\Delta_f G°$ =		−703.79		
$\ln K_f$ =		283.91		
Solid phase				
$\Delta_f H°$ =	−1032.70	−1027.68	−5.02	33VER/HAR
$C_p°$ =		265.72		

TABLE 19. Acids (89) — Continued

meso-2,3-Diethyl-1,4-butanedioic acid; meso-2,3-Diethylsuccinic acid $C_8H_{14}O_4$
$(2\times O-(H)(CO))+(2\times CO-(C)(O))+(2\times C-(H)(CO)(C)_2)+(2\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−909.36		
Liquid phase				
$\Delta_f H°$ =		−1024.48		
$C_p°$ =		334.22		
$S°$ =		324.32		
$\Delta_f S°$ =		−1045.68		
$\Delta_f G°$ =		−712.71		
$\ln K_f$ =		287.50		
Solid phase				
$\Delta_f H°$ =	−1019.20	−1043.46	24.26	33VER/HAR
$C_p°$ =		196.88		

racemic-2,3-Diethyl-1,4-butanedioic acid; racemic-2,3-Diethylsuccinic acid $C_8H_{14}O_4$
$(2\times O-(H)(CO))+(2\times CO-(C)(O))+(2\times C-(H)(CO)(C)_2)+(2\times C-(H)_2(C)_2)+(2\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−909.36		
Liquid phase				
$\Delta_f H°$ =		−1024.48		
$C_p°$ =		334.22		
$S°$ =		324.32		
$\Delta_f S°$ =		−1045.68		
$\Delta_f G°$ =		−712.71		
$\ln K_f$ =		287.50		
Solid phase				
$\Delta_f H°$ =	−1026.30	−1043.46	17.16	33VER/HAR
$C_p°$ =		196.88		

Triethylbutanedioic acid; Triethylsuccinic acid $C_{10}H_{18}O_4$
$(2\times O-(H)(CO))+(2\times CO-(C)(O))+(1\times C-(H)(CO)(C)_2)+(1\times C-(CO)(C)_3)+(3\times C-(H)_2(C)_2)+(3\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−948.07		

TABLE 19. Acids (89) — Continued

Triethylbutanedioic acid; Triethylsuccinic acid (Continued) $C_{10}H_{18}O_4$
$(2\times O-(H)(CO))+(2\times CO-(C)(O))+(1\times C-(H)(CO)(C)_2)+(1\times C-(CO)(C)_3)+(3\times C-(H)_2(C)_2)+(3\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		−1067.78		
$C_p°$ =		391.70		
$S°$ =		378.54		
$\Delta_f S°$ =		−1264.08		
$\Delta_f G°$ =		−690.89		
$\ln K_f$ =		278.70		
Solid phase				
$\Delta_f H°$ =	−1066.30	−1085.76	19.46	33VER/HAR
$C_p°$ =		252.66		

Tetraethylbutanedioic acid; Tetraethylsuccinic acid $C_{12}H_{22}O_4$
$(2\times O-(H)(CO))+(2\times CO-(C)(O))+(2\times C-(CO)(C)_3)+(4\times C-(H)_2(C)_2)+(4\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−986.78		
Liquid phase				
$\Delta_f H°$ =		−1111.08		
$C_p°$ =		449.18		
$S°$ =		432.76		
$\Delta_f S°$ =		−1482.49		
$\Delta_f G°$ =		−669.08		
$\ln K_f$ =		269.90		
Solid phase				
$\Delta_f H°$ =	−1096.50	−1128.06	31.56	33VER/HAR
$C_p°$ =		308.44		

Benzoic acid $C_7H_6O_2$
$(5\times C_B-(H)(C_B)_2)+(1\times C_B-(CO)(C_B)_2)+(1\times CO-(O)(C_B))+(1\times O-(H)(CO))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−295.70	−294.75	−0.95	72MOR2
Liquid phase				
$\Delta_f H°$ =	−372.80	−374.34	1.54	51FUR/MCC
$C_p°$ =		203.77		

TABLE 19. Acids (89) – Continued

Benzoic acid (Continued) $C_7H_6O_2$
$(5 \times C_B\text{-}(H)(C_B)_2) + (1 \times C_B\text{-}(CO)(C_B)_2) + (1 \times CO\text{-}(O)(C_B)) + (1 \times O\text{-}(H)(CO))$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	−385.20	−386.35	1.15	68CHU/ARM
$C_p°$ =	146.79	146.11	0.68	76ARV/FAL
$S°$ =	167.73	167.74	−0.01	76ARV/FAL
$\Delta_f S°$ =		−469.20		
$\Delta_f G°$ =		−246.46		
$\ln K_f$ =		99.42		

2-Methyl benzoic acid $C_8H_8O_2$
$(1 \times O\text{-}(H)(CO)) + (1 \times CO\text{-}(O)(C_B)) + (1 \times C_B\text{-}(CO)) + (1 \times C_B\text{-}(C)(C_B)_2) + (4 \times C_B\text{-}(H)(C_B)_2) + (1 \times C\text{-}(H)_3(C)) + (1 \times \textit{ortho}\text{ corr})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−325.92		
Liquid phase				
$\Delta_f H°$ =		−407.69		
$C_p°$ =		231.17		
Solid phase				
$\Delta_f H°$ =	−416.50	−420.72	4.22	61COL/BON
$C_p°$ =	174.89	170.17	4.72	26AND/LYN
$S°$ =		196.18		
$\Delta_f S°$ =		−577.07		
$\Delta_f G°$ =		−248.67		
$\ln K_f$ =		100.31		

3-Methyl benzoic acid $C_8H_8O_2$
$(1 \times O\text{-}(H)(CO)) + (1 \times CO\text{-}(O)(C_B)) + (1 \times C_B\text{-}(CO)) + (1 \times C_B\text{-}(C)(C_B)_2) + (1 \times C\text{-}(H)_3(C)) + (4 \times C_B\text{-}(H)(C_B)_2) + (1 \times \textit{meta}\text{ corr})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−327.81		
Liquid phase				
$\Delta_f H°$ =		−410.95		
$C_p°$ =		227.67		
Solid phase				
$\Delta_f H°$ =	−426.10	−423.72	−2.38	61COL/BON
$C_p°$ =	163.59	170.17	−6.58	26AND/LYN
$S°$ =		196.18		
$\Delta_f S°$ =		−577.07		
$\Delta_f G°$ =		−251.67		
$\ln K_f$ =		101.52		

4-Methyl benzoic acid $C_8H_8O_2$
$(1 \times O\text{-}(H)(CO)) + (1 \times CO\text{-}(O)(C_B)) + (1 \times C_B\text{-}(CO)) + (1 \times C_B\text{-}(C)(C_B)_2) + (1 \times C\text{-}(H)_3(C)) + (4 \times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−327.18		
Liquid phase				
$\Delta_f H°$ =		−410.95		
$C_p°$ =		227.67		
Solid phase				
$\Delta_f H°$ =	−429.20	−425.72	−3.48	61COL/BON
$C_p°$ =	169.03	170.17	−1.14	26AND/LYN
$S°$ =		196.18		
$\Delta_f S°$ =		−577.07		
$\Delta_f G°$ =		−253.67		
$\ln K_f$ =		102.33		

2,3-Dimethyl benzoic acid $C_9H_{10}O_2$
$(1 \times O\text{-}(H)(CO)) + (1 \times CO\text{-}(O)(C_B)) + (1 \times C_B\text{-}(CO)) + (2 \times C_B\text{-}(C)(C_B)_2) + (2 \times C\text{-}(H)_3(C)) + (3 \times C_B\text{-}(H)(C_B)_2) + (2 \times \textit{ortho}\text{ corr}) + (1 \times \textit{meta}\text{ corr})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−357.72		
Liquid phase				
$\Delta_f H°$ =		−441.04		
$C_p°$ =		258.57		
Solid phase				
$\Delta_f H°$ =	−450.40	−453.09	2.69	61COL/PER
$C_p°$ =		194.23		
$S°$ =		224.62		
$\Delta_f S°$ =		−684.94		
$\Delta_f G°$ =		−248.88		
$\ln K_f$ =		100.39		

2,4-Dimethyl benzoic acid $C_9H_{10}O_2$
$(1 \times O\text{-}(H)(CO)) + (1 \times CO\text{-}(O)(C_B)) + (1 \times C_B\text{-}(CO)) + (2 \times C_B\text{-}(C)(C_B)_2) + (2 \times C\text{-}(H)_3(C)) + (3 \times C_B\text{-}(H)(C_B)_2) + (1 \times \textit{ortho}\text{ corr}) + (1 \times \textit{meta}\text{ corr})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−358.98		

TABLE 19. Acids (89) – Continued

2,4-Dimethyl benzoic acid (Continued) $C_9H_{10}O_2$

(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+(2×C_B–(C)(C_B)$_2$)+(2×C–(H)$_3$(C))+(3×C_B–(H)(C_B)$_2$)+(1×*ortho* corr)+(1×*meta* corr)

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_f H°$ =		−444.30		
$C_p°$ =		255.07		
Solid phase				
$\Delta_f H°$ =	−458.50	−458.09	−0.41	61COL/PER
$C_p°$ =		194.23		
$S°$ =		224.62		
$\Delta_f S°$ =		−684.94		
$\Delta_f G°$ =		−253.88		
$\ln K_f$ =		102.41		

2,5-Dimethyl benzoic acid $C_9H_{10}O_2$

(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+(2×C_B–(C)(C_B)$_2$)+(2×C–(H)$_3$(C))+(3×C_B–(H)(C_B)$_2$)+(1×*ortho* corr)+(1×*meta* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−358.98		
Liquid phase				
$\Delta_f H°$ =		−444.30		
$C_p°$ =		255.07		
Solid phase				
$\Delta_f H°$ =	−456.10	−458.09	1.99	61COL/PER
$C_p°$ =		194.23		
$S°$ =		224.62		
$\Delta_f S°$ =		−684.94		
$\Delta_f G°$ =		−253.88		
$\ln K_f$ =		102.41		

2,6-Dimethyl benzoic acid $C_9H_{10}O_2$

(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+(2×C_B–(C)(C_B)$_2$)+(2×C–(H)$_3$(C))+(3×C_B–(H)(C_B)$_2$)+(2×*ortho* corr)+(1×*meta* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−357.72		
Liquid phase				
$\Delta_f H°$ =		−441.04		
$C_p°$ =		258.57		

TABLE 19. Acids (89) – Continued

2,6-Dimethyl benzoic acid (Continued) $C_9H_{10}O_2$

(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+(2×C_B–(C)(C_B)$_2$)+(2×C–(H)$_3$(C))+(3×C_B–(H)(C_B)$_2$)+(2×*ortho* corr)+(1×*meta* corr)

	Literature	– Calculated	= Residual	Reference
Solid phase				
$\Delta_f H°$ =	−440.70	−453.09	12.39	61COL/PER
$C_p°$ =		194.23		
$S°$ =		224.62		
$\Delta_f S°$ =		−684.94		
$\Delta_f G°$ =		−248.88		
$\ln K_f$ =		100.39		

3,4-Dimethyl benzoic acid $C_9H_{10}O_2$

(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+(2×C_B–(C)(C_B)$_2$)+(2×C–(H)$_3$(C))+(3×C_B–(H)(C_B)$_2$)+(1×*ortho* corr)+(1×*meta* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−358.98		
Liquid phase				
$\Delta_f H°$ =		−444.30		
$C_p°$ =		255.07		
Solid phase				
$\Delta_f H°$ =	−468.80	−458.09	−10.71	61COL/PER
$C_p°$ =		194.23		
$S°$ =		224.62		
$\Delta_f S°$ =		−684.94		
$\Delta_f G°$ =		−253.88		
$\ln K_f$ =		102.41		

3,5-Dimethyl benzoic acid $C_9H_{10}O_2$

(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+(2×C_B–(C)(C_B)$_2$)+(2×C–(H)$_3$(C))+(3×C_B–(H)(C_B)$_2$)+(3×*meta* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−361.50		
Liquid phase				
$\Delta_f H°$ =		−447.56		
$C_p°$ =		251.57		

TABLE 19. Acids (89) — Continued

3,5-Dimethyl benzoic acid (Continued) $C_9H_{10}O_2$
(1 × O–(H)(CO)) + (1 × CO–(O)(C_B)) + (1 × C_B–(CO)) + (2 × C_B–(C)(C_B)$_2$) + (2 × C–(H)$_3$(C)) + (3 × C_B–(H)(C_B)$_2$) + (3 × *meta* corr)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−466.40	−459.09	−7.31	61COL/PER
$C_p°$ =		194.23		
$S°$ =		224.62		
$\Delta_fS°$ =		−684.94		
$\Delta_fG°$ =		−254.88		
$\ln K_f$ =		102.82		

TABLE 19. Acids (89) — Continued

3,5-Dimethyl benzoic acid (Continued) $C_9H_{10}O_2$
(1 × O–(H)(CO)) + (1 × CO–(O)(C_B)) + (1 × C_B–(CO)) + (2 × C_B–(C)(C_B)$_2$) + (2 × C–(H)$_3$(C)) + (3 × C_B–(H)(C_B)$_2$) + (3 × *meta* corr)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−488.70	−490.46	1.76	64COL/TUR
$C_p°$ =		218.29		
$S°$ =		253.06		
$\Delta_fS°$ =		−792.81		
$\Delta_fG°$ =		−254.08		
$\ln K_f$ =		102.50		

2,3,4-Trimethyl benzoic acid $C_{10}H_{12}O_2$
(1 × O–(H)(CO)) + (1 × CO–(O)(C_D)) + (1 × C_D–(CO)) + (3 × C_B–(C)(C_B)$_2$) + (3 × C–(H)$_3$(C)) + (2 × C_B–(H)(C_B)$_2$) + (3 × *ortho* corr) + (2 × *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−389.52		
Liquid phase				
$\Delta_fH°$ =		−474.39		
$C_p°$ =		285.97		
Solid phase				
$\Delta_fH°$ =	−486.60	−485.46	−1.14	64COL/TUR
$C_p°$ =		218.29		
$S°$ =		253.06		
$\Delta_fS°$ =		−792.81		
$\Delta_fG°$ =		−249.08		
$\ln K_f$ =		100.48		

2,3,6-Trimethyl benzoic acid $C_{10}H_{12}O_2$
(1 × O–(H)(CO)) + (1 × CO–(O)(C_D)) + (1 × C_D–(CO)) + (3 × C_B–(C)(C_B)$_2$) + (3 × C–(H)$_3$(C)) + (2 × C_B–(H)(C_B)$_2$) + (3 × *ortho* corr) + (2 × *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−389.52		
Liquid phase				
$\Delta_fH°$ =		−474.39		
$C_p°$ =		285.97		
Solid phase				
$\Delta_fH°$ =	−475.70	−485.46	9.76	64COL/TUR
$C_p°$ =		218.29		
$S°$ =		253.06		
$\Delta_fS°$ =		−792.81		
$\Delta_fG°$ =		−249.08		
$\ln K_f$ =		100.48		

2,3,5-Trimethyl benzoic acid $C_{10}H_{12}O_2$
(1 × O–(H)(CO)) + (1 × CO–(O)(C_B)) + (1 × C_B–(CO)) + (3 × C_B–(C)(C_B)$_2$) + (3 × C–(H)$_3$(C)) + (2 × C_B–(H)(C_B)$_2$) + (2 × *ortho* corr) + (2 × *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−390.78		
Liquid phase				
$\Delta_fH°$ =		−477.65		
$C_p°$ =		282.47		

2,4,5-Trimethyl benzoic acid $C_{10}H_{12}O_2$
(1 × O–(H)(CO)) + (1 × CO–(O)(C_B)) + (1 × C_B–(CO)) + (3 × C_B–(C)(C_B)$_2$) + (3 × C–(H)$_3$(C)) + (2 × C_B–(H)(C_B)$_2$) + (2 × *ortho* corr) + (2 × *meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−390.78		
Liquid phase				
$\Delta_fH°$ =		−477.65		
$C_p°$ =		282.47		

TABLE 19. Acids (89) — Continued

2,4,5-Trimethyl benzoic acid (Continued) $C_{10}H_{12}O_2$
(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+
(3×C_B–(C)(C_B)$_2$)+(3×C–(H)$_3$(C))+(2×C_B–(H)(C_B)$_2$)+
(2×*ortho* corr)+(2×*meta* corr)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−495.70	−490.46	−5.24	64COL/TUR
$C_p°$ =		218.29		
$S°$ =		253.06		
$\Delta_fS°$ =		−792.81		
$\Delta_fG°$ =		−254.08		
$\ln K_f$ =		102.50		

2,4,6-Trimethyl benzoic acid $C_{10}H_{12}O_2$
(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+
(3×C_B–(C)(C_B)$_2$)+(3×C–(H)$_3$(C))+(2×C_B–(H)(C_B)$_2$)+
(2×*ortho* corr)+(3×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−391.41		
Liquid phase				
$\Delta_fH°$ =		−477.65		
$C_p°$ =		282.47		
Solid phase				
$\Delta_fH°$ =	−477.90	−488.46	10.56	64COL/TUR
$C_p°$ =		218.29		
$S°$ =		253.06		
$\Delta_fS°$ =		−792.81		
$\Delta_fG°$ =		−252.08		
$\ln K_f$ =		101.69		

3,4,5-Trimethyl benzoic acid $C_{10}H_{12}O_2$
(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+
(3×C_B–(C)(C_B)$_2$)+(3×C–(H)$_3$(C))+(2×C_B–(H)(C_B)$_2$)+
(2×*ortho* corr)+(1×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−390.15		
Liquid phase				
$\Delta_fH°$ =		−477.65		
$C_p°$ =		282.47		

TABLE 19. Acids (89) — Continued

3,4,5-Trimethyl benzoic acid (Continued) $C_{10}H_{12}O_2$
(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+
(3×C_B–(C)(C_B)$_2$)+(3×C–(H)$_3$(C))+(2×C_B–(H)(C_B)$_2$)+
(2×*ortho* corr)+(1×*meta* corr)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−500.90	−492.46	−8.44	64COL/TUR
$C_p°$ =		218.29		
$S°$ =		253.06		
$\Delta_fS°$ =		−792.81		
$\Delta_fG°$ =		−256.08		
$\ln K_f$ =		103.30		

2,3,4,5-Tetramethyl benzoic acid $C_{11}H_{14}O_2$
(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+
(4×C_B–(C)(C_B)$_2$)+(4×C–(H)$_3$(C))+(1×C_B–(H)(C_B)$_2$)+
(4×*ortho* corr)+(4×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−421.95		
Liquid phase				
$\Delta_fH°$ =		−507.74		
$C_p°$ =		313.37		
Solid phase				
$\Delta_fH°$ =	−514.40	−515.83	1.43	64COL/PER
$C_p°$ =		242.35		
$S°$ =		281.50		
$\Delta_fS°$ =		−900.68		
$\Delta_fG°$ =		−247.29		
$\ln K_f$ =		99.76		

2,3,4,6-Tetramethyl benzoic acid $C_{11}H_{14}O_2$
(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+
(4×C_B–(C)(C_B)$_2$)+(4×C–(H)$_3$(C))+(1×C_B–(H)(C_B)$_2$)+
(4×*ortho* corr)+(4×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−421.95		
Liquid phase				
$\Delta_fH°$ =		−507.74		
$C_p°$ =		313.37		

TABLE 19. Acids (89) – Continued

2,3,4,6-Tetramethyl benzoic acid (Continued) $C_{11}H_{14}O_2$

(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+(4×C_B–(C)(C_B)$_2$)+(4×C–(H)$_3$(C))+(1×C_B–(H)(C_B)$_2$)+(4×*ortho* corr)+(4×*meta* corr)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−507.70	−515.83	8.13	64COL/PER
$C_p°$ =		242.35		
$S°$ =		281.50		
$\Delta_fS°$ =		−900.68		
$\Delta_fG°$ =		−247.29		
$\ln K_f$ =		99.76		

2,3,5,6-Tetramethyl benzoic acid $C_{11}H_{14}O_2$

(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+(4×C_B–(C)(C_B)$_2$)+(4×C–(H)$_3$(C))+(1×C_B–(H)(C_B)$_2$)+(4×*ortho* corr)+(4×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−421.95		
Liquid phase				
$\Delta_fH°$ =		−507.74		
$C_p°$ =		313.37		
Solid phase				
$\Delta_fH°$ =	−506.10	−515.83	9.73	64COL/PER
$C_p°$ =		242.35		
$S°$ =		281.50		
$\Delta_fS°$ =		−900.68		
$\Delta_fG°$ =		−247.29		
$\ln K_f$ =		99.76		

3,5-Diethylbenzoic acid $C_{11}H_{14}O_2$

(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)(C_B))+(2×C_B–(C)(C_B)$_2$)+(3×C_B–(H)(C_B)$_2$)+(1×C_B–(CO))+(1×CO–(O)(C_B))+(1×O–(H)(CO))+(3×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−407.80	−404.18	−3.62	74ROU/TUR
Liquid phase				
$\Delta_fH°$ =		−497.18		
$C_p°$ =		297.37		
Solid phase				
$\Delta_fH°$ =	−511.90	−503.29	−8.61	74ROU/TUR
$C_p°$ =		292.99		
$S°$ =		278.42		
$\Delta_fS°$ =		−903.76		
$\Delta_fG°$ =		−233.83		
$\ln K_f$ =		94.33		

Pentamethyl benzoic acid $C_{12}H_{16}O_2$

(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO))+(5×C_B–(C)(C_B)$_2$)+(5×C–(H)$_3$(C))+(6×*ortho* corr)+(5×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−452.49		
Liquid phase				
$\Delta_fH°$ =		−537.83		
$C_p°$ =		344.27		
Solid phase				
$\Delta_fH°$ =	−536.10	−543.20	7.10	64COL/PER
$C_p°$ =		266.41		
$S°$ =		309.94		
$\Delta_fS°$ =		−1008.55		
$\Delta_fG°$ =		−242.50		
$\ln K_f$ =		97.82		

2-Hydroxybenzoic acid; Salicylic acid $C_7H_6O_3$

(1×O–(H)(C_B))+(1×C_B–(O))+(1×C_B–(CO))+(1×CO–(O)(C_B))+(1×O–(H)(CO))+(4×C_B–(H)(C_B)$_2$)+(1×OH–COOH *ortho* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−494.80	−493.61	−1.19	54DAV/JON
Liquid phase				
$\Delta_fH°$ =		−579.86		
$C_p°$ =		265.44		
Solid phase				
$\Delta_fH°$ =	−589.90	−591.13	1.23	35STI/HUF
$C_p°$ =		154.94		
$S°$ =		175.20		
$\Delta_fS°$ =		−564.26		
$\Delta_fG°$ =		−422.90		
$\ln K_f$ =		170.59		

1,2-Benzene dicarboxylic acid; Phthalic acid $C_8H_6O_4$

(2×O–(H)(CO))+(2×CO–(O)(C_B))+(2×C_B–(CO)(C_B)$_2$)+(4×C_B–(H)(C_B)$_2$)+(1×COOH–COOH (*ortho* corr))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−782.07	−777.74	−4.33	61SCH/WAG
$C_p°$ =	188.11	186.44	1.67	36PAR/TOD
$S°$ =	207.94	207.94	0.00	36PAR/TOD
$\Delta_fS°$ =		−639.78		
$\Delta_fG°$ =		−586.99		
$\ln K_f$ =		236.79		

TABLE 19. Acids (89) – Continued

1,3-Benzene dicarboxylic acid; Isophthalic acid $C_8H_6O_4$
(2×O–(H)(CO)) + (2×CO–(O)(C_B)) + (2×C_B–(CO)(C_B)$_2$) + (4×C_B–(H)(C_B)$_2$) + (1×COOH–COOH (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−696.30	−696.30	0.00	62KRA/BER
Solid phase				
$\Delta_fH°$ =	−803.00	−798.74	−4.26	71YUK/BIK
$C_p°$ =	201.70	201.44	0.26	39SAT/SOG2
$S°$ =		198.98		
$\Delta_fS°$ =		−648.74		
$\Delta_fG°$ =		−605.32		
$\ln K_f$ =		244.18		

1,4-Benzene dicarboxylic acid; Terephthalic acid $C_8H_6O_4$
(2×O–(H)(CO)) + (2×CO–(O)(C_B)) + (2×C_B–(CO)(C_B)$_2$) + (4×C_B–(H)(C_B)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−717.90	−672.36	−45.54	34HIR
Liquid phase				
$\Delta_fH°$ =		−797.64		
$C_p°$ =		271.46		
Solid phase				
$\Delta_fH°$ =	−816.18	−811.88	4.30	71YUK/BIK
$C_p°$ =		171.44		
$S°$ =		198.98		
$\Delta_fS°$ =		−648.74		
$\Delta_fG°$ =		−618.46		
$\ln K_f$ =		249.48		

1,2,3-Benzene tricarboxylic acid $C_9H_6O_6$
(3×O–(H)(CO)) + (3×CO–(O)(C_B)) + (3×C_B–(CO)(C_B)$_2$) + (3×C_B–(H)(C_B)$_2$) + (2×COOH–COOH (*ortho* corr)) + (1×COOH–COOH (*meta* corr))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−1160.30	−1155.99	−4.31	71YUK/BIK
$C_p°$ =		256.77		
$S°$ =		248.14		
$\Delta_fS°$ =		−810.36		
$\Delta_fG°$ =		−914.38		
$\ln K_f$ =		368.85		

TABLE 19. Acids (89) – Continued

1,3,5-Benzene tricarboxylic acid $C_9H_6O_6$
(3×O–(H)(CO)) + (3×CO–(O)(C_B)) + (3×C_B–(CO)(C_B)$_2$) + (3×C_B–(H)(C_B)$_2$) + (3×COOH–COOH (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−1121.79		
Solid phase				
$\Delta_fH°$ =	−1190.10	−1197.99	7.89	71YUK/BIK
$C_p°$ =		286.77		
$S°$ =		230.22		
$\Delta_fS°$ =		−828.28		
$\Delta_fG°$ =		−951.04		
$\ln K_f$ =		383.64		

1-Naphthoic acid $C_{11}H_8O_2$
(7×C_B–(H)(C_B)$_2$) + (2×C_{BF}–(C_{BF})(C_B)$_2$) + (1×C_B–(CO)) + (1×CO–(O)(C_B)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−223.10	−226.93	3.83	74COL/ROU
Liquid phase				
$\Delta_fH°$ =		−326.36		
$C_p°$ =		268.17		
Solid phase				
$\Delta_fH°$ =	−333.50	−345.09	11.59	74COL/ROU
$C_p°$ =		190.97		
$S°$ =		201.24		
$\Delta_fS°$ =		−589.23		
$\Delta_fG°$ =		169.41		
$\ln K_f$ =		68.34		

2-Naphthoic acid $C_{11}H_8O_2$
(7×C_B–(H)(C_B)$_2$) + (2×C_{BF}–(C_{BF})(C_B)$_2$) + (1×C_B–(CO)) + (1×CO–(O)(C_B)) + (1×O–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−232.50	−226.93	−5.57	74COL/ROU
Liquid phase				
$\Delta_fH°$ =		−326.36		
$C_p°$ =		268.17		

TABLE 19. Acids (89) — Continued

2-Naphthoic acid (Continued) $C_{11}H_8O_2$

$(7\times C_B-(H)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(1\times C_B-(CO))+(1\times CO-(O)(C_B))+(1\times O-(H)(CO))$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−346.10	−345.09	−1.01	74COL/ROU
$C_p°$ =		190.97		
$S°$ =		201.24		
$\Delta_fS°$ =		−589.23		
$\Delta_fG°$ =		−169.41		
$\ln K_f$ =		68.34		

3-Hydroxy-2-naphthoic acid $C_{11}H_8O_3$

$(1\times O-(H)(C_B))+(1\times O-(H)(CO))+(1\times CO-(O)(C_B))+(1\times C_B-(CO))+(1\times C_B-(O))+(6\times C_B-(H)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(1\times OH-COOH$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−425.79		
Liquid phase				
$\Delta_fH°$ =		−531.88		
$C_p°$ =		329.84		
Solid phase				
$\Delta_fH°$ =	−547.80	−549.87	2.07	56YOU/KEI
$C_p°$ =		199.80		
$S°$ =		208.70		
$\Delta_fS°$ =		−684.29		
$\Delta_fG°$ =		−345.85		
$\ln K_f$ =		139.51		

Phenylbutanedioic acid; Phenylsuccinic acid $C_{10}H_{10}O_4$

$(2\times O-(H)(CO))+(2\times CO-(C)(O))+(1\times C-(H)_2(CO)(C))+(1\times C-(H)(CO)(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(5\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−841.00	−838.04	−2.96	33VER/HAR

meso-2,3-Diphenylbutanedioic acid; meso-2,3-Diphenylsuccinic acid $C_{16}H_{14}O_4$

$(2\times O-(H)(CO))+(2\times CO-(C)(O))+(2\times C-(H)(CO)(C)(C_B))+(2\times C_B-(C)(C_B)_2)+(10\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−733.50	−748.78	15.28	33VER/HAR

racemic-2,3-Diphenylbutandedioic acid; racemic-2,3-Diphenylsuccinic acid $C_{16}H_{14}O_4$

$(2\times O-(H)(CO))+(2\times CO-(C)(O))+(2\times C-(H)(CO)(C)(C_B))+(2\times C_B-(C)(C_B)_2)+(10\times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−740.10	−748.78	8.68	33VER/HAR

2-Methoxybenzoic acid $C_8H_8O_3$

$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(CO)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times CO-(O)(C_B))+(1\times O-(H)(CO))+(1\times O-(C)(C_B))+(1\times C-(H)_3(O))+(1\times CH_3O-COOH$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−433.80	−433.12	−0.68	78COL/JIM
Solid phase				
$\Delta_fH°$ =	−538.50	−538.49	−0.01	78COL/JIM

3-Methoxybenzoic acid $C_8H_8O_3$

$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(CO)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times CO-(O)(C_B))+(1\times O-(H)(CO))+(1\times O-(C)(C_B))+(1\times C-(H)_3(O))+(1\times CH_3-COOH$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−446.10	−443.12	−2.98	78COL/JIM
Solid phase				
$\Delta_fH°$ =	−553.50	−556.49	2.99	78COL/JIM

4-Methoxybenzoic acid $C_8H_8O_3$

$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(CO)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times CO-(O)(C_B))+(1\times O-(H)(CO))+(1\times O-(C)(C_B))+(1\times C-(H)_3(O))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−451.90	−448.12	−3.78	78COL/JIM
Liquid phase				
$\Delta_fH°$ =		−540.57		
$C_p°$ =		265.38		
Solid phase				
$\Delta_fH°$ =	−561.70	−561.49	−0.21	78COL/JIM

TABLE 20. Anhydrides (11)

Ethanoic anhydride; Acetic anhydride $C_4H_6O_3$
(2×C–(H)$_3$(C))+(2×CO–(C)(O))+
(1×O–(CO)$_2$, aliphatic), σ = 18

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	−573.50	−573.50	0.00	47STU
$C_p°$ =	99.50	99.50	0.00	69STU/WES
$S°$ =	389.95	389.95	0.00	69STU/WES
$\Delta_fS°$ =		−332.29		
$\Delta_fG°$ =		−474.43		
$\ln K_f$ =		191.38		
Liquid phase				
$\Delta_fH°$ =	−624.40	−624.46	0.06	62WAD
$C_p°$ =	168.20	168.20	0.00	62WAD

Propanoic anhydride; Propionic anhydride $C_6H_{10}O_3$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(CO)(C))+(2×CO–(C)(O))+
(1×O–(CO)$_2$, aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	−626.51	−617.18	−9.33	47STU
$C_p°$ =		148.88		
Liquid phase				
$\Delta_fH°$ =	−679.10	−672.74	−6.36	42CON/KIS
$C_p°$ =		226.78		

2,2-Dimethylpropanoic anhydride; Pivalic anhydride $C_{10}H_{18}O_3$
(6×C–(H)$_3$(C))+(6×–CH$_3$ corr (quaternary))+
(2×C–(CO)(C)$_3$)+(2×CO–(C)(O))+(1×O–(CO)$_2$, aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		−722.04		
Liquid phase				
$\Delta_fH°$ =	−780.00	−788.94	8.94	42CON/KIS
$C_p°$ =		330.10		

Dihydrofuran-2,5-dione; Succinic anhydride $C_4H_4O_3$
(2×C–(H)$_2$(CO)(C))+(2×CO–(C)(O))+(1×O–(CO)$_2$, aliphatic)+
(1×Succinic anhydride rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	−527.90	−527.90	0.00	90YAN/PIL

TABLE 20. Anhydrides (11) – Continued

Dihydrofuran-2,5-dione; Succinic anhydride (Continued) $C_4H_4O_3$
(2×C–(H)$_2$(CO)(C))+(2×CO–(C)(O))+(1×O–(CO)$_2$, aliphatic)+
(1×Succinic anhydride rsc)

	Literature	– Calculated	– Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−588.60	−588.60	0.00	13TAM
Solid phase				
$\Delta_fH°$ =	−608.60	−608.60	0.00	90YAN/PIL

Glutaric anhydride $C_5H_6O_3$
(1×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(CO)(C))+(2×CO–(C)(O))+
(1×O–(CO)$_2$, aliphatic)+(1×Glutaric anhydride rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	−532.40	−532.40	0.00	90YAN/PIL
Solid phase				
$\Delta_fH°$ =	−618.50	−618.50	0.00	90YAN/PIL

Methylsuccinic anhydride $C_5H_6O_3$
(1×C–(H)$_3$(C))+(1×C–(H)(CO)(C)$_2$)+(1×C–(H)$_2$(CO)(C))+
(2×CO–(C)(O))+(1×O–(CO)$_2$, aliphatic)+
(1×–CH$_3$ corr (tertiary))+(1×Succinic anhydride rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		−550.83		
Liquid phase				
$\Delta_fH°$ =	−617.60	−618.14	0.54	42CON/KIS
Solid phase				
$\Delta_fH°$ =	−620.00	−639.61	19.61	33VER/HAR

2,2-Dimethylsuccinic anhydride $C_6H_8O_3$
(2×C–(H)$_3$(C))+(1×C–(CO)(C)$_3$)+(1×C–(H)$_2$(CO)(C))+
(2×CO–(C)(O))+(1×O–(CO)$_2$, aliphatic)+
(2×–CH$_3$ corr (quaternary))+(1×Succinic anhydride rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	−581.70	−575.77	−5.93	47STU

TABLE 20. Anhydrides (11) – Continued

2,2-Dimethylsuccinic anhydride (Continued) $C_6H_8O_3$

(2 × C–(H)$_3$(C)) + (1 × C–(CO)(C)$_3$) + (1 × C–(H)$_2$(CO)(C)) + (2 × CO–(C)(O)) + (1 × O–(CO)$_2$, aliphatic) + (2 × –CH$_3$ corr (quaternary)) + (1 × Succinic anhydride rsc)

	Literature	– Calculated	= Residual	Reference
Liquid phase $\Delta_fH°$ =	–645.50	–642.31	–3.19	42CON/KIS
Solid phase $\Delta_fH°$ =	–651.50	–658.86	7.36	33VER/HAR

Tetramethylsuccinic anhydride $C_8H_{12}O_3$

(4 × C–(H)$_3$(C)) + (4 × –CH$_3$ corr (quaternary)) + (2 × C–(CO)(C)$_3$) + (2 × CO–(C)(O)) + (1 × O–(CO)$_2$, aliphatic) + (1 × Succinic anhydride rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_fH°$ =		–623.64		
Liquid phase $\Delta_fH°$ =		–696.02		
Solid phase $\Delta_fH°$ =	–712.80	–709.12	–3.68	33VER/HAR

2,2-Diethylsuccinic anhydride $C_8H_{12}O_3$

(2 × C–(H)$_3$(C)) + (2 × C–(H)$_2$(C)$_2$) + (1 × C–(CO)(C)$_3$) + (1 × C–(H)$_2$(CO)(C)) + (2 × CO–(C)(O)) + (1 × O–(CO)$_2$, aliphatic) + (1 × Succinic anhydride rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_fH°$ =		–607.91		
Liquid phase $\Delta_fH°$ =		–684.99		
Solid phase $\Delta_fH°$ =	–688.80	–708.98	20.18	33VER/HAR

TABLE 20. Anhydrides (11) – Continued

Benzoic anhydride $C_{14}H_{10}O_3$

(10 × C$_B$–(H)(C$_B$)$_2$) + (2 × C$_B$–(CO)(C$_B$)$_2$) + (2 × CO–(O)(C$_B$)) + (1 × O–(CO)$_2$, aromatic)

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_fH°$ =	–319.23	–319.20	–0.03	71CAR/FIN
Liquid phase $\Delta_fH°$ =	–398.32	–398.30	–0.02	71CAR/FIN
Solid phase $\Delta_fH°$ =	–415.47	–415.40	–0.07	71CAR/FIN

Phthalic anhydride $C_8H_4O_3$

(4 × C$_B$–(H)(C$_B$)$_2$) + (2 × C$_B$–(CO)(C$_B$)$_2$) + (2 × CO–(O)(C$_B$)) + (1 × O–(CO)$_2$, aromatic) + (1 × Phthalic anhydride rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_fH°$ =	–371.40	–371.40	0.00	46CRO/FEE
Solid phase $\Delta_fH°$ =	–460.10	–460.10	0.00	50PAR/MOS

TABLE 21. Esters (74)

Methyl methanoate; Methyl formate $C_2H_4O_2$
(1×C–(H)$_3$(C))+(1×CO–(H)(O))+(1×O–(C)(CO)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−355.50	−355.52	0.02	71HAL/BAL
$C_p°$ =	66.53	66.53	0.00	69STU/WES
$S°$ =	301.25	301.25	0.00	69STU/WES
$\Delta_fS°$ =		−176.42		
$\Delta_fG°$ =		−302.92		
$\ln K_f$ =		122.20		
Liquid phase				
$\Delta_fH°$ =	−386.10	−386.05	−0.05	71HAL/BAL
$C_p°$ =	119.66	121.16	−1.50	79FUC
$S°$ =		216.26		
$\Delta_fS°$ =		−261.40		
$\Delta_fG°$ =		−308.11		
$\ln K_f$ =		124.29		

Methyl ethanoate; Methyl acetate $C_3H_6O_2$
(2×C–(H)$_3$(C))+(1×O–(C)(CO))+(1×CO–(C)(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−410.00	−410.63	0.63	71HAL/BAL
$C_p°$ =		87.82		
Liquid phase				
$\Delta_fH°$ =	−445.80	−440.61	−5.19	71HAL/BAL
$C_p°$ =	123.85	137.52	−13.67	71HAL/BAL
$S°$ =		237.60		
$\Delta_fS°$ =		−376.38		
$\Delta_fG°$ =		−328.39		
$\ln K_f$ =		132.47		

Methyl propanoate; Methyl propionate $C_4H_8O_2$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(O))+(1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−432.47		
$C_p°$ =		112.51		
Liquid phase				
$\Delta_fH°$ =		−464.75		
$C_p°$ =	174.05	166.81	7.24	79FUC
$S°$ =		277.47		
$\Delta_fS°$ =		−472.82		
$\Delta_fG°$ =		−323.78		
$\ln K_f$ =		130.61		

TABLE 21. Esters (74) – Continued

Methyl butanoate; Methyl butyrate $C_5H_{10}O_2$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(O))+(1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−453.10		
$C_p°$ =		135.40		
Liquid phase				
$\Delta_fH°$ =		−490.48		
$C_p°$ =	200.83	197.23	3.60	79FUC
$S°$ =		309.85		
$\Delta_fS°$ =		−576.75		
$\Delta_fG°$ =		−318.52		
$\ln K_f$ =		128.49		

Methyl pentanoate; Methyl valerate $C_6H_{12}O_2$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(O))+(1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−471.10	−473.73	2.63	77MAN/SEL
$C_p°$ =		158.29		
Liquid phase				
$\Delta_fH°$ =	−514.20	−516.21	2.01	65ADR/DEK
$C_p°$ =	229.28	227.65	1.63	79FUC
$S°$ =		342.23		
$\Delta_fS°$ =		−680.68		
$\Delta_fG°$ =		−313.27		
$\ln K_f$ =		126.37		

Methyl hexanoate; Methyl caproate $C_7H_{14}O_2$
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(O))+(1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−492.20	−494.36	2.16	77MAN/SEL
$C_p°$ =		181.18		
Liquid phase				
$\Delta_fH°$ =	−540.20	−541.94	1.74	65ADR/DEK
$C_p°$ =		258.07		
$S°$ =		374.61		
$\Delta_fS°$ =		−784.61		
$\Delta_fG°$ =		−308.01		
$\ln K_f$ =		124.25		

TABLE 21. Esters (74) – Continued

Methyl heptanoate; Methyl enanthate $C_8H_{16}O_2$

(2×C–(H)$_3$(C)) + (4×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−515.50	−514.99	−0.51	77MAN/SEL
$C_p°$ =		204.07		
Liquid phase				
$\Delta_f H°$ =	−567.10	−567.67	0.57	65ADR/DEK
$C_p°$ =	285.10	288.49	−3.39	79FUC
$S°$ =		406.99		
$\Delta_f S°$ =		−888.54		
$\Delta_f G°$ =		−302.75		
$\ln K_f$ =		122.13		

Methyl octanoate; Methyl caprylate $C_9H_{18}O_2$

(2×C–(H)$_3$(C)) + (5×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−533.90	−535.62	1.72	77MAN/SEL
$C_p°$ =		226.96		
Liquid phase				
$\Delta_f H°$ =	−590.30	−593.40	3.10	65ADR/DEK
$C_p°$ =		318.91		
$S°$ =		439.37		
$\Delta_f S°$ =		−992.47		
$\Delta_f G°$ =		−297.49		
$\ln K_f$ =		120.01		

Methyl nonanoate; Methyl perlargonate $C_{10}H_{20}O_2$

(2×C–(H)$_3$(C)) + (6×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−554.20	−556.25	2.05	77MAN/SEL
$C_p°$ =		249.85		
Liquid phase				
$\Delta_f H°$ =	−616.20	−619.13	2.93	65ADR/DEK
$C_p°$ =		349.33		
$S°$ =		471.75		
$\Delta_f S°$ =		−1096.40		
$\Delta_f G°$ =		−292.24		
$\ln K_f$ =		117.89		

TABLE 21. Esters (74) – Continued

Methyl decanoate; Methyl caprate $C_{11}H_{22}O_2$

(2×C–(H)$_3$(C)) + (7×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−573.80	−576.88	3.08	77MAN/SEL
$C_p°$ =		272.74		
Liquid phase				
$\Delta_f H°$ =	−640.50	−644.86	4.36	65ADR/DEK
$C_p°$ =	382.80	379.75	3.05	79FUC
$S°$ =		504.13		
$\Delta_f S°$ =		−1200.33		
$\Delta_f G°$ =		−286.98		
$\ln K_f$ =		115.77		

Methyl undecanoate; Methyl undecylate $C_{12}H_{24}O_2$

(2×C–(H)$_3$(C)) + (8×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−593.80	−597.51	3.71	77MAN/SEL
$C_p°$ =		295.63		
Liquid phase				
$\Delta_f H°$ =	−665.20	−670.59	5.39	65ADR/DEK
$C_p°$ =		410.17		
$S°$ =		536.51		
$\Delta_f S°$ =		−1304.27		
$\Delta_f G°$ =		−281.72		
$\ln K_f$ =		113.65		

Methyl dodecanoate; Methyl laurate $C_{13}H_{26}O_2$

(2×C–(H)$_3$(C)) + (9×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−615.90	−618.14	2.24	77MAN/SEL
$C_p°$ =		318.52		
Liquid phase				
$\Delta_f H°$ =	−693.00	−696.32	3.32	65ADR/DEK
$C_p°$ =		440.59		
$S°$ =		568.89		
$\Delta_f S°$ =		−1408.20		
$\Delta_f G°$ =		−276.47		
$\ln K_f$ =		111.52		

TABLE 21. Esters (74) – Continued

Methyl tridecanoate; Methyl tridecylate $C_{14}H_{28}O_2$
(2×C–(H)3(C)) + (10×C–(H)2(C)2) + (1×C–(H)2(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−635.30	−638.77	3.47	77MAN/SEL
C_p° =		341.41		
Liquid phase				
$\Delta_f H°$ =	−717.90	−722.05	4.15	65ADR/DEK
C_p° =		471.01		
$S°$ =		601.27		
$\Delta_f S°$ =		−1512.13		
$\Delta_f G°$ =		−271.21		
$\ln K_f$ =		109.40		

Methyl tetradecanoate; Methyl myristate $C_{15}H_{30}O_2$
(2×C–(H)3(C)) + (11×C–(H)2(C)2) + (1×C–(H)2(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−656.90	−659.40	2.50	77MAN/SEL
C_p° =		364.30		
Liquid phase				
$\Delta_f H°$ =	−743.90	−747.78	3.88	65ADR/DEK
C_p° =	505.40	501.43	3.97	79FUC
$S°$ =		633.65		
$\Delta_f S°$ =		−1616.06		
$\Delta_f G°$ =		−265.95		
$\ln K_f$ =		107.28		

Methyl pentadecanoate; Methyl pentadecylate $C_{16}H_{32}O_2$
(2×C–(H)3(C)) + (12×C–(H)2(C)2) + (1×C–(H)2(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−677.50	−680.03	2.53	77MAN/SEL
C_p° =		387.19		
Liquid phase				
$\Delta_f H°$ =	−771.00	−773.51	2.51	65ADR/DEK
C_p° =		531.85		
$S°$ =		666.03		
$\Delta_f S°$ =		−1719.99		
$\Delta_f G°$ =		−260.70		
$\ln K_f$ =		105.16		

TABLE 21. Esters (74) – Continued

Methyl hexadecanoate; Methyl palmitate $C_{17}H_{34}O_2$
(2×C–(H)3(C)) + (1×O–(C)(CO)) + (1×C–(H)2(CO)(C)) + (13×C–(H)2(C)2) + (1×CO–(C)(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−700.66		
C_p° =		410.08		
Liquid phase				
$\Delta_f H°$ =		−799.24		
C_p° =		562.27		
$S°$ =		698.41		
$\Delta_f S°$ =		−1823.92		
$\Delta_f G°$ =		−255.44		
$\ln K_f$ =		103.04		
Solid phase				
$\Delta_f H°$ =		−867.91		
C_p° =	474.47	480.76	−6.29	56WIR/DRO
$S°$ =	495.09	481.46	13.63	56WIR/DRO
$\Delta_f S°$ =		−2040.87		
$\Delta_f G°$ =		−259.42		
$\ln K_f$ =		104.65		

Ethyl methanoate; Ethyl formate $C_3H_6O_2$
(1×C–(H)3(C)) + (1×C–(H)2(O)(C)) + (1×O–(C)(CO)) + (1×CO–(H)(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−388.42		
C_p° =		86.86		
Liquid phase				
$\Delta_f H°$ =		−421.85		
C_p° =	144.35	154.80	−10.45	79FUC
$S°$ =		248.85		
$\Delta_f S°$ =		−365.13		
$\Delta_f G°$ =		−312.99		
$\ln K_f$ =		126.26		

Ethyl ethanoate; Ethyl acetate $C_4H_8O_2$
(2×C–(H)3(C)) + (1×C–(H)2(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−444.10	−443.53	−0.57	66WAD2
C_p° =	113.64	108.15	5.49	69STU/WES
$S°$ =	362.75	378.42	−15.67	69STU/WES
$\Delta_f S°$ =		−371.87		
$\Delta_f G°$ =		−332.66		
$\ln K_f$ =		134.19		

TABLE 21. Esters (74) — Continued

Ethyl ethanoate; Ethyl acetate (Continued) $C_4H_8O_2$
(2×C–(H)3(C))+(1×C–(H)2(O)(C))+(1×O–(C)(CO))+(1×CO–(C)(O)), σ = 9

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−478.80	−476.41	−2.39	78FEN/HAR
$C_p°$ =	169.20	171.16	−1.96	33PAR/HUF
$S°$ =	259.41	270.19	−10.78	33PAR/HUF
$\Delta_fS°$ =		−480.10		
$\Delta_fG°$ =		−333.27		
$\ln K_f$ =		134.44		

Propyl ethanoate; Propyl acetate $C_5H_{10}O_2$
(2×C–(H)3(C))+(1×C–(H)2(C)2)+(1×C–(H)2(O)(C))+(1×O–(C)(CO))+(1×CO–(C)(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−464.16		
$C_p°$ =		131.04		
Liquid phase				
$\Delta_fH°$ =		−502.14		
$C_p°$ =	196.07	201.58	−5.51	86JIM/ROM
$S°$ =		302.57		
$\Delta_fS°$ =		−584.03		
$\Delta_fG°$ =		−328.01		
$\ln K_f$ =		132.32		

Isopropyl ethanoate; Isopropyl acetate $C_5H_{10}O_2$
(3×C–(H)3(C))+(1×C–(H)(O)(C)2 (ethers,esters))+(1×O–(C)(CO))+(1×CO–(C)(O))+(2×–CH3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−481.70	−476.87	−4.83	66WAD2
$C_p°$ =		131.33		
Liquid phase				
$\Delta_fH°$ =	−518.80	−513.58	−5.22	58WAD
$C_p°$ =	196.65	199.56	−2.91	79FUC
$S°$ =		295.59		
$\Delta_fS°$ =		−591.01		
$\Delta_fG°$ =		−337.37		
$\ln K_f$ =		136.09		

TABLE 21. Esters (74) — Continued

2-Methylpropyl methanoate; Isobutyl formate $C_5H_{10}O_2$
(2×C–(H)3(C))+(1×C–(H)(C)3)+(1×C–(H)2(O)(C))+(1×O–(C)(CO))+(1×CO–(H)(O))+(2×–CH3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−436.37		
$C_p°$ =		132.67		
Liquid phase				
$\Delta_fH°$ =		−478.59		
$C_p°$ =	214.22	212.66	1.56	36KUR/VOS
$S°$ =		308.26		
$\Delta_fS°$ =		−578.34		
$\Delta_fG°$ =		−306.16		
$\ln K_f$ =		123.50		

Butyl ethanoate; Butyl acetate $C_6H_{12}O_2$
(2×C–(H)3(C))+(2×C–(H)2(C)2)+(1×C–(H)2(O)(C))+(1×O–(C)(CO))+(1×CO–(C)(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−485.60	−484.79	−0.81	66WAD2
$C_p°$ =		153.93		
Liquid phase				
$\Delta_fH°$ =	−529.20	−527.87	−1.33	58WAD
$C_p°$ =	228.45	232.00	−3.55	79FUC
$S°$ =		334.95		
$\Delta_fS°$ =		−687.96		
$\Delta_fG°$ =		−322.76		
$\ln K_f$ =		130.20		

2-Methylpropyl ethanoate; Isobutyl acetate $C_6H_{12}O_2$
(3×C–(H)3(C))+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)2(O)(C))+(1×C–(H)(C)3)+(2×–CH3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−491.48		
$C_p°$ =		153.96		
Liquid phase				
$\Delta_fH°$ =		−533.15		
$C_p°$ =	240.20	229.02	11.18	36KUR/VOS
$S°$ =		329.60		
$\Delta_fS°$ =		−693.31		
$\Delta_fG°$ =		−326.44		
$\ln K_f$ =		131.68		

TABLE 21. Esters (74) – Continued

2,2-Dimethylpropyl ethanoate; tert-Butyl acetate $C_6H_{12}O_2$
(4×C–(H)$_3$(C))+(1×C–(O)(C)$_3$ (ethers,esters))+(1×O–(C)(CO))+(1×CO–(C)(O))+(3×–CH_3 corr (quaternary))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		–499.33		
$C_p°$ =		153.88		
Liquid phase				
$\Delta_f H°$ =		–548.21		
$C_p°$ =	230.96	230.94	0.02	79FUC
$S°$ =		309.52		
$\Delta_f S°$ =		–713.39		
$\Delta_f G°$ =		–335.51		
$\ln K_f$ =		135.34		

Ethyl propanoate; Ethyl propionate $C_5H_{10}O_2$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(O)(C))+(1×O–(C)(CO))+(1×CO–(C)(O))+(1×C–(H)$_2$(CO)(C))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	–463.60	–465.37	1.77	72MAN2
$C_p°$ =		132.84		
Liquid phase				
$\Delta_f H°$ =	–502.70	–500.55	–2.15	72MAN2
$C_p°$ =	199.58	200.45	–0.87	87ZAB/HYN
$S°$ =		310.06		
$\Delta_f S°$ =		–576.54		
$\Delta_f G°$ =		–328.66		
$\ln K_f$ =		132.58		

Ethyl pentanoate; Ethyl valerate $C_7H_{14}O_2$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		–506.63		
$C_p°$ =		178.62		
Liquid phase				
$\Delta_f H°$ =	–553.00	–552.01	–0.99	37SCH
$C_p°$ =		261.29		
$S°$ =		374.82		
$\Delta_f S°$ =		–784.40		
$\Delta_f G°$ =		–318.14		
$\ln K_f$ =		128.34		

TABLE 21. Esters (74) – Continued

Propyl pentanoate; Propyl valerate $C_8H_{16}O_2$
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		–527.26		
$C_p°$ =		201.51		
Liquid phase				
$\Delta_f H°$ =	–583.00	–577.74	–5.26	37SCH
$C_p°$ =		291.71		
$S°$ =		407.20		
$\Delta_f S°$ =		–888.33		
$\Delta_f G°$ =		–312.88		
$\ln K_f$ =		126.22		

Butyl pentanoate; Butyl valerate $C_9H_{18}O_2$
(2×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		–547.89		
$C_p°$ =		224.40		
Liquid phase				
$\Delta_f H°$ =	–613.30	–603.47	–9.83	37SCH
$C_p°$ =		322.13		
$S°$ =		439.58		
$\Delta_f S°$ =		–992.26		
$\Delta_f G°$ =		–307.63		
$\ln K_f$ =		124.09		

Methyl 2-methylbutanoate $C_6H_{12}O_2$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)(CO)(C)$_2$)+(1×–CH_3 corr (tertiary))+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_3$(O))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	–492.50	–476.03	–16.47	70COX/PIL
Liquid phase				
$\Delta_f H°$ =	–534.30	–520.02	–14.28	54HAN/WAT
$C_p°$ =		221.83		
$S°$ =		328.76		
$\Delta_f S°$ =		–694.15		
$\Delta_f G°$ =		–313.06		
$\ln K_f$ =		126.29		

TABLE 21. Esters (74) – Continued

Methyl 3-methylbutanoate; Methyl isovalerate $C_6H_{12}O_2$
(2×C–(H)$_3$(C)) + (1×C–(H)(C)$_3$) + (2×–CH$_3$ corr (tertiary)) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO)) + (1×C–(H)$_3$(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−497.90	−480.42	−17.48	70COX/PIL
$C_p°$ =		158.32		
Liquid phase				
$\Delta_f H°$ =	−538.90	−521.49	−17.41	54HAN/WAT
$C_p°$ =		224.67		
$S°$ =		336.88		
$\Delta_f S°$ =		−686.03		
$\Delta_f G°$ =		−316.95		
$\ln K_f$ =		127.86		

Methyl 2,2-dimethylpropanoate; Methyl pivalate $C_6H_{12}O_2$
(3×C–(H)$_3$(C)) + (1×C–(CO)(C)$_3$) + (1×CO–(C)(O)) + (1×O–(C)(CO)) + (3×–CH$_3$ corr (quaternary)) + (1×C–(H)$_3$(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−494.51	−484.90	−9.61	71HAL/BAL
Liquid phase				
$\Delta_f H°$ =	−530.00	−522.85	−7.15	71HAL/BAL
$C_p°$ =	223.01	218.47	4.54	71HAL/BAL
$S°$ =		318.22		
$\Delta_f S°$ =		−704.69		
$\Delta_f G°$ =		−312.75		
$\ln K_f$ =		126.16		

Ethyl 2-methylbutanoate; Ethyl sec-valerate $C_7H_{14}O_2$
(3×C–(H)$_3$(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×C–(H)(CO)(C)$_2$) + (1×C–(H)$_2$(C)$_2$) + (1×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−522.41	−508.93	−13.48	70COX/PIL
Liquid phase				
$\Delta_f H°$ =	−566.81	−555.82	−10.99	54HAN/WAT
$C_p°$ =		255.47		
$S°$ =		361.35		
$\Delta_f S°$ =		−797.87		
$\Delta_f G°$ =		−317.94		
$\ln K_f$ =		128.25		

TABLE 21. Esters (74) – Continued

Ethenyl ethanoate; Vinyl acetate $C_4H_6O_2$
(1×C$_d$–(H)$_2$) + (1×C$_d$–(O)(H)) + (1×O–(C$_d$)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_3$(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−314.90	−314.89	−0.01	38DOL/GRE
Liquid phase				
$\Delta_f H°$ =	−349.70	−345.60	−4.10	47STU
$C_p°$ =	165.40	154.01	11.39	59BEN/THO

Methyl propenoate; Methyl acrylate $C_4H_6O_2$
(1×C$_d$–(H)$_2$) + (1×C$_d$–(H)(CO)) + (1×CO–(C$_d$)(O)) + (1×O–(C)(CO)) + (1×C–(H)$_3$(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−333.00	−309.24	−23.76	71HAL/BAL
$C_p°$ =		99.08		
Liquid phase				
$\Delta_f H°$ =	−362.20	−350.83	−11.37	71HAL/BAL
$C_p°$ =	161.50	160.71	0.79	79FUC

Methyl 2-methylpropenoate; Methyl methacrylate $C_5H_8O_2$
(1×C$_d$–(H)$_2$) + (1×C$_d$–(C)(CO)) + (2×C–(H)$_3$(C)) + (1×CO–(C$_d$)(O)) + (1×O–(C)(CO))

	Literature	Calculated	Residual	Reference
Liquid phase				
$C_p°$ =	188.49	187.69	0.80	52ERD/JAG

Methyl (E)-2-butenoate; Methyl *trans*-2-butenoate; Methyl crotonate $C_5H_8O_2$
(2×C–(H)$_3$(C)) + (1×O–(C)(CO)) + (1×CO–(C$_d$)(O)) + (1×C$_d$–(H)(CO)) + (1×C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−341.92	−341.50	−0.42	70COX/PIL
$C_p°$ =		122.17		
Liquid phase				
$\Delta_f H°$ =	−382.90	−389.14	6.24	36SCH
$C_p°$ =		193.42		

TABLE 21. Esters (74) — Continued

Ethyl (E)-2-butenoate; Ethyl *trans*-2-butenoate $C_6H_{10}O_2$
(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C$_d$)(O)) + (1×C$_d$–(H)(CO)) + (1×C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−375.60	−374.40	−1.20	70COX/PIL
$C_p°$ =		142.50		
Liquid phase				
$\Delta_f H°$ =	−420.00	−424.94	4.94	36SCH
$C_p°$ =		227.06		

Ethyl-3-pentynoate $C_7H_{10}O_2$
(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_2$(CO)(C$_t$)) + (2×C$_t$–(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−237.82	−238.81	0.99	70COX/PIL
Liquid phase				
$\Delta_f H°$ =	−287.60	−288.72	1.12	38SCH

Ethyl-4-pentynoate $C_7H_{10}O_2$
(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_2$(CO)(C)) + (1×C–(H)$_2$(C)(C$_t$)) + (1×C$_t$–(C)) + (1×C$_t$–(H))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−233.22	−214.21	−19.01	70COX/PIL
$C_p°$ =		163.85		
Liquid phase				
$\Delta_f H°$ =	−281.71	−263.45	−18.26	38SCH
$C_p°$ =		259.91		
$S°$ =		340.94		
$\Delta_f S°$ =		−557.14		
$\Delta_f G°$ =		−97.34		
$\ln K_f$ =		39.27		

TABLE 21. Esters (74) — Continued

Ethyl (Z)-2-pentenoate; Ethyl *cis*-2-pentenoate $C_7H_{12}O_2$
(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C$_d$)(O)) + (1×C$_d$–(H)(CO)) + (1×C$_d$–(H)(C)) + (1×C–(H)$_2$(C)(C$_d$)) + (1×*cis*(unsat) corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−394.72	−390.43	−4.29	70COX/PIL
$C_p°$ =		155.10		
Liquid phase				
$\Delta_f H°$ =	−440.80	−445.40	4.60	38SCH2
$C_p°$ =		256.35		

Ethyl (E)-2-pentenoate; Ethyl *trans*-2-pentenoate $C_7H_{12}O_2$
(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C$_d$)(O)) + (1×C$_d$–(H)(CO)) + (1×C$_d$–(H)(C)) + (1×C–(H)$_2$(C)(C$_d$))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−394.30	−395.28	0.98	70COX/PIL
$C_p°$ =		163.13		
Liquid phase				
$\Delta_f H°$ =	−442.50	−450.67	8.17	38SCH2
$C_p°$ =		256.35		

Ethyl (Z)-3-pentenoate; Ethyl *cis*-3-pentenoate $C_7H_{12}O_2$
(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_2$(CO)(C$_d$)) + (2×C$_d$–(H)(C)) + (1×*cis*(unsat) corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−387.61	−382.99	−4.62	70COX/PIL
Liquid phase				
$\Delta_f H°$ =	−432.40	−428.66	−3.74	38SCH2

Ethyl (E)-3-pentenoate; Ethyl *trans*-3-pentenoate $C_7H_{12}O_2$
(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_2$(CO)(C$_d$)) + (2×C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−390.12	−387.84	−2.28	70COX/PIL

TABLE 21. Esters (74) — Continued

Ethyl (E)-3-pentenoate; Ethyl *trans*-3-pentenoate (Continued) $C_7H_{12}O_2$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(O)(C))+(1×O–(C)(CO))+
(1×CO–(C)(O))+(1×C–(H)$_2$(CO)(C$_d$))+(2×C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−437.00	−433.93	−3.07	38SCH2

Ethyl 4-pentenoate $C_7H_{12}O_2$
(1×C–(H)$_3$(C))+(1×C–(H)$_2$(O)(C))+(1×O–(C)(CO))+
(1×CO–(C)(O))+(1×C–(H)$_2$(CO)(C))+(1×C–(H)$_2$(C)(C$_d$))+
(1×C$_d$–(H)(C))+(1×C$_d$–(H)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−385.51	−381.35	−4.16	70COX/PIL
$C_p°$ =		167.86		
Liquid phase				
$\Delta_f H°$ =	−431.60	−425.87	−5.73	37SCH
$C_p°$ =		246.23		
$S°$ =		373.20		
$\Delta_f S°$ =		−655.45		
$\Delta_f G°$ =		−230.45		
$\ln K_f$ =		92.96		

Ethyl-2,4-pentadienoate $C_7H_{10}O_2$
(1×C–(H)$_3$(C))+(1×C–(H)$_2$(O)(C))+(1×O–(C)(CO))+
(1×CO–(C)(O))+(1×C$_d$–(H)(CO))+(2×C$_d$–(H)(C$_d$))+
(1×C$_d$–(H)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−289.70	−286.09	−3.61	70COX/PIL
$C_p°$ =		156.49		
Liquid phase				
$\Delta_f H°$ =	−338.20	−336.08	−2.12	38SCH
$C_p°$ =		254.51		

Propyl (E)-2-butenoate; Propyl *trans*-2-butenoate $C_7H_{12}O_2$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(O)(C))+
(1×O–(C)(CO))+(1×CO–(C$_d$)(O))+(1×C$_d$–(H)(CO))+
(1×C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−394.30	−395.03	0.73	70COX/PIL
$C_p°$ =		165.39		

TABLE 21. Esters (74) — Continued

Propyl (E)-2-butenoate; Propyl *trans*-2-butenoate $C_7H_{12}O_2$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(O)(C))+
(1×O–(C)(CO))+(1×CO–(C$_d$)(O))+(1×C$_d$–(H)(CO))+
(1×C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−443.30	−450.67	7.37	36SCH
$C_p°$ =		257.48		

Isopropyl (E)-2-butenoate; Isopropyl *trans*-2-butenoate $C_7H_{12}O_2$
(3×C–(H)$_3$(C))+(1×C$_d$–(H)(C))+(1×C$_d$–(H)(CO))+
(1×CO–(C$_d$)(O))+(1×O–(C)(CO))+
(1×C–(H)(O)(C)$_2$ (ethers,esters))+
(2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−411.10	−407.74	−3.36	70COX/PIL
$C_p°$ =		165.68		
Liquid phase				
$\Delta_f H°$ =	−457.10	−462.11	5.01	36SCH
$C_p°$ =		255.46		

Butyl (E)-2-butenoate; Butyl *trans*-2-butenoate $C_8H_{14}O_2$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(O)(C))+
(1×O–(C)(CO))+(1×CO–(C$_d$)(O))+(1×C$_d$–(H)(CO))+
(1×C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−415.89	−415.66	−0.23	70COX/PIL
$C_p°$ =		188.28		
Liquid phase				
$\Delta_f H°$ =	−467.80	−476.40	8.60	36SCH
$C_p°$ =		287.90		

Propyl 2-pentenoate $C_8H_{14}O_2$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(O)(C))+
(1×O–(C)(CO))+(1×CO–(C$_d$)(O))+(1×C$_d$–(H)(CO))+
(1×C$_d$–(H)(C))+(1×C–(H)$_2$(C)(C$_d$))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−413.00	−415.91	2.91	70COX/PIL
$C_p°$ =		186.02		

TABLE 21. Esters (74) – Continued

Propyl 2-pentenoate (Continued) $C_8H_{14}O_2$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(O)(C))+(1×O–(C)(CO))+(1×CO–(C$_d$)(O))+(1×C$_d$–(H)(CO))+(1×C$_d$–(H)(C))+(1×C–(H)$_2$(C)(C$_d$))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−464.90	−476.40	11.50	37SCH
$C_p°$ =		286.77		

Propyl 3-pentenoate $C_8H_{14}O_2$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(O)(C))+(1×O–(C)(CO))+(1×CO–(C)(O))+(1×C–(H)$_2$(CO)(C$_d$))+(2×C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−404.22	−408.47	4.25	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−454.40	−459.66	5.26	37SCH

Isopropyl 3-pentenoate $C_8H_{14}O_2$
(3×C–(H)$_3$(C))+(1×C–(H)(O)(C)$_2$ (ethers,esters))+(1×O–(C)(CO))+(1×CO–(C)(O))+(1×C–(H)$_2$(CO)(C$_d$))+(2×C$_d$–(H)(C))+(2×–CH$_3$ corr (tertiary))+(1×C–(H)$_2$(C)(C$_d$))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−425.09	−442.06	16.97	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−473.30	−496.83	23.53	37SCH

Dimethyl ethanedioate; Dimethyl oxalate $C_4H_6O_4$
(2×C–(H)$_3$(C))+(2×O–(C)(CO))+(2×CO–(O)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−708.90	−709.76	0.86	76ANT/CAR
Liquid phase				
$\Delta_fH°$ =	−735.20	−733.86	−1.34	76ANT/CAR
$C_p°$ =		193.38		
Solid phase				
$\Delta_fH°$ =	−756.30	−756.30	0.00	76ANT/CAR

TABLE 21. Esters (74) – Continued

Dimethyl (Z)-2-butenedioate; Dimethyl maleate $C_6H_8O_4$
(2×C–(H)$_3$(C))+(2×O–(C)(CO))+(2×CO–(C$_d$)(O))+(2×C$_d$–(H)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−671.12		
$C_p°$ =		155.40		
Liquid phase				
$\Delta_fH°$ =		−745.16		
$C_p°$ =	263.17	264.68	−1.51	30WAS

Diethyl ethanedioate; Diethyl oxalate $C_6H_{10}O_4$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(O)(C))+(2×O–(C)(CO))+(2×CO–(O)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−742.00	−775.56	33.56	47STU
Liquid phase				
$\Delta_fH°$ =	−805.50	−805.46	−0.04	66ZIM/ROB
$C_p°$ =	260.66	260.66	0.00	1881REI

Diethyl propanedioate; Diethyl malonate $C_7H_{12}O_4$
(2×C–(H)$_3$(C))+(2×O–(C)(CO))+(2×CO–(C)(O))+(1×C–(H)$_2$(CO)$_2$)+(2×C–(H)$_2$(O)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−833.26		
Liquid phase				
$\Delta_fH°$ =		−880.65		
$C_p°$ =	284.93	284.92	0.01	33KOL/UDO

Diethyl butanedioate; Diethyl succinate $C_8H_{14}O_4$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(O)(C))+(2×O–(C)(CO))+(2×CO–(C)(O))+(2×C–(H)$_2$(CO)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−846.22		
$C_p°$ =		214.22		

TABLE 21. Esters (74) – Continued

Diethyl butanedioate; Diethyl succinate (Continued) $C_8H_{14}O_4$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(O)(C)) + (2×O–(C)(CO)) + (2×CO–(C)(O)) + (2×C–(H)$_2$(CO)(C))

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_f H°$ =		−905.88		
$C_p°$ =	330.54	327.94	2.60	79FUC
$S°$ =		453.52		
$\Delta_f S°$ =		−916.48		
$\Delta_f G°$ =		−632.63		
$\ln K_f$ =		255.20		

2-Oxetanone; 3-Propanolactone; β-Propiolactone $C_3H_4O_2$
(1×C–(H)$_2$(CO)(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×β-propiolactone rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−282.90	−282.90	0.00	66BOR/NAK
Liquid phase				
$\Delta_f H°$ =	−329.90	−329.90	0.00	66BOR/NAK
$C_p°$ =	122.09	122.09	0.00	83LEB/YEV
$S°$ =	175.31	175.31	0.00	83LEB/YEV
$\Delta_f S°$ =		−308.10		
$\Delta_f G°$ =		−238.04		
$\ln K_f$ =		96.02		

4-Butanolactone; τ-Butyrolactone $C_4H_6O_2$
(1×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×τ-butyrolactone rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−366.50	−366.50	0.00	90LEI/PIL
Liquid phase				
$\Delta_f H°$ =	−420.90	−420.90	0.00	90LEI/PIL
$C_p°$ =	141.29	141.30	−0.01	83LEB/YEV
$S°$ =	197.40	197.40	0.00	83LEB/YEV
$\Delta_f S°$ =		−422.32		
$\Delta_f G°$ =		−294.99		
$\ln K_f$ =		119.00		

TABLE 21. Esters (74) – Continued

4-Pentanolactone; τ-Valerolactone $C_5H_8O_2$
(1×C–(H)$_2$(C)$_2$) + (1×C–(H)(O)(C)$_2$ (ethers,esters)) + (1×C–(H)$_3$(C)) + (1×–CH_3 corr (tertiary)) + (1×C–(H)$_2$(CO)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×τ-Valerolactone rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−406.50	−406.50	0.00	90LEI/PIL
Liquid phase				
$\Delta_f H°$ =	−461.30	−461.30	0.00	90LEI/PIL

5-Pentanolactone; δ-Valerolactone $C_5H_8O_2$
(2×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×δ-valerolactone rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−379.60	−379.60	0.00	90LEI/PIL
Liquid phase				
$\Delta_f H°$ =	−437.60	−437.60	0.00	90LEI/PIL
$C_p°$ =	171.59	171.59	0.00	83LEB/YEV
$S°$ =	218.99	218.99	0.00	83LEB/YEV
$\Delta_f S°$ =		−537.04		
$\Delta_f G°$ =		−277.48		
$\ln K_f$ =		111.93		

Hexanolactone; Caprolactone $C_6H_{10}O_2$
(3×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×caprolactone rsc)

	Literature	-Calculated	= Residual	Reference
Liquid phase				
$C_p°$ =	196.82	196.83	−0.01	83LEB/YEV
$S°$ =	235.68	235.68	0.00	83LEB/YEV
$\Delta_f S°$ =		−656.66		

Undecanolactone $C_{11}H_{20}O_2$
(8×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×undecanolactone rsc)

	Literature	-Calculated	= Residual	Reference
Liquid phase				
$C_p°$ =	342.71	342.73	−0.02	83LEB/YEV
$S°$ =	369.49	369.45	0.04	83LEB/YEV
$\Delta_f S°$ =		−1204.44		

TABLE 21. Esters (74) – Continued

Methyl benzoate $C_8H_8O_2$
(1×C–(H)$_3$(C)) + (1×O–(C)(CO)) + (1×CO–(O)(C$_B$)) + (1×C$_B$–(CO)(C$_B$)$_2$) + (5×C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−287.90	−271.58	−16.32	71KUS/WAD
Liquid phase				
$\Delta_f H°$ =	−343.50	−332.33	−11.17	71HAL/BAL
$C_p°$ =		222.01		

Phenyl ethanoate; Phenyl acetate $C_8H_8O_2$
(1×C–(H)$_3$(C)) + (1×CO–(C)(O)) + (1×O–(C$_B$)(CO)) + (1×C$_B$–(O)(C$_B$)$_2$) + (5×C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−279.70	−282.20	2.50	72LEB/KAT
Liquid phase				
$\Delta_f H°$ =	−325.40	−327.29	1.89	72LEB/KAT

Ethyl benzoate $C_9H_{10}O_2$
(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(O)(C$_B$)) + (1×C$_B$–(CO)(C$_B$)$_2$) + (5×C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−304.48		
Liquid phase				
$\Delta_f H°$ =		−368.13		
$C_p°$ =	246.00	255.65	−9.65	79FUC

3-Methylphenyl ethanoate; 3-Methylphenyl acetate $C_9H_{10}O_2$
(2×C–(H)$_3$(C)) + (1×CO–(C)(O)) + (1×O–(C$_B$)(CO)) + (1×C$_B$–(O)(C$_B$)$_2$) + (4×C$_B$–(H)(C$_B$)$_2$) + (1×C$_B$–(C)(C$_B$)$_2$) + (1×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−313.40	−315.26	1.86	47BAL
Liquid phase				
$\Delta_f H°$ =	−374.20	−363.90	−10.30	57SUN

TABLE 21. Esters (74) – Continued

Phenyl benzoate $C_{13}H_{10}O_2$
(10×C$_B$–(H)(C$_B$)$_2$) + (1×C$_B$–(CO)(C$_B$)$_2$) + (1×CO–(O)(C$_B$)) + (1×O–(C$_B$)(CO)) + (1×C$_B$–(O)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−142.60	−143.15	0.55	71CAR/FIN
Liquid phase				
$\Delta_f H°$ =		−219.01		
Solid phase				
$\Delta_f H°$ =	−241.60	−240.55	−1.05	67ADA/FIN
$C_p°$ =		230.95		
$S°$ =		306.62		
$\Delta_f S°$ =		−625.90		
$\Delta_f G°$ =		−53.94		
$\ln K_f$ =		21.76		

Dimethyl 1,2-phthalate; Dimethyl o-phthalate; Dimethyl phthalate $C_{10}H_{10}O_4$
(2×C–(H)$_3$(C)) + (2×O–(C)(CO)) + (2×CO–(O)(C$_B$)) + (2×C$_B$–(CO)(C$_B$)$_2$) + (4×C$_B$–(H)(C$_B$)$_2$) + (1×*ortho* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−624.76		
Liquid phase				
$\Delta_f H°$ =		−710.36		
$C_p°$ =	309.28	311.44	−2.16	78MIL

Dimethyl 1,3-phthalate; Dimethyl m-phthalate; Dimethyl isophthalate $C_{10}H_{10}O_4$
(2×C–(H)$_3$(C)) + (2×O–(C)(CO)) + (2×CO–(O)(C$_B$)) + (2×C$_B$–(CO)(C$_B$)$_2$) + (4×C$_B$–(H)(C$_B$)$_2$) + (1×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−626.65		
Liquid phase				
$\Delta_f H°$ =		−713.62		
$C_p°$ =		307.94		

TABLE 21. Esters (74) — Continued

Dimethyl 1,3-phthalate; Dimethyl m-phthalate; Dimethyl isophthalate (Continued) $C_{10}H_{10}O_4$

(2×C–(H)$_3$(C)) + (2×O–(C)(CO)) + (2×CO–(O)(C$_B$)) + (2×C$_B$–(CO)(C$_B$)$_2$) + (4×C$_B$–(H)(C$_B$)$_2$) + (1×*meta* corr)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	−730.90	−760.26	29.36	72COL/LAY
$C_p°$ =		205.14		
$S°$ =		292.98		
$\Delta_f S°$ =		−827.36		
$\Delta_f G°$ =		−513.58		
$\ln K_f$ =		207.18		

Dimethyl 1,4-phthalate; Dimethyl p-phthalate; Dimethyl terephthalate $C_{10}H_{10}O_4$

(2×C–(H)$_3$(C)) + (2×O–(C)(CO)) + (2×C$_B$–(CO)(C$_B$)$_2$) + (4×C$_B$–(H)(C$_B$)$_2$) + (2×CO–(O)(C$_B$))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−626.02		
Liquid phase				
$\Delta_f H°$ =		−713.62		
$C_p°$ =		307.94		
Solid phase				
$\Delta_f H°$ =	−732.60	−762.26	29.66	72COL/LAY
$C_p°$ =	261.08	205.14	55.94	68ELL/CHR
$S°$ =		292.98		
$\Delta_f S°$ =		827.36		
$\Delta_f G°$ =		−515.58		
$\ln K_f$ =		207.98		

Diethyl 1,2-phthalate; Diethyl o-phthalate; Diethyl phthalate $C_{12}H_{14}O_4$

(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(O)(C)) + (2×O–(C)(CO)) + (2×CO–(O)(C$_B$)) + (2×C$_B$–(CO)(C$_B$)$_2$) + (4×C$_B$–(H)(C$_B$)$_2$) + (1×*ortho* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−688.40	−690.56	2.16	58HOY/PEP
Liquid phase				
$\Delta_f H°$ =	−776.60	−781.96	5.36	52MED/THO
$C_p°$ =	366.15	378.72	−12.57	67CHA/HOR

TABLE 21. Esters (74) — Continued

Cyclobutane methyl carboxylate $C_6H_{10}O_2$

(3×C–(H)$_2$(C)$_2$) + (1×C–(H)(CO)(C)$_2$) + (1×CO–(C)(O)) + (1×O–(C)(CO)) + (1×C–(H)$_3$(O)) + (1×Cyclobutane methyl carboxylate rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−355.30	−355.30	0.00	71HAL/BAL
Liquid phase				
$\Delta_f H°$ =	−395.00	−395.00	0.00	71HAL/BAL

Bicyclobutane methyl carboxylate $C_6H_8O_2$

(2×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_3$) + (1×C–(CO)(C)$_3$) + (1×CO–(C)(O)) + (1×O–(C)(CO)) + (1×C–(H)$_3$(O)) + (1×Bicyclobutane methyl carboxylate rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−164.60	−164.60	0.00	71HAL/BAL
Liquid phase				
$\Delta_f H°$ =	−203.10	−203.10	0.00	71HAL/BAL

Cubane 1,4-dimethyldicarboxylate $C_{12}H_{12}O_4$

(6×C–(H)(C)$_3$) + (2×C–(CO)(C)$_3$) + (2×CO–(C)(O)) + (2×O–(C)(CO)) + (2×C–(H)$_3$(O)) + (1×1,4-Dimethylcubane dicarboxylate)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−100.10	−100.10	0.00	66KYB/CAR
Solid phase				
$\Delta_f H°$ =	−218.99	−218.99	0.00	89KIR/CHU

TABLE 22. Peroxides (7)

Dimethylperoxide $C_2H_6O_2$
(2×C–(H)$_3$(C))+(2×O–(C)(O))

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	–125.90	–126.02	0.12	65BAK/LIT

Diethylperoxide $C_4H_{10}O_2$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(O)(C))+(2×O–(C)(O))

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	–192.80	–191.82	–0.98	39BLA/GER
Liquid phase $\Delta_f H°$ =	–223.30	–213.82	–9.48	65BAK/LIT

Di-*tert*-butyl peroxide $C_8H_{18}O_2$
(6×C–(H)$_3$(C))+(2×O–(C)(O))+
(2×C–(O)(C)$_3$ (alcohols,peroxides))+
(6×–CH_3 corr (quaternary))

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	–349.11	–349.42	0.31	51EGE/EMT
Liquid phase $\Delta_f H°$ =	–380.91	–381.26	0.35	65BAK/LIT

Dibenzoyl peroxide $C_{14}H_{10}O_4$
(10×C_B–(H)(C_B)$_2$)+(2×C_B–(CO)(C_B)$_2$)+(2×CO–(O)(C_B))+
(2×O–(CO)(O))

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	–271.70	–256.90	–14.80	75CAR/LAY
Liquid phase $\Delta_f H°$ =		–357.40		
Solid phase $\Delta_f H°$ =	–369.60	–369.40	–0.20	75CAR/LAY

TABLE 22. Peroxides (7) – Continued

Diacetyl peroxide; Diethanoyl peroxide $C_4H_6O_4$
(2×C–(H)$_3$(CO))+(2×CO–(C)(O))+(2×O–(CO)(O))

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =		–535.00		
Liquid phase $\Delta_f H°$ =	–535.30	–573.96	38.66	57JAF/PRO

Dipropionyl peroxide; Dipropanoyl peroxide $C_6H_{10}O_4$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(CO)(C))+(2×CO–(C)(O))+
(2×O–(CO)(O))

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =		–578.68		
Liquid phase $\Delta_f H°$ =	–620.10	–622.24	2.14	57JAF/PRO

Dibutyryl peroxide; Dibutanoyl peroxide $C_8H_{14}O_4$
(2×C–(H)$_3$(C))+(4×C–(H)$_2$(CO)(C))+(2×CO–(C)(O))+
(2×O–(CO)(O))

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =		–622.36		
Liquid phase $\Delta_f H°$ =	–673.60	–670.52	–3.08	57JAF/PRO

TABLE 23. Hydroperoxides (9)

***tert*-Butyl hydroperoxide** $C_4H_{10}O_2$

(3 × C–(H)$_3$(C)) + (1 × C–(O)(C)$_3$ (alcohols,peroxides)) + (1 × O–(C)(O)) + (1 × O–(H)(O)) + (3 × –CH_3 corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =	−245.90	−246.97	1.07	64KOZ/RAB
Liquid phase $\Delta_f H°$ =	−293.60	−292.38	−1.22	64KOZ/RAB
Solid phase $\Delta_f H°$ =		−301.02		

***n*-Hexyl-1-hydroperoxide** $C_6H_{14}O_2$

(1 × O–(H)(O)) + (1 × O–(C)(O)) + (1 × C–(H)$_2$(O)(C)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_3$(C))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−250.69		
Liquid phase $\Delta_f H°$ =	−299.62	−311.58	11.96	56PRI/MUL
Solid phase $\Delta_f H°$ =		−332.88		

***n*-Hexyl-2-hydroperoxide** $C_6H_{14}O_2$

(2 × C–(H)$_3$(C)) + (3 × C–(H)$_2$(C)$_2$) + (1 × C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (1 × O–(C)(O)) + (1 × O–(H)(O)) + (1 × –CH_3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−267.78		
Liquid phase $\Delta_f H°$ =	−310.12	−327.44	17.32	56PRI/MUL
Solid phase $\Delta_f H°$ =		−348.63		

TABLE 23. Hydroperoxides (9) – Continued

***n*-Hexyl-3-hydroperoxide** $C_6H_{14}O_2$

(2 × C–(H)$_3$(C)) + (3 × C–(H)$_2$(C)$_2$) + (1 × C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (1 × O–(C)(O)) + (1 × O–(H)(O))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−265.52		
Liquid phase $\Delta_f H°$ =	−305.10	−325.26	20.16	56PRI/MUL
Solid phase $\Delta_f H°$ =		−346.29		

***n*-Heptyl-1-hydroperoxide** $C_7H_{16}O_2$

(1 × C–(H)$_3$(C)) + (5 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(O)(C)) + (1 × O–(C)(O)) + (1 × O–(H)(O))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−271.32		
Liquid phase $\Delta_f H°$ =	−343.00	−337.31	−5.69	56PRI/MUL
Solid phase $\Delta_f H°$ =		−362.29		

***n*-Heptyl-2-hydroperoxide** $C_7H_{16}O_2$

(2 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (1 × O–(C)(O)) + (1 × O–(H)(O)) + (1 × –CH_3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−288.41		
Liquid phase $\Delta_f H°$ =	−346.20	−353.17	6.97	56PRI/MUL
Solid phase $\Delta_f H°$ =		−378.04		

TABLE 23. Hydroperoxides (9) — Continued

n-Heptyl-3-hydroperoxide $C_7H_{16}O_2$

(2 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (1 × O–(C)(O)) + (1 × O–(H)(O))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−286.15		
Liquid phase $\Delta_f H°$ =	−346.81	−350.99	4.18	56PRI/MUL
Solid phase $\Delta_f H°$ =		−375.70		

n-Heptyl-4-hydroperoxide $C_7H_{16}O_2$

(2 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (1 × O–(C)(O)) + (1 × O–(H)(O))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−286.15		
Liquid phase $\Delta_f H°$ =	−333.80	−350.99	17.19	56PRI/MUL
Solid phase $\Delta_f H°$ =		−375.70		

1-Methyl-1-phenylethyl hydroperoxide; Cumyl hydroperoxide $C_9H_{12}O_2$

(5 × C$_B$–(H)(C$_B$)$_2$) + (1 × C$_B$–(C)(C$_B$)$_2$) + (1 × C–(C)$_2$(O)(C$_B$)) + (2 × C–(H)$_3$(C)) + (2 × –CH$_3$ corr (quaternary)) + (1 × O–(C)(O)) + (1 × O–(H)(O))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =	−78.40	−78.66	0.26	64KOZ/RAB
Liquid phase $\Delta_f H°$ =		−143.49		
Solid phase $\Delta_f H°$ =	−161.80	−161.83	0.03	64KOZ/RAB

TABLE 24. Peroxyacids (8)

Perbenzoic acid $C_7H_6O_3$

(1 × C$_B$–(CO)(C$_B$)$_2$) + (1 × CO–(O)(C$_B$)) + (1 × O–(CO)(O)) + (1 × O–(H)(O)) + (5 × C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−200.71		
Liquid phase $\Delta_f H°$ =		−280.45		
Solid phase $\Delta_f H°$ =	−367.00	−290.00	−77.00	54BRI/DEC

Perdodecanoic acid; Peroxylauric acid $C_{12}H_{24}O_3$

(1 × C–(H)$_3$(C)) + (9 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)(O)) + (1 × O–(CO)(O)) + (1 × O–(H)(O))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−547.27		
Liquid phase $\Delta_f H°$ =		−644.44		
Solid phase $\Delta_f H°$ =	−680.30	−678.73	−1.57	64SWA/SIL

Pertetradecanoic acid; Peroxymyristic acid $C_{14}H_{28}O_3$

(1 × C–(H)$_3$(C)) + (11 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)(O)) + (1 × O–(CO)(O)) + (1 × O–(H)(O))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−588.53		
Liquid phase $\Delta_f H°$ =		−695.90		
Solid phase $\Delta_f H°$ =	−749.90	−737.55	−12.35	64SWA/SIL

TABLE 24. Peroxyacids (8) – Continued

Perhexadecanoic acid; Peroxypalmitic acid $C_{16}H_{32}O_3$
(1 × C–(H)$_3$(C)) + (13 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)(O)) + (1 × O–(CO)(O)) + (1 × O–(H)(O))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−629.79		
Liquid phase $\Delta_f H°$ =		−747.36		
Solid phase $\Delta_f H°$ =	−801.90	−796.37	−5.53	64SWA/SIL

Peroctadecanoic acid; Peroxystearic acid $C_{18}H_{36}O_3$
(1 × C–(H)$_3$(C)) + (15 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)(O)) + (1 × O–(CO)(O)) + (1 × O–(H)(O))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−671.05		
Liquid phase $\Delta_f H°$ =		−798.82		
Solid phase $\Delta_f H°$ =	−857.30	−855.19	−2.11	64SWA/SIL

***tert*-Butyl perdecanoate** $C_{14}H_{28}O_3$

(4 × C–(H)$_3$(C)) + (1 × O–(C)(O)) + (1 × O–(CO)(O)) + (1 × CO–(C)(O)) + (1 × C–(H)$_2$(CO)(C)) + (7 × C–(H)$_2$(C)$_2$) + (3 × –CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−594.96		
Liquid phase $\Delta_f H°$ =	−688.80	−670.73	−18.07	64SWA/SIL

TABLE 24. Peroxyacids (8) – Continued

***tert*-Butyl perdodecanoate** $C_{16}H_{32}O_3$
(4 × C–(H)$_3$(C)) + (1 × C–(O)(C)$_3$ (ethers,esters)) + (1 × O–(C)(O)) + (1 × O–(CO)(O)) + (1 × CO–(C)(O)) + (1 × C–(H)$_2$(CO)(C)) + (9 × C–(H)$_2$(C)$_2$) + (3 × –CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−626.72		
Liquid phase $\Delta_f H°$ =	−738.30	−721.40	−16.90	64SWA/SIL

***tert*-Butyl pertetradecanoate** $C_{18}H_{36}O_3$
(4 × C–(H)$_3$(C)) + (1 × C–(O)(C)$_3$ (ethers,esters)) + (1 × O–(C)(O)) + (1 × O–(CO)(O)) + (1 × CO–(C)(O)) + (1 × C–(H)$_2$(CO)(C)) + (11 × C–(H)$_2$(C)$_2$) + (3 × –CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =		−667.98		
Liquid phase $\Delta_f H°$ =	−795.80	−772.86	−22.94	64SWA/SIL

TABLE 25. Carbonates (3)

Diethyl carbonate $C_5H_{10}O_3$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(O)(C))+(2×O–(C)(CO))+(1×CO–(O)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−637.90	−639.94	2.04	72MAN
Liquid phase				
$\Delta_fH°$ =	−681.50	−680.86	−0.64	72MAN2
$C_p°$ =	210.90	210.86	0.04	34KOL/UDO
Solid phase				
$\Delta_fH°$ =		−703.68		
$C_p°$ =		170.99		
$S°$ =		144.10		
$\Delta_fS°$ =		−845.02		
$\Delta_fG°$ =		−451.74		
$\ln K_f$ =		182.23		

Diphenyl carbonate $C_{13}H_{10}O_3$
(10×C$_B$–(H)(C$_B$)$_2$)+(2×C$_B$–(O)(C$_B$)$_2$)+(2×O–(C$_B$)(CO))+(1×CO–(O)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−311.30	−317.28	5.98	71CAR/FIN
Liquid phase				
$\Delta_fH°$ =	−377.70	−382.62	4.92	71CAR/FIN
Solid phase				
$\Delta_fH°$ =	−401.20	−395.70	−5.50	58SIN/HIL
$C_p°$ =	263.13	263.13	0.00	58SIN/HIL
$S°$ =	278.40	278.40	0.00	58SIN/HIL
$\Delta_fS°$ =		−756.64		
$\Delta_fG°$ =		−170.11		
$\ln K_f$ =		68.62		

1,3-Dioxolan-2-one; Ethylene carbonate $C_3H_4O_3$
(2×C–(H)$_2$(O)(C))+(2×O–(C)(CO))+(1×CO–(O)$_2$)+(1×Ethyl carbonate rsc)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−586.30	−586.30	0.00	83CAL

TABLE 26. Amines (50)

Aminomethane; Methyl amine CH_5N
(1×C–(H)$_3$(C))+(1×N–(H)$_2$(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−23.01	−23.01	0.00	37AST/SIL
$C_p°$ =	50.08	50.08	0.00	69STU/WES
$S°$ =	242.59	242.59	0.00	69STU/WES
$\Delta_fS°$ =		−185.33		
$\Delta_fG°$ =		32.25		
$\ln K_f$ =		−13.01		
Liquid phase				
$\Delta_fH°$ =	−47.27	−47.28	0.01	90CHA/GAD
$C_p°$ =	102.09	99.07	3.02	90CHA/GAD
$S°$ =	150.43	155.01	−4.58	90CHA/GAD
$\Delta_fS°$ =		−272.91		
$\Delta_fG°$ =		34.09		
$\ln K_f$ =		−13.75		

Aminoethane; Ethyl amine C_2H_7N
(1×C–(H)$_3$(C))+(1×N–(H)$_2$(C))+(1×C–(H)$_2$(C)(N)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−47.47	−51.31	3.84	90CHA/GAD
$C_p°$ =	72.63	72.76	−0.13	69STU/WES
$S°$ =	284.85	284.85	0.00	69STU/WES
$\Delta_fS°$ =		−279.38		
$\Delta_fG°$ =		31.99		
$\ln K_f$ =		−12.90		
Liquid phase				
$\Delta_fH°$ =	−74.13	−78.08	3.95	90CHA/GAD
$C_p°$ =		129.49		
$S°$ =		187.39		
$\Delta_fS°$ =		−376.84		
$\Delta_fG°$ =		34.27		
$\ln K_f$ =		−13.83		

1-Aminopropane; *n*-Propyl amine C_3H_9N
(1×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(N))+(1×N–(H)$_2$(C)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−70.10	−71.94	1.84	90CHA/GAD
$C_p°$ =	95.77	95.65	0.12	69STU/WES
$S°$ =	324.18	324.01	0.17	69STU/WES
$\Delta_fS°$ =		−376.53		
$\Delta_fG°$ =		40.32		
$\ln K_f$ =		−16.27		

TABLE 26. Amines (50) – Continued

1-Aminopropane; *n*-Propyl amine (Continued) C_3H_9N
$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(N))+(1\times N-(H)_2(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Liquid phase				
Δ_fH° =	−101.47	−103.81	2.34	90CHA/GAD
C_p° =	162.54	159.91	2.63	90CHA/GAD
S° =	227.44	219.77	7.67	90CHA/GAD
Δ_fS° =		−480.77		
Δ_fG° =		39.53		
$\ln K_f$ =		−15.95		

1-Aminobutane; *n*-Butyl amine $C_4H_{11}N$
$(1\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(N))+(1\times N-(H)_2(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−92.00	−92.57	0.57	69WAD
C_p° =	118.53	118.54	−0.01	69STU/WES
S° =	363.00	363.17	−0.17	69STU/WES
Δ_fS° =		−473.68		
Δ_fG° =		48.66		
$\ln K_f$ =		−19.63		
Liquid phase				
Δ_fH° =	−127.70	−129.54	1.84	59EVA/FAI
C_p° =	188.00	190.33	−2.33	71KON/WAD
S° =		252.15		
Δ_fS° =		−584.70		
Δ_fG° =		44.79		
$\ln K_f$ =		−18.07		

1-Aminopentane; *n*-Pentyl amine $C_5H_{13}N$
$(1\times C-(H)_3(C))+(3\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(N))+(1\times N-(H)_2(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−113.20		
C_p° =		141.43		
S° =		402.33		
Δ_fS° =		−570.84		
Δ_fG° =		56.99		
$\ln K_f$ =		−22.99		
Liquid phase				
Δ_fH° =		−155.27		
C_p° =	218.00	220.75	−2.75	71KON/WAD
S° =		284.53		
Δ_fS° =		−688.63		
Δ_fG° =		50.05		
$\ln K_f$ =		−20.19		

TABLE 26. Amines (50) – Continued

1-Aminohexane; *n*-Hexyl amine $C_6H_{15}N$
$(1\times C-(H)_3(C))+(4\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(N))+(1\times N-(H)_2(C))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−133.83		
C_p° =		164.32		
S° =		441.49		
Δ_fS° =		−667.99		
Δ_fG° =		65.33		
$\ln K_f$ =		−26.35		
Liquid phase				
Δ_fH° =		−181.00		
C_p° =	252.00	251.17	0.83	71KON/WAD
S° =		316.91		
Δ_fS° =		−792.56		
Δ_fG° =		55.30		
$\ln K_f$ =		−22.31		

2-Methylpropyl amine; Isobutyl amine $C_4H_{11}N$
$(2\times C-(H)_3(C))+(1\times C-(H)(C)_3)+(2\times -CH_3 \text{ corr (tertiary)})+(1\times C-(H)_2(C)(N))+(1\times N-(H)_2(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−98.80	−99.26	0.46	69WAD
C_p° =		118.57		
Liquid phase				
Δ_fH° =	−132.60	−134.82	2.22	70GOO/MOO
C_p° =	194.00	187.35	6.65	71KON/WAD
S° =		246.80		
Δ_fS° =		−590.05		
Δ_fG° =		41.10		
$\ln K_f$ =		−16.58		

1,2-Ethanediamine; Ethylenediamine $C_2H_8N_2$
$(2\times C-(H)_2(C)(N))+(2\times N-(H)_2(C))$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−17.60	−18.10	0.50	69WAD
C_p° =		94.06		
S° =	321.80	309.29	12.51	75MES/FIN
Δ_fS° =		−415.98		
Δ_fG° =		105.92		
$\ln K_f$ =		−42.73		

TABLE 26. Amines (50) — Continued

1,2-Ethanediamine; Ethylenediamine (Continued) $C_2H_8N_2$
(2×C–(H)$_2$(C)(N)) + (2×N–(H)$_2$(C)), σ = 18

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−63.00	−60.94	−2.06	70GOO/MOO
$C_p°$ =	172.59	186.02	−13.43	75MES/FIN
$S°$ =	202.42	208.18	−5.76	75MES/FIN
$\Delta_f S°$ =		−517.08		
$\Delta_f G°$ =		93.23		
lnK_f =		−37.61		

1,2-Propanediamine $C_3H_{10}N_2$
(1×C–(H)$_2$(C)(N)) + (2×N–(H)$_2$(C)) + (1×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(N)) + (1×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−53.60	−51.02	−2.58	69WAD
$C_p°$ =		115.73		
Liquid phase				
$\Delta_f H°$ =	−97.80	−94.58	−3.22	70GOO/MOO
$C_p°$ =		220.36		
$S°$ =		239.10		
$\Delta_f S°$ =		−622.47		
$\Delta_f G°$ =		91.01		
lnK_f =		−36.71		

1,2-Butanediamine $C_4H_{12}N_2$
(2×N–(H)$_2$(C)) + (1×C–(H)$_2$(C)(N)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(N))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−74.00	−69.39	−4.61	70GOO/MOO
$C_p°$ =		138.62		
Liquid phase				
$\Delta_f H°$ =	−120.20	−118.13	−2.07	70GOO/MOO
$C_p°$ =		250.78		
$S°$ =		271.48		
$\Delta_f S°$ =		−726.41		
$\Delta_f G°$ =		98.45		
lnK_f =		−39.71		

TABLE 26. Amines (50) — Continued

2-Aminopropane; Isopropyl amine C_3H_9N
(1×N–(H)$_2$(C)) + (2×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(N)) + (2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−83.70	−86.49	2.79	90CHA/GAD
$C_p°$ =		94.43		
Liquid phase				
$\Delta_f H°$ =	−112.30	−113.90	1.60	90CHA/GAD
$C_p°$ =	163.85	163.83	0.02	72FIN/MES
$S°$ =	218.32	218.31	0.01	72FIN/MES
$\Delta_f S°$ =		−482.23		
$\Delta_f G°$ =		29.88		
lnK_f =		−12.05		

2-Aminobutane; sec-Butyl amine $C_4H_{11}N$
(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(N)) + (1×–CH$_3$ corr (tertiary)) + (1×N–(H)$_2$(C)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−104.90	−104.86	−0.04	69WAD
$C_p°$ =	117.11	117.32	−0.21	69STU/WES
$S°$ =	351.04	342.14	8.90	69STU/WES
$\Delta_f S°$ =		−494.71		
$\Delta_f G°$ =		42.64		
lnK_f =		−17.20		
Liquid phase				
$\Delta_f H°$ =	−137.49	−137.45	−0.04	59EVA/FAI
$C_p°$ =		194.25		
$S°$ =		250.69		
$\Delta_f S°$ =		−586.16		
$\Delta_f G°$ =		37.31		
lnK_f =		−15.05		

2-Amino-2-methylpropane; tert-Butyl amine $C_4H_{11}N$
(3×C–(H)$_3$(C)) + (1×N–(H)$_2$(C)) + (1×C–(C)$_3$(N)) + (3×–CH$_3$ corr (quaternary)), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−121.00	−120.92	−0.08	69WAD
$C_p°$ =	119.96	119.95	0.01	69STU/WES
$S°$ =	337.10	317.23	19.87	69STU/WES
$\Delta_f S°$ =		−519.62		
$\Delta_f G°$ =		34.00		
lnK_f =		−13.72		

TABLE 26. Amines (50) – Continued

2-Amino-2-methylpropane; tert-Butyl amine (Continued) $C_4H_{11}N$
(3×C–(H)$_3$(C)) + (1×N–(H)$_2$(C)) + (1×C–(C)$_3$(N)) + (3×–CH$_3$ corr (quaternary)), σ = 81

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−150.60	−150.57	−0.03	67SMI/GOO
$C_p°$ =	191.71	191.69	0.02	72FIN/MES
$S°$ =	233.63	233.62	0.01	72FIN/MES
$\Delta_fS°$ =		−603.23		
$\Delta_fG°$ =		29.28		
$\ln K_f$ =		−11.81		

2-Methyl-1,2-propanediamine $C_4H_{12}N_2$
(2×N–(H)$_2$(C)) + (1×C–(H)$_2$(C)(N)) + (2×C–(H)$_3$(C)) + (2×–CH$_3$ corr (quaternary)) + (1×C–(C)$_3$(N))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−90.20	−83.15	−7.05	70GOO/MOO
$C_p°$ =		141.25		
Liquid phase				
$\Delta_fH°$ =	−133.90	−129.04	−4.86	70GOO/MOO
$C_p°$ =		248.22		
$S°$ =		254.41		
$\Delta_fS°$ =		−743.48		
$\Delta_fG°$ =		92.63		
$\ln K_f$ =		−37.37		

Dimethylamine C_2H_7N
(2×C–(H)$_3$(C)) + (1×N–(H)(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−18.50	−16.97	−1.53	39AST/EID
$C_p°$ =	69.04	63.74	5.30	69STU/WES
$S°$ =	272.96	270.33	2.63	69STU/WES
$\Delta_fS°$ =		−293.90		
$\Delta_fG°$ =		70.66		
$\ln K_f$ =		−28.50		
Liquid phase				
$\Delta_fH°$ =	−43.90	−43.72	−0.18	58JAF
$C_p°$ =		132.33		
$S°$ =		198.69		
$\Delta_fS°$ =		−365.54		
$\Delta_fG°$ =		65.27		
$\ln K_f$ =		−26.33		

TABLE 26. Amines (50) – Continued

Diethylamine $C_4H_{11}N$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)(N)) + (1×N–(H)(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−72.50	−73.57	1.07	69WAD
$C_p°$ =	103.81	109.10	−5.29	69STU/WES
$S°$ =	352.21	354.85	−2.64	69STU/WES
$\Delta_fS°$ =		−482.00		
$\Delta_fG°$ =		70.14		
$\ln K_f$ =		−28.29		
Liquid phase				
$\Delta_fH°$ =	−103.70	−105.32	1.62	58JAF
$C_p°$ =		193.17		
$S°$ =		263.45		
$\Delta_fS°$ =		−573.40		
$\Delta_fG°$ =		65.64		
$\ln K_f$ =		−26.48		

Di-*n*-propylamine $C_6H_{15}N$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(C)(N)) + (1×N–(H)(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−116.10	−114.83	−1.27	69WAD
$C_p°$ =		154.88		
$S°$ =		433.17		
$\Delta_fS°$ =		−676.30		
$\Delta_fG°$ =		86.81		
$\ln K_f$ =		−35.02		
Liquid phase				
$\Delta_fH°$ =	−156.11	−156.78	0.67	71LEB/KAT
$C_p°$ =		254.01		
$S°$ =		328.21		
$\Delta_fS°$ =		−781.26		
$\Delta_fG°$ =		76.15		
$\ln K_f$ =		−30.72		

Diisopropylamine $C_6H_{15}N$
(4×C–(H)$_3$(C)) + (2×C–(H)(C)$_2$(N)) + (4×–CH$_3$ corr (tertiary)) + (1×N–(H)(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−144.00	−143.93	−0.07	69WAD
$C_p°$ =		152.44		

TABLE 26. Amines (50) — Continued

Diisopropylamine $C_6H_{15}N$

$(4\times C\text{-}(H)_3(C)) + (2\times C\text{-}(H)(C)_2(N)) + (4\times\text{-}CH_3\text{ corr (tertiary)}) + (1\times N\text{-}(H)(C)_2)$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H^\circ$ =	−178.50	−176.96	−1.54	71LEB/KAT
C_p° =		261.85		
S° =		325.29		
$\Delta_f S^\circ$ =		−784.18		
$\Delta_f G^\circ$ =		56.84		
$\ln K_f$ =		−22.93		

Di-*n*-butylamine $C_8H_{19}N$

$(2\times C\text{-}(H)_3(C)) + (4\times C\text{-}(H)_2(C)_2) + (2\times C\text{-}(H)_2(C)(N)) + (1\times N\text{-}(H)(C)_2)$, $\sigma = 9$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−156.61	−156.09	−0.52	69WAD
C_p° =		200.66		
S° =		511.49		
$\Delta_f S^\circ$ =		−870.60		
$\Delta_f G^\circ$ =		103.48		
$\ln K_f$ =		−41.74		
Liquid phase				
$\Delta_f H^\circ$ =	−206.00	−208.24	2.24	71LEB/KAT
C_p° =		314.85		
S° =		392.97		
$\Delta_f S^\circ$ =		−989.12		
$\Delta_f G^\circ$ =		86.67		
$\ln K_f$ =		−34.96		

Diisobutylamine $C_8H_{19}N$

$(4\times C\text{-}(H)_3(C)) + (2\times C\text{-}(H)(C)_3) + (4\times\text{-}CH_3\text{ corr (tertiary)}) + (2\times C\text{-}(H)_2(C)(N)) + (1\times N\text{-}(H)(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−179.20	−169.47	−9.73	71LEB/KAT
C_p° =		200.72		
Liquid phase				
$\Delta_f H^\circ$ =	−218.50	−218.80	0.30	71LEB/KAT
C_p° =		308.89		
S° =		382.27		
$\Delta_f S^\circ$ =		−999.82		
$\Delta_f G^\circ$ =		79.30		
$\ln K_f$ =		−31.99		

TABLE 26. Amines (50) — Continued

***n*-Butylisobutylamine** $C_8H_{19}N$

$(3\times C\text{-}(H)_3(C)) + (2\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)(C)_3) + (2\times\text{-}CH_3\text{ corr (tertiary)}) + (2\times C\text{-}(H)_2(C)(N)) + (1\times N\text{-}(H)(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−171.00	−162.78	−8.22	62BED/EDM
C_p° =		200.69		
Liquid phase				
$\Delta_f H^\circ$ =	−215.90	−213.52	−2.38	62BED/EDM
C_p° =		311.87		
S° =		387.62		
$\Delta_f S^\circ$ =		−994.47		
$\Delta_f G^\circ$ =		82.98		
$\ln K_f$ =		−33.47		

Trimethylamine C_3H_9N

$(3\times C\text{-}(H)_3(C)) + (1\times N\text{-}(C)_3) + (3\times\text{-}CH_3\text{ corr (quaternary)})$, $\sigma = 81$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−23.70	−23.96	0.26	44AST/SAG
C_p° =	91.76	92.29	−0.53	44AST/SAG
S° =	288.78	283.71	5.07	44AST/SAG
$\Delta_f S^\circ$ =		−416.83		
$\Delta_f G^\circ$ =		100.32		
$\ln K_f$ =		−40.47		
Liquid phase				
$\Delta_f H^\circ$ =	−45.70	−44.00	−1.70	58JAF
C_p° =		135.55		
S° =		211.28		
$\Delta_f S^\circ$ =		−489.26		
$\Delta_f G^\circ$ =		101.87		
$\ln K_f$ =		−41.09		

Triethylamine $C_6H_{15}N$

$(3\times C\text{-}(H)_3(C)) + (3\times C\text{-}(H)_2(C)(N)) + (1\times N\text{-}(C)_3)$, $\sigma = 81$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−92.80	−95.18	2.38	69WAD
C_p° =	160.92	160.33	0.59	69STU/WES
S° =	405.43	410.49	−5.06	69STU/WES
$\Delta_f S^\circ$ =		−698.98		
$\Delta_f G^\circ$ =		113.22		
$\ln K_f$ =		−45.67		

TABLE 26. Amines (50) – Continued

Triethylamine (Continued) $C_6H_{15}N$
$(3\times C\text{-}(H)_3(C)) + (3\times C\text{-}(H)_2(C)(N)) + (1\times N\text{-}(C)_3)$, $\sigma = 81$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H^\circ =$	−127.70	−123.23	−4.47	66LEB
$C_p^\circ =$		226.81		
$S^\circ =$		308.42		
$\Delta_f S^\circ =$		−801.05		
$\Delta_f G^\circ =$		115.60		
$\ln K_f =$		−46.63		

Tri-*n*-propylamine $C_9H_{21}N$
$(3\times C\text{-}(H)_3(C)) + (3\times C\text{-}(H)_2(C)_2) + (3\times C\text{-}(H)_2(C)(N)) + (1\times N\text{-}(C)_3)$, $\sigma = 81$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ =$	−161.00	−157.07	−3.93	69WAD
$C_p^\circ =$		229.00		
$S^\circ =$		527.97		
$\Delta_f S^\circ =$		−990.43		
$\Delta_f G^\circ =$		138.23		
$\ln K_f =$		−55.76		
Liquid phase				
$\Delta_f H^\circ =$	−207.11	−200.42	−6.69	66LEB
$C_p^\circ =$		318.07		
$S^\circ =$		405.56		
$\Delta_f S^\circ =$		−1112.85		
$\Delta_f G^\circ =$		131.37		
$\ln K_f =$		−53.00		

Tri-*n*-butylamine $C_{12}H_{27}N$
$(3\times C\text{-}(H)_3(C)) + (6\times C\text{-}(H)_2(C)_2) + (3\times C\text{-}(H)_2(C)(N)) + (1\times N\text{-}(C)_3)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ =$		−218.96		
$C_p^\circ =$		297.67		
Liquid phase				
$\Delta_f H^\circ =$	−281.60	−277.61	−3.99	66LEB
$C_p^\circ =$		409.33		
$S^\circ =$		502.70		
$\Delta_f S^\circ =$		−1424.64		
$\Delta_f G^\circ =$		147.15		
$\ln K_f =$		−59.36		

TABLE 26. Amines (50) – Continued

Tri-*n*-hexylamine $C_{18}H_{39}N$
$(3\times C\text{-}(H)_3(C)) + (12\times C\text{-}(H)_2(C)_2) + (3\times C\text{-}(H)_2(C)(N)) + (1\times N\text{-}(C)_3)$, $\sigma = 81$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ =$		−342.74		
$C_p^\circ =$		435.01		
$S^\circ =$		880.41		
$\Delta_f S^\circ =$		−1864.79		
$\Delta_f G^\circ =$		213.25		
$\ln K_f =$		−86.02		
Liquid phase				
$\Delta_f H^\circ =$	−433.00	−431.99	−1.01	66LEB
$C_p^\circ =$		591.85		
$S^\circ =$		696.98		
$\Delta_f S^\circ =$		−2048.22		
$\Delta_f G^\circ =$		178.69		
$\ln K_f =$		−72.08		

Tri-*n*-octylamine $C_{24}H_{51}N$
$(3\times C\text{-}(H)_3(C)) + (18\times C\text{-}(H)_2(C)_2) + (3\times C\text{-}(H)_2(C)(N)) + (1\times N\text{-}(C)_3)$, $\sigma = 81$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ =$		−466.52		
$C_p^\circ =$		572.35		
$S^\circ =$		1115.37		
$\Delta_f S^\circ =$		−2447.70		
$\Delta_f G^\circ =$		263.26		
$\ln K_f =$		−106.20		
Liquid phase				
$\Delta_f H^\circ =$	−585.01	−586.37	1.36	66LEB
$C_p^\circ =$		774.37		
$S^\circ =$		891.26		
$\Delta_f S^\circ =$		−2671.81		
$\Delta_f G^\circ =$		210.23		
$\ln K_f =$		−84.81		

Tri-*n*-nonylamine $C_{27}H_{57}N$
$(3\times C\text{-}(H)_3(C)) + (21\times C\text{-}(H)_2(C)_2) + (3\times C\text{-}(H)_2(C)(N)) + (1\times N\text{-}(C)_3)$, $\sigma = 81$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ =$		−528.41		
$C_p^\circ =$		641.02		
$S^\circ =$		1232.85		
$\Delta_f S^\circ =$		−2739.15		
$\Delta_f G^\circ =$		288.27		
$\ln K_f =$		−116.29		

TABLE 26. Amines (50) — Continued

Tri-*n*-nonylamine (Continued) $C_{27}H_{57}N$

(3×C–(H)$_3$(C)) + (21×C–(H)$_2$(C)$_2$) + (3×C–(H)$_2$(C)(N)) + (1×N–(C)$_3$), σ = 81

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−661.62	−663.56	1.94	66LEB
$C_p°$ =		865.63		
$S°$ =		988.40		
$\Delta_fS°$ =		−2983.60		
$\Delta_fG°$ =		226.00		
$\ln K_f$ =		−91.17		

Tri-*n*-decylamine $C_{30}H_{63}N$

(3×C–(H)$_3$(C)) + (24×C–(H)$_2$(C)$_2$) + (3×C–(H)$_2$(C)(N)) + (1×N–(C)$_3$), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−590.30		
$C_p°$ =		709.69		
$S°$ =		1350.33		
$\Delta_fS°$ =		−3030.60		
$\Delta_fG°$ =		313.27		
$\ln K_f$ =		−126.37		
Liquid phase				
$\Delta_fH°$ =	−738.02	−740.75	2.73	66LEB
$C_p°$ =		956.89		
$S°$ =		1085.54		
$\Delta_fS°$ =		−3295.40		
$\Delta_fG°$ =		241.77		
$\ln K_f$ =		−97.53		

Triphenylamine $C_{18}H_{15}N$

(15×C$_B$–(H)(C$_B$)$_2$) + (3×C$_B$–(N)) + (1×N–(C$_B$)$_3$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	326.77	326.40	0.37	78STE
Liquid phase				
$\Delta_fH°$ =	247.72	248.70	−0.98	78STE
Solid phase				
$\Delta_fH°$ =	234.72	234.70	0.02	78STE
$C_p°$ =	301.70	301.95	−0.25	78STE

TABLE 26. Amines (50) — Continued

Tribenzylamine $C_{21}H_{21}N$

(15×C$_B$–(H)(C$_B$)$_2$) + (3×C$_B$–(C)(C$_B$)$_2$) + (3×C–(H)$_2$(C$_B$)(N)) + (1×N–(C)$_3$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		322.15		
Liquid phase				
$\Delta_fH°$ =		213.61		
$C_p°$ =		455.98		
Solid phase				
$\Delta_fH°$ =	140.70	140.72	−0.02	56TAV/LAM

Cyclopropylamine C_3H_7N

(2×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(N)) + (1×N–(H)$_2$(C)) + (1×Cyclopropane rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	77.00	76.44	0.56	71GOO/MOO
$C_p°$ =		76.02		
Liquid phase				
$\Delta_fH°$ =	45.80	45.80	0.00	71GOO/MOO
$C_p°$ =		123.18		

Cyclobutylamine C_4H_9N

(3×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(N)) + (1×N–(H)$_2$(C)) + (1×Cyclobutane rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	41.20	51.55	−10.35	75GOO/MES
$C_p°$ =		92.30		
Liquid phase				
$\Delta_fH°$ =	5.60	15.13	−9.53	75GOO/MES
$C_p°$ =		171.45		
$S°$ =		200.33		
$\Delta_fS°$ =		−505.95		
$\Delta_fG°$ =		165.98		
$\ln K_f$ =		−66.95		

TABLE 26. Amines (50) — Continued

Cyclopentylamine $C_5H_{11}N$

(4×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(N)) + (1×N–(H)$_2$(C)) + (1×Cyclopentane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−54.90	−60.42	5.52	75GOO/MES
$C_p°$ =		106.66		
Liquid phase				
$\Delta_fH°$ =	−95.10	−93.65	−1.45	75GOO/MES
$C_p°$ =	181.21	189.23	−8.02	81FIN/MES
$S°$ =	241.04	237.88	3.16	81FIN/MES
$\Delta_fS°$ =		−604.71		
$\Delta_fG°$ =		86.64		
$\ln K_f$ =		−34.95		

Cyclohexylamine $C_6H_{13}N$

(5×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(N)) + (1×N–(H)$_2$(C)) + (1×Cyclohexane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−104.90	−100.99	−3.91	79STE
$C_p°$ =		134.60		
Liquid phase				
$\Delta_fH°$ =	−147.70	−145.03	−2.67	79STE
$C_p°$ =		216.76		
$S°$ =		238.71		
$\Delta_fS°$ =		−740.19		
$\Delta_fG°$ =		75.66		
$\ln K_f$ =		−30.52		

Benzenamine; Aniline C_6H_7N

(5×C$_B$–(H)(C$_B$)$_2$) + (1×N–(H)$_2$(C$_B$)) + (1×C$_B$–(N)(C$_B$)$_2$), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	87.46	87.00	0.46	90CHA/GAD
$C_p°$ =	108.41	108.47	−0.06	69STU/WES
$S°$ =	319.16	319.16	0.00	69STU/WES
$\Delta_fS°$ =		−268.03		
$\Delta_fG°$ =		166.91		
$\ln K_f$ =		−67.33		
Liquid phase				
$\Delta_fH°$ =	31.63	31.30	0.33	90CHA/GAD
$C_p°$ =	191.92	191.01	0.91	90CHA/GAD
$S°$ =	189.55	191.63	−2.08	90CHA/GAD
$\Delta_fS°$ =		−395.56		
$\Delta_fG°$ =		149.24		
$\ln K_f$ =		−60.20		

TABLE 26. Amines (50) — Continued

2-Methylaniline C_7H_9N

(4×C$_B$–(H)(C$_B$)$_2$) + (1×C$_B$–(C)(C$_B$)$_2$) + (1×C$_B$–(N)(C$_B$)$_2$) + (1×N–(H)$_2$(C$_B$)) + (1×C–(H)$_3$(C)) + (1×*ortho* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	56.40	55.83	0.57	90CHA/GAD
$C_p°$ =		136.74		
Liquid phase				
$\Delta_fH°$ =	−6.30	−2.05	−4.25	90CHA/GAD
$C_p°$ =	211.29	218.41	−7.12	1881REI
$S°$ =		226.56		
$\Delta_fS°$ =		−496.94		
$\Delta_fG°$ =		146.11		
$\ln K_f$ =		−58.94		

3-Methylaniline C_7H_9N

(4×C$_B$–(H)(C$_B$)$_2$) + (1×C$_B$–(C)(C$_B$)$_2$) + (1×C$_B$–(N)(C$_B$)$_2$) + (1×N–(H)$_2$(C$_B$)) + (1×C–(H)$_3$(C)) + (1×*meta* corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	54.60	53.94	0.66	90CHA/GAD
$C_p°$ =		131.05		
Liquid phase				
$\Delta_fH°$ =	−8.10	−5.31	−2.79	90CHA/GAD
$C_p°$ =	216.73	214.91	1.82	34KOL/UDO
$S°$ =		226.56		
$\Delta_fS°$ =		−496.94		
$\Delta_fG°$ =		142.85		
$\ln K_f$ =		−57.63		

4-Methylaniline C_7H_9N

(4×C$_B$–(H)(C$_B$)$_2$) + (1×C$_B$–(C)(C$_B$)$_2$) + (1×C–(H)$_3$(C)) + (1×C$_B$–(N)(C$_B$)$_2$) + (1×N–(H)$_2$(C$_B$))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	55.30	54.57	0.73	90CHA/GAD
$C_p°$ =		130.34		
Liquid phase				
$\Delta_fH°$ =		−5.31		
$C_p°$ =		214.91		
$S°$ =		226.56		
$\Delta_fS°$ =		−496.94		
$\Delta_fG°$ =		142.85		
$\ln K_f$ =		−57.63		

TABLE 26. Amines (50) — Continued

N-Methylaniline C_7H_9N

$(5 \times C_B-(H)(C_B)_2) + (1 \times C-(H)_3(C)) + (1 \times N-(H)(C)(C_B)) + (1 \times C_B-(N)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		84.49		
Liquid phase				
$\Delta_f H°$ =		20.94		
$C_p°$ =	230.10	230.10	0.00	36KUR/VOS

Benzylamine C_7H_9N

$(1 \times N-(H)_2(C)) + (5 \times C_B-(H)(C_B)_2) + (1 \times C_B-(C)(C_B)_2) + (1 \times C-(H)_2(C_B)(N))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	87.80	87.80	0.00	77CAR/LAY
Liquid phase				
$\Delta_f H°$ =	34.20	34.20	0.00	77CAR/LAY
$C_p°$ =	207.19	205.88	1.31	75NIC/WAD

2-Phenylethylamine $C_8H_{11}N$

$(1 \times N-(H)_2(C)) + (1 \times C-(H)_2(C)(N)) + (1 \times C-(H)_2(C)(C_B)) + (1 \times C_B-(C)(C_B)_2) + (5 \times C_B-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		62.30		
$C_p°$ =		150.44		
Liquid phase				
$\Delta_f H°$ =		4.68		
$C_p°$ =	239.24	239.41	−0.17	75NIC/WAD
$S°$ =		276.34		
$\Delta_f S°$ =		−583.47		
$\Delta_f G°$ =		178.64		
$\ln K_f$ =		−72.06		

N,N-Dimethylaniline $C_8H_{11}N$

$(5 \times C_B-(H)(C_B)_2) + (1 \times C_B-(N)(C_B)_2) + (1 \times N-(C)_2(C_B)) + (2 \times C-(H)_3(C)) + (2 \times -CH_3 \text{ corr (quaternary)})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	100.50	100.51	−0.01	82FUR/SAK

TABLE 26. Amines (50) — Continued

N,N-Dimethylaniline (Continued) $C_8H_{11}N$

$(5 \times C_B-(H)(C_B)_2) + (1 \times C_B-(N)(C_B)_2) + (1 \times N-(C)_2(C_B)) + (2 \times C-(H)_3(C)) + (2 \times -CH_3 \text{ corr (quaternary)})$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	47.70	47.70	0.00	82FUR/SAK
$C_p°$ =	212.00	212.13	−0.13	34KOL/UDO

N-Ethylaniline $C_8H_{11}N$

$(5 \times C_B-(H)(C_B)_2) + (1 \times C_B-(N)(C_B)_2) + (1 \times N-(H)(C)(C_B)) + (1 \times C-(H)_2(C)(N)) + (1 \times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	56.32	56.19	0.13	52VRI/HIL
Liquid phase				
$\Delta_f H°$ =	4.02	−9.86	13.88	52VRI/HIL
$C_p°$ =		260.52		

N-Phenylaniline $C_{12}H_{11}N$

$(10 \times C_B-(H)(C_B)_2) + (2 \times C_B-(N)(C_B)_2) + (1 \times N-(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	219.30	219.05	0.25	53AIH
Liquid phase				
$\Delta_f H°$ =		135.10		
Solid phase				
$\Delta_f H°$ =	130.00	130.20	−0.20	55MED
$C_p°$ =		223.30		

N-Methyl-N-phenylaniline $C_{13}H_{13}N$

$(10 \times C_B-(H)(C_B)_2) + (2 \times C_B-(N)(C_B)_2) + (1 \times C-(H)_3(C)) + (1 \times N-(C)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		213.68		
Liquid phase				
$\Delta_f H°$ =	120.50	134.37	−13.87	56TAV/LAM
$C_p°$ =	301.25	301.27	−0.02	

TABLE 26. Amines (50) — Continued

1,2-Benzenediamine $C_6H_8N_2$
$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(N)(C_B)_2)+(2\times N\text{–}(H)_2(C_B))+(1\times NH_2\text{–}NH_2$ *ortho* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		91.14		
$C_p°$ =		135.28		
Liquid phase				
$\Delta_f H°$ =		13.64		
$C_p°$ =		245.94		
$S°$ =		210.04		
$\Delta_f S°$ =		−538.18		
$\Delta_f G°$ =		174.10		
$\ln K_f$ =		−70.23		
Solid phase				
$\Delta_f H°$ =	−0.30	−0.58	0.28	73KUN/KAR
$C_p°$ =		158.52		
$S°$ =		155.86		
$\Delta_f S°$ =		−592.36		
$\Delta_f G°$ =		176.03		
$\ln K_f$		−71.01		

1,3-Benzenediamine $C_6H_8N_2$
$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(N)(C_B)_2)+(2\times N\text{–}(H)_2(C_B))+(1\times NH_2\text{–}NH_2$ *meta* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		91.14		
$C_p°$ =		135.28		
Liquid phase				
$\Delta_f H°$ =		13.64		
$C_p°$ =		245.94		
$S°$ =		210.04		
$\Delta_f S°$ =		−538.18		
$\Delta_f G°$ =		174.10		
$\ln K_f$ =		−70.23		
Solid phase				
$\Delta_f H°$ =	−7.80	−7.58	−0.22	73KUN/KAR
$C_p°$ =	159.60	158.52	1.08	84RAB/KAR
$S°$ =		155.86		
$\Delta_f S°$ =		−592.36		
$\Delta_f G°$ =		169.03		
$\ln K_f$		−68.19		

TABLE 26. Amines (50) — Continued

1,4-Benzenediamine $C_6H_8N_2$
$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(N)(C_B)_2)+(2\times N\text{–}(H)_2(C_B))$

	Literature	Calculated	– Residual	Reference
Gas phase				
$\Delta_f H°$ =		91.14		
$C_p°$ =		135.28		
Liquid phase				
$\Delta_f H°$ =		13.64		
$C_p°$ =		245.94		
$S°$ =		210.04		
$\Delta_f S°$ =		−538.18		
$\Delta_f G°$ =		174.10		
$\ln K_f$ =		−70.23		
Solid phase				
$\Delta_f H°$ =	6.40	2.42	3.98	73KUN/KAR
$C_p°$ =		158.52		
$S°$ =		155.86		
$\Delta_f S°$ =		−592.36		
$\Delta_f G°$ =		179.03		
$\ln K_f$		−72.22		

4-Aminobiphenyl $C_{12}H_{11}N$
$(1\times N\text{–}(H)_2(C_B))+(1\times C_B\text{–}(N)(C_B)_2)+(9\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(C_B)_3)$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		185.56		
$C_p°$ =		189.15		
Liquid phase				
$\Delta_f H°$ =		98.36		
$C_p°$ =		315.87		
Solid phase				
$\Delta_f H°$ =	81.00	80.98	0.02	35BRU
$C_p°$ =		216.73		
$S°$ =		225.18		
$\Delta_f S°$ =		−657.59		
$\Delta_f G°$ =		277.04		
$\ln K_f$		−111.76		

TABLE 27. Imines (2)

N-(2-Methylpropylidene)butylamine; N-Butylisobutyleneimine $C_8H_{17}N$

$(3\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(N))+(1\times N_I-(C))+(1\times C_d-(H)(C))+(1\times C-(H)(C)_2(C_d))+(2\times -CH_3 \text{ corr (tertiary)})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−84.71		
Liquid Phase				
$\Delta_f H°$ =	−132.80	−129.74	−3.06	62BED/EDM

N-(Phenylmethylene)benzenimine; Benzylideneaniline $C_{13}H_{11}N$

$(10\times C_B-(H)(C_B)_2)+(1\times C_B-(N))+(1\times C_B-(C_d)(C_B)_2)+(1\times C_d-(H)(C_B))+(1\times N_I-(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	253.60	258.25	−4.65	48COA/SUT
$C_p°$ =		194.90		
Liquid Phase				
$\Delta_f H°$ =		178.90		
$C_p°$ =		302.68		
$S°$ =		304.93		
$\Delta_f S°$ =		−583.58		
$\Delta_f G°$ =		352.89		
$\ln K_f$ =		−142.36		
Solid phase				
$\Delta_f H°$ =	167.80	169.85	−2.05	48COA/SUT

TABLE 28. Nitriles (27)

Ethanenitrile; Acetonitrile C_2H_3N

$(1\times C-(H)_3(CN)$, Acetonitrile), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	74.04	74.04	0.00	83AN/MAN
$C_p°$ =	52.22	52.22	0.00	69STU/WES
$S°$ =	243.47	243.47	0.00	69STU/WES
$\Delta_f S°$ =		−59.62		
$\Delta_f G°$ =		91.82		
$\ln K_f$ =		−37.04		
Liquid phase				
$\Delta_f H°$ =	40.56	40.56	0.00	83AN/MAN
$C_p°$ =	91.46	91.46	0.00	65PUT/MCE
$S°$ =	149.62	149.62	0.00	65PUT/MCE
$\Delta_f S°$ =		−153.47		
$\Delta_f G°$ =		86.32		
$\ln K_f$ =		−34.82		

Propanenitrile; Propionitrile C_3H_5N

$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)(CN))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	51.50	52.26	−0.76	70HOW/WAD
$C_p°$ =	73.05	73.59	−0.54	69STU/WES
$S°$ =	286.60	285.44	1.16	69STU/WES
$\Delta_f S°$ =		−153.96		
$\Delta_f G°$ =		98.16		
$\ln K_f$ =		−39.60		
Liquid phase				
$\Delta_f H°$ =	15.50	18.46	−2.96	71HAL/BAL
$C_p°$ =	119.50	119.49	0.01	62WEB/KIL
$S°$ =	189.33	189.32	0.01	62WEB/KIL
$\Delta_f S°$ =		−250.08		
$\Delta_f G°$ =		93.02		
$\ln K_f$ =		−37.52		

Butanenitrile; Butyronitrile C_4H_7N

$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(CN))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	33.60	31.63	1.97	70HOW/WAD
$C_p°$ =	97.03	96.48	0.55	69STU/WES
$S°$ =	325.43	324.60	0.83	69STU/WES
$\Delta_f S°$ =		−251.11		
$\Delta_f G°$ =		106.50		
$\ln K_f$ =		−42.96		

TABLE 28. Nitriles (27) — Continued

Butanenitrile; Butyronitrile (Continued) C_4H_7N

$(1\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(CN))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−5.82	−7.27	1.45	59EVA/SKI
$C_p°$ =		149.91		
$S°$ =		221.70		
$\Delta_fS°$ =		−354.01		
$\Delta_fG°$ =		98.28		
$\ln K_f$ =		−39.64		

Pentanenitrile; Valeronitrile C_5H_9N

$(1\times C\text{-}(H)_3(C)) + (2\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(CN))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	10.50	11.00	−0.50	70HOW/WAD
$C_p°$ =		119.37		
$S°$ =		363.76		
$\Delta_fS°$ =		−348.26		
$\Delta_fG°$ =		114.83		
$\ln K_f$ =		−46.32		
Liquid phase				
$\Delta_fH°$ =	−33.10	−33.00	−0.10	69KON/PRO
$C_p°$ =		180.33		
$S°$ =		254.08		
$\Delta_fS°$ =		−457.94		
$\Delta_fG°$ =		103.53		
$\ln K_f$ =		−41.77		

Heptanenitrile; Enanthonitrile $C_7H_{13}N$

$(1\times C\text{-}(H)_3(C)) + (4\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(CN))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−31.00	−30.26	−0.74	73LEB/KAT
$C_p°$ =		165.15		
$S°$ =		442.08		
$\Delta_fS°$ =		−542.57		
$\Delta_fG°$ =		131.51		
$\ln K_f$ =		−53.05		
Liquid phase				
$\Delta_fH°$ =	−82.89	−84.46	1.57	73LEB/KAT
$C_p°$ =		241.17		
$S°$ =		318.84		
$\Delta_fS°$ =		−665.80		
$\Delta_fG°$ =		114.05		
$\ln K_f$ =		−46.01		

TABLE 28. Nitriles (27) — Continued

Octanenitrile; Capryonitrile $C_8H_{15}N$

$(1\times C\text{-}(H)_3(C)) + (5\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(CN))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−50.60	−50.89	0.29	77STR/SUN
$C_p°$ =		188.04		
$S°$ =		481.24		
$\Delta_fS°$ =		−639.72		
$\Delta_fG°$ =		139.84		
$\ln K_f$ =		−56.41		
Liquid phase				
$\Delta_fH°$ =	−107.40	−110.19	2.79	77STR/SUN
$C_p°$ =		271.59		
$S°$ =		351.22		
$\Delta_fS°$ =		−769.73		
$\Delta_fG°$ =		119.31		
$\ln K_f$ =		−48.13		

Decanenitrile; Caprinitrile $C_{10}H_{19}N$

$(1\times C\text{-}(H)_3(C)) + (7\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(CN))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−91.60	−92.15	0.55	77STR/SUN
$C_p°$ =		233.82		
$S°$ =		559.56		
$\Delta_fS°$ =		−834.02		
$\Delta_fG°$ =		156.51		
$\ln K_f$ =		−63.14		
Liquid phase				
$\Delta_fH°$ =	−158.40	−161.65	3.25	77STR/SUN
$C_p°$ =		332.43		
$S°$ =		415.98		
$\Delta_fS°$ =		−977.59		
$\Delta_fG°$ =		129.82		
$\ln K_f$ =		−52.37		

Undecanenitrile; Undecylnitrile $C_{11}H_{21}N$

$(1\times C\text{-}(H)_3(C)) + (8\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(C)(CN))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−113.40	−112.78	−0.62	77STR/SUN
$C_p°$ =		256.71		
$S°$ =		598.72		
$\Delta_fS°$ =		−931.17		
$\Delta_fG°$ =		164.85		
$\ln K_f$ =		−66.50		

TABLE 28. Nitriles (27) – Continued

Undecanenitrile; Undecylnitrile (Continued) $C_{11}H_{21}N$

(1 × C–(H)$_3$(C)) + (8 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(C)(CN)), σ = 3

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	–184.50	–187.38	2.88	77STR/SUN
$C_p°$ =		362.85		
$S°$ =		448.36		
$\Delta_f S°$ =		–1081.53		
$\Delta_f G°$ =		135.08		
$\ln K_f$ =		–54.49		

Tetradecanenitrile; Myristonitrile $C_{14}H_{27}N$

(1 × C–(H)$_3$(C)) + (11 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(C)(CN)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	–174.80	–174.67	–0.13	77STR/SUN
$C_p°$ =		325.38		
$S°$ =		716.20		
$\Delta_f S°$ =		–1222.62		
$\Delta_f G°$ =		189.86		
$\ln K_f$ =		–76.59		
Liquid phase				
$\Delta_f H°$ =	–260.10	–264.57	4.47	77STR/SUN
$C_p°$ =		454.11		
$S°$ =		545.50		
$\Delta_f S°$ =		–1393.32		
$\Delta_f G°$ =		150.85		
$\ln K_f$ =		–60.85		

Propenenitrile; Acrylonitrile C_3H_3N

(1 × C$_d$–(H)$_2$) + (1 × C$_d$–(H)(CN)), σ = 1

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	183.68	172.97	10.71	72FIN/MES
$C_p°$ =	64.18	63.76	0.42	72FIN/MES
$S°$ =	275.31	273.93	1.38	72FIN/MES
$\Delta_f S°$ =		–34.90		
$\Delta_f G°$ =		183.37		
$\ln K_f$ =		–73.97		
Liquid phase				
$\Delta_f H°$ =	150.21	139.03	11.18	72FIN/MES
$C_p°$ =	108.80	108.79	0.01	72FIN/MES
$S°$ =	178.91	178.91	0.00	72FIN/MES
$\Delta_f S°$ =		–129.92		
$\Delta_f G°$ =		177.76		
$\ln K_f$ =		–71.71		

TABLE 28. Nitriles (27) – Continued

***trans*-2-Butenenitrile** C_4H_5N

(1 × C–(H)$_3$(C)) + (1 × C$_d$–(H)(C)) + (1 × C$_d$–(H)(CN))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	140.71	140.71	0.00	73KON
$C_p°$ =		86.85		
Liquid phase				
$\Delta_f H°$ =	100.71	100.72	–0.01	69KON/PRO
$C_p°$ =		141.50		
$S°$ =		204.60		
$\Delta_f S°$ =		–240.54		
$\Delta_f G°$ =		172.44		
$\ln K_f$ =		–69.56		

***cis*-2-Butenenitrile** C_4H_5N

(1 × C–(H)$_3$(C)) + (1 × C$_d$–(H)(C)) + (1 × C$_d$–(H)(CN)) + (1 × *cis*(unsat) corr)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	134.10	145.56	–11.46	73KON
$C_p°$ =		78.82		
Liquid phase				
$\Delta_f H°$ =	95.10	105.99	–10.89	69KON/PRO
$C_p°$ =		141.50		
$S°$ =		204.60		
$\Delta_f S°$ =		–240.54		
$\Delta_f G°$ =		177.71		
$\ln K_f$ =		–71.69		

2-Methylpropanenitrile; Isobutryonitrile C_4H_7N

(2 × C–(H)$_3$(C)) + (1 × C–(H)(C)$_2$(CN)) + (2 × –CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	23.30	24.46	–1.16	70HOW/WAD
$C_p°$ =		96.40		
Liquid phase				
$\Delta_f H°$ =	–13.80	–18.08	4.28	71HAL/BAL
$C_p°$ =	156.06	156.05	0.01	71HAL/BAL

TABLE 28. Nitriles (27) – Continued

***trans*-2-Pentenenitrile** C_5H_7N
(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)(C$_d$)) + (1×C$_d$–(H)(C)) + (1×C$_d$–(H)(CN))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	119.79	119.83	−0.04	73KON
$C_p°$ =		107.48		
Liquid phase				
$\Delta_fH°$ =	74.89	74.99	−0.10	69KON/PRO
$C_p°$ =		170.79		
$S°$ =		236.27		
$\Delta_fS°$ =		−345.18		
$\Delta_fG°$ =		177.90		
$\ln K_f$ =		−71.77		

***trans*-3-Pentenenitrile** C_5H_7N
(1×C–(H)$_3$(C)) + (2×C$_d$–(H)(C)) + (1×C–(H)$_2$(C$_d$)(CN))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	125.69	125.69	0.00	73KON
Liquid phase				
$\Delta_fH°$ =	80.88	80.89	−0.01	69KON/PRO

2,2-Dimethylpropanenitrile C_5H_9N
(3×C–(H)$_3$(C)) + (1×C–(C)$_3$(CN)) + (3×–CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−2.50	−2.50	0.00	70HOW/WAD
Liquid phase				
$\Delta_fH°$ =	−39.80	−39.80	0.00	71HAL/BAL
$C_p°$ =	179.37	179.35	0.02	67WES/RIB
$S°$ =	232.00	231.99	0.01	67WES/RIB
$\Delta_fS°$ =		−480.03		
$\Delta_fG°$ =		103.32		
$\ln K_f$ =		−41.68		

TABLE 28. Nitriles (27) – Continued

Cyclopropanenitrile C_4H_5N
(2×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(CN)) + (1×cyclopropanenitrile rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	182.80	182.80	0.00	82FUC/HAL
Liquid phase				
$\Delta_fH°$ =	140.80	140.80	0.00	71HAL/BAL
$C_p°$ =	115.40	115.40	0.00	71HAL/BAL

Cyclobutanenitrile C_5H_7N
(3×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(CN)) + (1×cyclobutanenitrile rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	143.00	143.00	0.00	71HAL/BAL
Liquid phase				
$\Delta_fH°$ =	103.00	103.00	0.00	71HAL/BAL
$C_p°$ =	146.00	146.00	0.00	71HAL/BAL

Cyclopentanenitrile C_6H_9N
(4×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(CN)) + (1×cyclopentanenitrile rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	41.80	41.80	0.00	71HAL/BAL
Liquid phase				
$\Delta_fH°$ =	0.70	0.70	0.00	71HAL/BAL
$C_p°$ =	167.50	167.50	0.00	71HAL/BAL

Cyclohexanenitrile $C_7H_{11}N$
(5×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(CN)) + (1×cyclohexanenitrile rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	4.80	4.80	0.00	71HAL/BAL
Liquid phase				
$\Delta_fH°$ =	−47.20	−47.20	0.00	71HAL/BAL
$C_p°$ =	177.90	177.90	0.00	71HAL/BAL

TABLE 28. Nitriles (27) — Continued

Benzonitrile C_7H_5N
$(5\times C_B-(H)(C_B)_2)+(1\times C_B-(CN)(C_B)_2)$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	218.82	220.05	−1.23	59EVA/SKI
$C_p°$ =	109.08	109.14	−0.06	69STU/WES
$S°$ =	321.04	321.04	0.00	69STU/WES
$\Delta_fS°$ =		−141.32		
$\Delta_fG°$ =		262.18		
$\ln K_f$ =		−105.76		
Liquid phase				
$\Delta_fH°$ =	163.18	163.18	0.00	59EVA/SKI
$C_p°$ =	165.20	165.20	0.00	84LEB/BYK
$S°$ =	209.10	209.10	0.00	84LEB/BYK
$\Delta_fS°$ =		−253.26		
$\Delta_fG°$ =		238.69		
$\ln K_f$ =		−96.29		

2-Butyne-1,4-dinitrile C_4N_2
$(2\times C_t-(CN))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	529.28	529.20	0.08	57SAG
Liquid phase				
$\Delta_fH°$ =	500.41	500.40	0.01	63ARM/MAR

1,4-Butanedinitrile; Succinonitrile $C_4H_4N_2$
$(2\times C-(H)_2(C)(CN))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	209.70	189.04	20.66	71RAP/WES
$C_p°$ =		95.72		
Liquid phase				
$\Delta_fH°$ =		132.14		
$C_p°$ =		166.02		
$S°$ =		212.04		
$\Delta_fS°$ =		−263.56		
$\Delta_fG°$ =		210.72		
$\ln K_f$ =		−85.00		
Solid phase				
$\Delta_fH°$ =	139.70	139.70	0.00	71RAP/WES
$C_p°$ =	145.60	145.60	0.00	63WUL/WES
$S°$ =	191.59	192.30	−0.71	63WUL/WES
$\Delta_fS°$ =		−283.30		
$\Delta_fG°$ =		224.17		
$\ln K_f$ =		−90.43		

TABLE 27. Nitriles (27) — Continued

1,5-Pentanedinitrile; Glutaronitrile $C_5H_6N_2$
$(1\times C-(H)_2(C)_2)+(2\times C-(H)_2(C)(CN))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		168.41		
$C_p°$ =		118.61		
Liquid phase				
$\Delta_fH°$ =		106.41		
$C_p°$ =	186.26	196.44	−10.18	65CLE/WUL
$S°$ =	239.45	244.42	−4.97	65CLE/WUL
$\Delta_fS°$ =		−367.49		
$\Delta_fG°$ =		215.98		
$\ln K_f$ =		−87.12		
Solid phase				
$\Delta_fH°$ =	102.90	110.29	−7.39	1889BER/PE
$C_p°$ =		167.52		
$S°$ =		215.31		
$\Delta_fS°$ =		−396.60		
$\Delta_fG°$ =		228.54		
$\ln K_f$ =		−92.19		

2,2-Dimethylpropane-1,3-dinitrile $C_5H_6N_2$
$(2\times C-(H)_3(C))+(1\times C-(C)_2(CN)_2)+$
$(2\times -CH_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Solid phase				
$C_p°$ =	179.49	179.50	−0.01	67RIB/WES
$S°$ =	187.95	187.95	0.00	67RIB/WES
$\Delta_fS°$ =		−423.96		

1,6-Hexanedinitrile; Adiponitrile $C_6H_8N_2$
$(2\times C-(H)_2(C)_2)+(2\times C-(H)_2(C)(CN))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	149.50	147.78	1.72	73LEB/KAT
$C_p°$ =		141.50		
Liquid phase				
$\Delta_fH°$ =	85.10	80.68	4.42	73LEB/KAT
$C_p°$ =		226.86		
$S°$ =		276.80		
$\Delta_fS°$ =		−471.42		
$\Delta_fG°$ =		221.24		
$\ln K_f$ =		−89.24		

TABLE 28. Nitriles (27) — Continued

1,4-Benzodinitrile; 1,4-Dicyanobenzene $C_8H_4N_2$
$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(CN)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	358.30	357.24	1.06	92ACR/TUC
$C_p°$ =		136.62		
Liquid phase				
$\Delta_fH°$ =		277.40		
$C_p°$ =		194.32		
$S°$ =		244.98		
$\Delta_fS°$ =		−253.58		
$\Delta_fG°$ =		353.01		
$\ln K_f$ =		−142.40		
Solid phase				
$\Delta_fH°$ =	268.50	268.52	−0.02	92ACR/TUC
$S°$ =		191.90		
$\Delta_fS°$ =		−306.66		
$\Delta_fG°$ =		359.95		
$\ln K_f$ =		−145.20		

TABLE 29. Hydrazines (6)

Hydrazine N_2H_4
$(2\times N\text{–}(H)_2(N))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	95.19	95.40	−0.21	49SCO/OLI
$C_p°$ =	52.71	52.72	−0.01	49SCO/OLI
$S°$ =	238.36	238.60	−0.24	49SCO/OLI
$\Delta_fS°$ =		−214.05		
$\Delta_fG°$ =		159.22		
$\ln K_f$ =		−64.23		
Liquid phase				
$\Delta_fH°$ =	50.42	50.60	−0.18	39HUG/COR
$C_p°$ =	98.83	98.82	0.01	49SCO/OLI
$S°$ =	121.21	121.16	0.05	49SCO/OLI
$\Delta_fS°$ =		−331.48		
$\Delta_fG°$ =		149.43		
$\ln K_f$ =		−60.28		

Methylhydrazine CH_6N_2
$(1\times C\text{–}(H)_3(N))+(1\times N\text{–}(H)(C)(N))+(1\times N\text{–}(H)_2(N))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	94.60	94.60	0.00	51AST/FIN
Liquid phase				
$\Delta_fH°$ =	54.20	52.69	1.51	51AST/ROC
$C_p°$ =	134.93	134.93	0.00	51AST/FIN
$S°$ =	165.94	165.93	0.01	51AST/FIN
$\Delta_fS°$ =		−423.02		
$\Delta_fG°$ =		178.81		
$\ln K_f$ =		−72.13		

1,1-Dimethylhydrazine $C_2H_8N_2$
$(2\times C\text{–}(H)_3(N))+(1\times N\text{–}(C)_2(N))+(1\times N\text{–}(H)_2(N))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	83.89	83.89	0.00	53AST/WOO
Liquid phase				
$\Delta_fH°$ =	49.30	49.08	0.22	60DON/SHO
$C_p°$ =	164.05	164.04	0.01	53AST/WOO
$S°$ =	200.25	200.24	0.01	53AST/WOO
$\Delta_fS°$ =		−525.02		
$\Delta_fG°$ =		205.62		
$\ln K_f$ =		−82.94		

TABLE 29. Hydrazines (6) — Continued

1,2-Dimethylhydrazine $C_2H_8N_2$
(2×C–(H)$_3$(N)) + (2×N–(H)(C)(N))

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	92.01	93.80	−1.79	51AST/JAN
Liquid phase				
$\Delta_f H°$ =	52.70	54.78	−2.08	52AST/ROC
$C_p°$ =		171.04		
$S°$ =		210.70		
$\Delta_f S°$ =		−514.56		
$\Delta_f G°$ =		208.20		
$\ln K_f$ =		−83.99		

Phenylhydrazine $C_6H_8N_2$
(5×C_B–(H)(C_B)$_2$) + (1×C_B–(N)(C_B)$_2$) + (1×N–(H)(C_B)(N)) + (1×N–(H)$_2$(N))

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	202.90	202.95	−0.05	72LEB/KAT
Liquid phase				
$\Delta_f H°$ =	141.00	141.00	0.00	72LEB/KAT
Solid phase				
$\Delta_f H°$ =	124.60	128.27	−3.67	11LOU/DUP

1,2-Diphenylhydrazine; Hydrazobenzene $C_{12}H_{12}N_2$
(10×C_B–(H)(C_B)$_2$) + (2×C_B–(N)(C_B)$_2$) + (2×N–(H)(C_B)(N))

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		310.50		
Liquid phase				
$\Delta_f H°$ =		231.40		
Solid phase				
$\Delta_f H°$ =	221.30	218.60	2.70	51COL/GIL

TABLE 30. Diazenes (14)

Dimethyldiazene; Azomethane $C_2H_6N_2$
(2×C–(H)$_3$(N_A)) + (2×N_A–(C))

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	134.47	134.48	−0.01	76ROS

Methylethyldiazene; Methyl azoethane $C_3H_8N_2$
(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)(N_A)) + (2×N_A–(C)) + (1×C–(H)$_3$(N_A))

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	113.85	113.78	0.07	76ROS

Diethyldiazene; Azoethane $C_4H_{10}N_2$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)(N_A)) + (2×N_A–(C))

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	93.26	93.08	0.18	76ROS

Di-*n*-propyldiazene; Azopropane $C_6H_{14}N_2$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(C)(N_A)) + (2×N_A–(C))

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	51.34	51.82	−0.48	76ENG/MEL
Liquid phase				
$\Delta_f H°$ =	11.50	11.62	−0.12	76ENG/MEL

Methyl-*n*-butyldiazene $C_5H_{12}N_2$
(1×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(N_A)) + (2×N_A–(C)) + (1×C–(H)$_3$(N_A))

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	78.90	72.52	6.38	78ENG/MON
Liquid phase				
$\Delta_f H°$ =	42.50	37.32	5.18	78ENG/MON

TABLE 30. Diazenes (14) – Continued

Diisopropyldiazene; Azoisopropane $C_6H_{14}N_2$
(4 × C–(H)$_3$(C)) + (4 × –CH$_3$ corr (tertiary)) + (2 × C–(H)(C)$_2$(N_A)) + (2 × N_A–(C))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	35.60	35.60	0.00	76ENG/MEL
Liquid phase $\Delta_fH°$ =	−0.30	−0.30	0.00	76ENG/MEL

Di-*n*-butyldiazene; Azobutane $C_8H_{18}N_2$
(2 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(C)(N_A)) + (2 × N_A–(C))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	9.20	10.56	−1.36	78ENG/MON
Liquid phase $\Delta_fH°$ =	−40.10	−39.84	−0.26	78ENG/MON

Di-tert-butyldiazene; Azo-tert-butane $C_8H_{18}N_2$
(6 × C–(H)$_3$(C)) + (2 × C–(C)$_3$(N_A)) + (6 × –CH$_3$ corr (quaternary)) + (2 × N_A–(C))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−35.61	−38.92	3.31	76ENG/MEL
Liquid phase $\Delta_fH°$ =	−74.70	−71.30	−3.40	76ENG/MEL

tert-Butyl-(1,1,3,3-tetramethylbutyl)diazene $C_{12}H_{26}N_2$
(8 × C–(H)$_3$(C)) + (2 × N_A–(C)) + (1 × C–(H)$_2$(C)$_2$) + (1 × C–(C)$_4$) + (3 × –CH$_3$ corr (quaternary)) + (2 × C–(C)$_3$(N_A)) + (5 × –CH$_3$ corr (*quat/quat*))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−119.30	−114.39	−4.91	76ENG/MEL
Liquid phase $\Delta_fH°$ =	−172.90	−164.29	−8.61	76ENG/MEL

TABLE 30. Diazenes (14) – Continued

Di-(1,1,3,3-tetramethylbutyl)diazene $C_{16}H_{34}N_2$
(10 × C–(H)$_3$(C)) + (2 × N_A–(C)) + (2 × C–(H)$_2$(C)$_2$) + (2 × C–(C)$_4$) + (10 × –CH$_3$ corr (*quat/quat*)) + (2 × C–(C)$_3$(N_A))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−196.80	−189.86	−6.94	76ENG/MEL
Liquid phase $\Delta_fH°$ =	−263.30	−257.28	−6.02	76ENG/MEL

1,1,3,3-Tetramethylcyclotrimethylenediazene; 3,3,5,5-Tetramethyl-1-pyrazoline $C_7H_{14}N_2$
(4 × C–(H)$_3$(C)) + (1 × C–(H)$_2$(C)$_2$) + (2 × N_A–(C)) + (2 × C–(C)$_3$(N_A)) + (4 × –CH$_3$ corr (*quat/quat*)) + (1 × Cyclotrimethylenediazene rsc)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	39.30	39.30	0.00	76ENG/MEL
Solid phase $\Delta_fH°$ =	−22.30	−22.30	0.00	76ENG/MEL

1,1,4,4-Tetramethylcyclotetramethylenediazene; 3,4,5,6-Tetrahydro-3,3,6,6-tetramethyl-pyridazine $C_8H_{16}N_2$
(4 × C–(H)$_3$(C)) + (4 × –CH$_3$ corr (*quat/quat*)) + (2 × C–(H)$_2$(C)$_2$) + (2 × N_A–(C)) + (2 × C–(C)$_3$(N_A)) + (1 × Cyclotetramethylenediazene rsc)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	42.00	42.00	0.00	76ENG/MEL
Liquid phase $\Delta_fH°$ =	−8.10	−8.10	0.00	76ENG/MEL

***trans*-Azobenzene** $C_{12}H_{10}N_2$
(10 × C_B–(H)(C_B)$_2$) + (2 × C_B–(N_A)(C_B)$_2$) + (2 × N_A–(C_B))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	402.20	402.20	0.00	92DIA/MIN

TABLE 30. Diazenes (14) – Continued

trans-Azobenzene (Continued) $C_{12}H_{10}N_2$
$(10\times C_B-(H)(C_B)_2)+(2\times C_B-(N_A)(C_B)_2)+(2\times N_A-(C_B))$

	Literature	– Calculated	= Residual	Reference
Liquid phase $\Delta_f H°$ =	331.45	331.46	–0.01	77SCH/PET
Solid phase $\Delta_f H°$ =	308.60	308.60	0.00	92DIA/MIN

cis-Azobenzene $C_{12}H_{10}N_2$
$(10\times C_B-(H)(C_B)_2)+(2\times C_B-(N_A)(C_B)_2)+(2\times N_A-(C_B))+$
(1 × *cis*-azobenzene corr)

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	450.60	450.60	0.00	92DIA/MIN
Solid phase $\Delta_f H°$ =	357.70	357.70	0.00	92DIA/MIN

TABLE 31. Azides (6)

2-Azidoethanol $C_2H_5N_3O$
$(1\times C-(H)_2(C)(N_3))+(1\times C-(H)_2(O)(C))+(1\times O-(H)(C))$

	Literature	– Calculated	= Residual	Reference
Liquid phase $\Delta_f H°$ =	94.40	94.40	0.00	53FAG/KLE

Azidocyclopentane $C_5H_9N_3$
$(4\times C-(H)_2(C)_2)+(1\times C-(H)(C)_2(N_3))+$
(1 × azidocyclopentane rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	220.90	220.90	0.00	54FAG/MYE
Liquid phase $\Delta_f H°$ =	179.10	179.10	0.00	54FAG/MYE

Azidocyclohexane $C_6H_{11}N_3$
$(5\times C-(H)_2(C)_2)+(1\times C-(H)(C)_2(N_3))+$
(1 × azidocyclohexane rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	154.40	154.40	0.00	54FAG/MYE
Liquid phase $\Delta_f H°$ =	108.40	108.40	0.00	54FAG/MYE

Azidobenzene; Phenylazide $C_6H_5N_3$
$(5\times C_B-(H)(C_B)_2)+(1\times C_B-(N_3))$

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	389.10	389.05	0.05	74PEP/ERL
Liquid phase $\Delta_f H°$ =	344.30	344.30	0.00	29ROT/MUL

Benzylazide $C_7H_7N_3$
$(5\times C_B-(H)(C_B)_2)+(1\times C-(H)_2(C_B)(N_3))$

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	416.10	416.05	0.05	74PEP/ERL

TABLE 31. Azides (6) — Continued

Benzylazide (Continued) $C_7H_7N_3$
$(5\times C_B-(H)(C_B)_2)+(1\times C-(H)_2(C_B)(N_3))$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	368.20	368.20	0.00	74PEP/ERL

Triphenylazidomethane; Triphenylmethylazide $C_{19}H_{15}N_3$
$(15\times C_B-(H)(C_B)_2)+(3\times C_B-(C)(C_B)_2)+(1\times C-(C_B)_3(N_3))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	606.70	606.67	0.03	74PEP/ERL
Solid phase				
$\Delta_fH°$ =	486.20	486.15	0.05	74PEP/ERL

TABLE 32. Cyclic CHN (32)

Aziridine; Ethyleneimine C_2H_5N
$(2\times C-(H)_2(C)(N))+(1\times N-(H)(C)_2)+$
$(1\times$ ethyleneimine rsc), $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	126.48	126.48	0.00	56BUR/GOO
$C_p°$ =	52.51	52.51	0.00	69STU/WES
$S°$ =	250.62	250.62	0.00	69STU/WES
$\Delta_fS°$ =		−183.04		
$\Delta_fG°$ =		181.05		
$\ln K_f$ =		−73.04		
Liquid phase				
$\Delta_fH°$ =	91.88	91.88	0.00	52NEL/JES

Pyrrolidine C_4H_9N
$(2\times C-(H)_2(C)_2)+(2\times C-(H)_2(C)(N))+(1\times N-(H)(C)_2)+$
$(1\times$ pyrrolidine rsc), $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−3.60	−3.60	0.00	59MCC/DOU
$C_p°$ =	81.13	81.13	0.00	59MCC/DOU
$S°$ =	309.49	309.49	0.00	59MCC/DOU
$\Delta_fS°$ =		−396.37		
$\Delta_fG°$ =		115.90		
$\ln K_f$ =		−46.75		
Liquid phase				
$\Delta_fH°$ =	−41.20	−41.20	0.00	59MCC/DOU
$C_p°$ =	156.57	156.57	0.00	59MCC/DOU
$S°$ =	204.01	204.01	0.00	59MCC/DOU
$\Delta_fS°$ =		−502.27		
$\Delta_fG°$ =		108.55		
$\ln K_f$ =		−43.79		

Pyridine C_5H_5N
$(5\times C_B-(H)(C_B)_2)+(1\times N_I-(C_B))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	140.20	138.05	2.15	57MCC/DOU
$C_p°$ =	78.12	78.12	0.00	57MCC/DOU
$S°$ =	282.80	282.80	0.00	57MCC/DOU
$\Delta_fS°$ =		−168.08		
$\Delta_fG°$ =		188.16		
$\ln K_f$ =		−75.90		

TABLE 32. Cyclic CHN (32) — Continued

Pyridine (Continued) C_5H_5N
$(5\times C_B-(H)(C_B)_2)+(1\times N_I-(C_B))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	100.20	95.30	4.90	61HUB/FRO
$C_p°$ =	132.72	133.15	−0.43	57MCC/DOU
$S°$ =	177.90	180.75	−2.85	57MCC/DOU
$\Delta_fS°$ =		−270.13		
$\Delta_fG°$ =		175.84		
$\ln K_f$ =		−70.93		

1,3,5-Triazine $C_3H_3N_3$
$(3\times C_B-(H)(N_I)_2)+(3\times N_I-(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	225.90	225.90	0.00	82BYS
Solid phase				
$\Delta_fH°$ =	171.75	171.75	0.00	82BYS

Pyrrole C_4H_5N
$(4\times C_B-(H)(C_B)_2)+(1\times N-(H)(C_B)_2)+(1\times$ pyrrole rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	108.31	108.31	0.00	67SCO/BER
Liquid phase				
$\Delta_fH°$ =	63.11	63.11	0.00	67SCO/BER

N-Methylpyrrole C_5H_7N
$(4\times C_B-(H)(C_B)_2)+(1\times N-(C)(C_B)_2)+(1\times C-(H)_3(N))+$
$(1\times$ pyrrole rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	103.14	102.94	0.20	72GOO
Liquid phase				
$\Delta_fH°$ =	62.38	62.38	0.00	72GOO

TABLE 32. Cyclic CHN (32) — Continued

2,5-Dimethylpyrrole C_6H_9N
$(2\times C_B-(H)(C_B)_2)+(2\times C_B-(C)(C_B)_2)+(2\times C-(H)_3(C))+$
$(1\times N-(H)(C_B)_2)+(1\times$ pyrrole rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	39.80	43.45	−3.65	72GOO
Liquid phase				
$\Delta_fH°$ =	−16.70	−10.11	−6.59	72GOO

2,2′,5,5′-Tetramethyl-N,N-dipyrryl $C_{12}H_{16}N_2$
$(4\times C_B-(H)(C_B)_2)+(4\times C_B-(C)(C_B)_2)+(4\times C-(H)_3(C))+$
$(2\times N-(C_B)_2(N))+(2\times$ pyrrole rsc)

	Literature	*Calculated*	*Residual*	*Reference*
Solid phase				
$\Delta_fH°$ =	132.30	133.78	−1.48	66COL/SKI

Piperidine $C_5H_{11}N$
$(3\times C-(H)_2(C)_2)+(2\times C-(H)_2(C)(N))+(1\times N-(H)(C)_2)+$
$(1\times$ piperidine rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−47.20	−47.80	0.60	63BED/BEE
Liquid phase				
$\Delta_fH°$ =	−86.40	−88.38	1.98	72GOO
$C_p°$ =	179.86	181.68	−1.82	88MES/TOD
$S°$ =	209.97	209.97	0.00	88MES/TOD
$\Delta_fS°$ =		−632.62		
$\Delta_fG°$ =		100.24		
$\ln K_f$ =		−40.43		

Pyridazine $C_4H_4N_2$
$(4\times C_B-(H)(C_B)_2)+(2\times N_I-(C_B))+(1\times N_I-N_I$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	278.30	278.30	0.00	62TJE2
$C_p°$ =		74.58		
Liquid phase				
$\Delta_fH°$ =	224.80	224.80	0.00	62TJE2
$C_p°$ =		130.22		
$S°$ =		188.28		
$\Delta_fS°$ =		−287.32		
$\Delta_fG°$ =		310.47		
$\ln K_f$ =		−125.24		

TABLE 32. Cyclic CHN (32) — Continued

Pyrimidine $C_4H_4N_2$
$(4\times C_B-(H)(C_B)_2)+(2\times N_I-(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	195.80	193.24	2.56	77NAB/SAB
$C_p°$ =		74.58		
Liquid phase				
$\Delta_f H°$ =	143.80	141.64	2.16	77NAB/SAB
$C_p°$ =		130.22		
$S°$ =		188.28		
$\Delta_f S°$ =		−287.32		
$\Delta_f G°$ =		227.31		
$\ln K_f$ =		−91.69		

Pyrazine $C_4H_4N_2$
$(4\times C_B-(H)(C_B)_2)+(2\times N_I-(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	196.10	193.24	2.86	62TJE
$C_p°$ =		74.58		
Liquid phase				
$\Delta_f H°$ =	139.80	141.64	−1.84	62TJE
$C_p°$ =		130.22		
$S°$ =		188.28		
$\Delta_f S°$ =		−287.32		
$\Delta_f G°$ =		227.31		
$\ln K_f$ =		−91.69		

Hexamethyleneimine $C_6H_{13}N$
$(4\times C-(H)_2(C)_2)+(2\times C-(H)_2(C)(N))+(1\times N-(H)(C)_2)+$
$(1\times \text{hexamethyleneimine rsc})$

	Literature	Calculated	Residual	Reference
Liquid phase				
$C_p°$ =	205.00	205.03	−0.03	76CON/GIN

Quinoline C_9H_7N
$(7\times C_B-(H)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(1\times N_I-(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	200.52	205.87	−5.35	88STE/ARC
$C_p°$ =		105.34		

TABLE 32. Cyclic CHN (32) — Continued

Quinoline (Continued) C_9H_7N
$(7\times C_B-(H)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)+(1\times N_I-(C_B))$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	141.22	143.28	−2.06	88STE/ARC
$C_p°$ =	194.89	197.55	−2.66	88STE/ARC
$S°$ =	219.72	227.41	−7.69	88STE/ARC
$\Delta_f S°$ =		−377.00		
$\Delta_f G°$ =		255.68		
$\ln K_f$ =		−103.14		

N-Methylpyrrolidine $C_5H_{11}N$
$(2\times C-(H)_2(C)_2)+(2\times C-(H)_2(C)(N))+(1\times N-(C)_3)+$
$(1\times C-(H)_3(C))+(1\times \text{pyrrolidine rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		4.41		
$C_p°$ =		109.68		
Liquid phase				
$\Delta_f H°$ =		−28.42		
$C_p°$ =	161.10	161.09	0.01	76CON/GIN
$S°$ =		216.60		
$\Delta_f S°$ =		−625.99		
$\Delta_f G°$ =		158.22		
$\ln K_f$ =		−63.82		

N-Methylpiperidine $C_6H_{13}N$
$(3\times C-(H)_2(C)_2)+(2\times C-(H)_2(C)(N))+(1\times C-(H)_3(N))+$
$(1\times N-(C)_3)+(1\times \text{piperidine rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−41.11		
Liquid phase				
$\Delta_f H°$ =		−75.49		
$C_p°$ =	184.93	184.90	0.03	76CON/GIN
$S°$ =		222.56		
$\Delta_f S°$ =		−756.34		
$\Delta_f G°$ =		150.01		
$\ln K_f$ =		−60.51		

TABLE 32. Cyclic CHN (32) — Continued

2-Methylpiperidine $C_6H_{13}N$

(3×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(N))+(1×C–(H)(C)$_2$(N))+(1×–CH$_3$ corr (tertiary))+(1×C–(H)$_3$(C))+(1×N–(H)(C)$_2$)+(1×piperidine rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−84.40	−80.72	−3.68	72GOO
Liquid phase				
$\Delta_fH°$ =	−124.90	−122.02	−2.88	72GOO
$C_p°$ =	205.02	216.02	−11.00	76CON/GIN
$S°$ =		240.89		
$\Delta_fS°$ =		−738.01		
$\Delta_fG°$ =		98.02		
$\ln K_f$ =		−39.54		

4-Methylpiperidine $C_6H_{13}N$

(1×C–(H)$_3$(C))+(1×C–(H)(C)$_2$(N))+(1×–CH$_3$ corr (tertiary))+(1×C–(H)$_2$(C)(N))+(3×C–(H)$_2$(C)$_2$)+(1×N–(H)(C)$_2$)+(1×piperidine rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−80.72		
Liquid phase				
$\Delta_fH°$ =		−122.02		
$C_p°$ =	209.00	216.02	−7.02	76CON/GIN
$S°$ =		240.89		
$\Delta_fS°$ =		−738.01		
$\Delta_fG°$ =		98.02		
$\ln K_f$ =		−39.54		

2-Methylpyridine; 2-Picoline C_6H_7N

(4×C$_B$–(H)(C$_B$)$_2$)+(1×C–(H)$_3$(C))+(1×C$_B$–(C)(C$_B$)$_2$)+(1×N$_I$–(C$_B$))+(1×N$_I$–CH$_3$ (*ortho* corr)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	99.20	99.32	−0.12	63SCO/HUB
$C_p°$ =	100.00	99.99	0.01	69STU/WES
$S°$ =	325.01	322.83	2.18	69STU/WES
$\Delta_fS°$ =		−264.36		
$\Delta_fG°$ =		178.14		
$\ln K_f$ =		−71.86		
Liquid phase				
$\Delta_fH°$ =	56.70	54.69	2.01	63SCO/HUB
$C_p°$ =	158.41	157.05	1.36	63SCO/HUB
$S°$ =	217.86	215.68	2.18	63SCO/HUB
$\Delta_fS°$ =		−371.51		
$\Delta_fG°$ =		165.46		
$\ln K_f$ =		−66.74		

TABLE 32. Cyclic CHN (32) — Continued

3-Methylpyridine; 3-Picoline C_6H_7N

(4×C$_B$–(H)(C$_B$)$_2$)+(1×C–(H)$_3$(C))+(1×C$_B$–(C)(C$_B$)$_2$)+(1×N$_I$–(C$_B$)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	106.40	105.62	0.78	63SCO/HUB
$C_p°$ =	99.58	99.99	−0.41	69STU/WES
$S°$ =	324.97	322.83	2.14	69STU/WES
$\Delta_fS°$ =		−264.36		
$\Delta_fG°$ =		184.44		
$\ln K_f$ =		−74.40		
Liquid phase				
$\Delta_fH°$ =	61.90	58.69	3.21	63SCO/GOO
$C_p°$ =	158.70	157.05	1.65	63SCO/GOO
$S°$ =	216.31	215.68	0.63	63SCO/GOO
$\Delta_fS°$ =		−371.51		
$\Delta_fG°$ =		169.46		
$\ln K_f$ =		−68.36		

4-Methylpyridine; 4-Picoline C_6H_7N

(4×C$_B$–(H)(C$_B$)$_2$)+(1×C–(H)$_3$(C))+(1×C$_B$–(C)(C$_B$)$_2$)+(1×N$_I$–(C$_B$))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	104.10	105.62	−1.52	72GOO
$C_p°$ =		99.99		
Liquid phase				
$\Delta_fH°$ =	59.20	58.69	0.51	72GOO
$C_p°$ =		157.05		
$S°$ =		215.68		
$\Delta_fS°$ =		−371.51		
$\Delta_fG°$ =		169.46		
$\ln K_f$ =		−68.36		

2,3-Dimethylpyridine; 2,3-Lutidine C_7H_9N

(2×C–(H)$_3$(C))+(2×C$_B$–(C)(C$_B$)$_2$)+(3×C$_B$–(H)(C$_B$)$_2$)+(1×N$_I$–(C$_B$))+(1×*ortho* corr, hydrocarbons)+(1×N$_I$–CH$_3$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	68.30	68.15	0.15	60COX
Liquid phase				
$\Delta_fH°$ =	19.40	21.34	−1.94	58COX/GUN

TABLE 32. Cyclic CHN (32) – Continued

2,4-Dimethylpyridine; 2,4-Lutidine C_7H_9N

$(3\times C_B\text{-}(H)(C_B)_2)+(2\times C\text{-}(H)_3(C))+(2\times C_B\text{-}(C)(C_B)_2)+(1\times N_I\text{-}(C_B))+(1\times$ *meta* corr, hydrocarbons$)+(1\times N_I\text{-}CH_3$ (*ortho* corr))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	63.90	66.26	−2.36	60COX
Liquid phase				
$\Delta_f H°$ =	16.20	18.08	−1.88	58COX/GUN

2,5-Dimethylpyridine; 2,5-Lutidine C_7H_9N

$(3\times C_B\text{-}(H)(C_B)_2)+(2\times C\text{-}(H)_3(C))+(2\times C_B\text{-}(C)(C_B)_2)+(1\times N_I\text{-}(C_B))+(1\times N_I\text{-}CH_3$ (*ortho* corr))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	66.50	66.89	−0.39	60COX
Liquid phase				
$\Delta_f H°$ =	18.70	18.08	0.62	58COX/GUN

2,6-Dimethylpyridine; 2,6-Lutidine C_7H_9N

$(3\times C_B\text{-}(H)(C_B)_2)+(2\times C\text{-}(H)_3(C))+(2\times C_B\text{-}(C)(C_B)_2)+(1\times N_I\text{-}(C_B))+(1\times$ *meta* corr, hydrocarbons$)+(2\times N_I\text{-}CH_3$ (*ortho* corr))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	58.70	59.96	−1.26	60COX
Liquid phase				
$\Delta_f H°$ =	12.72	14.08	−1.36	58COX/GUN

3,4-Dimethylpyridine; 3,4-Lutidine C_7H_9N

$(3\times C_B\text{-}(H)(C_B)_2)+(2\times C\text{-}(H)_3(C))+(2\times C_B\text{-}(C)(C_B)_2)+(1\times N_I\text{-}(C_B))+(1\times$ *ortho* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	70.08	74.45	−4.37	60COX
$C_p°$ =		128.26		

TABLE 32. Cyclic CHN (32) – Continued

3,4-Dimethylpyridine; 3,4-Lutidine C_7H_9N

$(3\times C_B\text{-}(H)(C_B)_2)+(2\times C\text{-}(H)_3(C))+(2\times C_B\text{-}(C)(C_B)_2)+(1\times N_I\text{-}(C_B))+(1\times$ *ortho* corr)

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_f H°$ =	18.28	25.34	−7.06	58COX/GUN
$C_p°$ =		184.45		
$S°$ =		250.61		
$\Delta_f S°$ =		−472.89		
$\Delta_f G°$ =		166.33		
$\ln K_f$ =		−67.10		

3,5-Dimethylpyridine; 3,5-Lutidine C_7H_9N

$(3\times C_B\text{-}(H)(C_B)_2)+(2\times C\text{-}(H)_3(C))+(2\times C_B\text{-}(C)(C_B)_2)+(1\times N_I\text{-}(C_B))+(1\times$ *meta* corr)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	72.80	72.56	0.24	60COX
$C_p°$ =		122.57		
Liquid phase				
$\Delta_f H°$ =	22.50	22.08	0.42	58COX/GUN
$C_p°$ =		180.95		
$S°$ =		250.61		
$\Delta_f S°$ =		−472.89		
$\Delta_f G°$ =		163.07		
$\ln K_f$ =		−65.78		

Octahydroazocine $C_7H_{15}N$

$(5\times C\text{-}(H)_2(C)_2)+(2\times C\text{-}(H)_2(C)(N))+(1\times N\text{-}(H)(C)_2)+(1\times$ octahydroazocine rsc)

	Literature	-Calculated	= Residual	Reference
Liquid phase				
$C_p°$ =	230.00	230.00	0.00	76CON/GIN

N-Propylpiperidine $C_8H_{17}N$

$(4\times C\text{-}(H)_2(C)_2)+(1\times C\text{-}(H)_3(C))+(3\times C\text{-}(H)_2(C)(N))+(1\times N\text{-}(C)_3)+(1\times$ piperidine rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−90.04		

TABLE 32. Cyclic CHN (32) – Continued

N-Propylpiperidine (Continued) $C_8H_{17}N$

(4×C-(H)$_2$(C)$_2$)+(1×C-(H)$_3$(C))+(3×C-(H)$_2$(C)(N))+(1×N-(C)$_3$)+(1×piperidine rsc)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−147.00	−132.02	−14.98	70PRO/KRE
$C_p°$ =		245.74		
$S°$ =		287.32		
$\Delta_f S°$ =		−964.20		
$\Delta_f G°$ =		155.46		
$\ln K_f$ =		−62.71		

Pyrrolizidine; 1-Azabicyclo[3.3.0]octane $C_7H_{13}N$

(4×C-(H)$_2$(C)$_2$)+(2×C-(H)$_2$(C)(N))+(1×C-(H)(C)$_2$(N))+(1×Pyrrolizidine rsc)+(1×N-(C)$_3$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−3.90	−3.90	0.00	81KOZ/TIM
Liquid phase				
$\Delta_f H°$ =	−48.30	−48.30	0.00	81KOZ/TIM

(*cis*-3,7a-H)-(*cis*-5,7a-H)-3,5-Dimethylpyrrolizidine $C_9H_{17}N$

(4×C-(H)$_2$(C)$_2$)+(3×C-(H)(C)$_2$(N))+(1×N-(C)$_3$)+(2×C-(H)$_3$(C))+(2×-CH$_3$ corr (tertiary))+(1×3,5-Dimethylpyrrolizidine rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−66.70	−66.70	0.00	81KOZ/TIM
Liquid phase				
$\Delta_f H°$ =	−114.40	−114.40	0.00	81KOZ/TIM

TABLE 33. Amides (28)

Methanamide; Formamide CH_3NO

(1×CO-(H)(N))+(1×N-(H)$_2$(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−186.19	−187.39	1.20	58BAU/GUN
$C_p°$ =		46.00		
Liquid phase				
$\Delta_f H°$ =	−251.00	−251.90	0.90	58BAU/GUN
$C_p°$ =	108.11	108.11	0.00	77VOR/PRI

Ethanamide; Acetamide C_2H_5NO

(1×C-(H)$_3$(C))+(1×CO-(C)(N))+(1×N-(H)$_2$(CO) (amides, ureas)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−238.30	−238.52	0.22	75BAR/PIL
$C_p°$ =	63.22	65.23	−2.01	67PUR/SIR
$S°$ =	272.21	263.14	9.07	67PUR/SIR
$\Delta_f S°$ =		−273.04		
$\Delta_f G°$ =		−157.11		
$\ln K_f$ =		63.38		
Liquid phase				
$\Delta_f H°$ =		−296.51		
$C_p°$ =		128.65		
Solid phase				
$\Delta_f H°$ =	−317.00	−306.59	−10.41	75BAR/PIL
$C_p°$ =	91.30	90.95	0.35	84NUR/BER
$S°$ =	115.00	114.69	0.31	84NUR/BER
$\Delta_f S°$ =		−421.49		
$\Delta_f G°$ =		−180.92		
$\ln K_f$ =		72.98		

Propanamide; Propionamide C_3H_7NO

(1×C-(H)$_3$(C))+(1×C-(H)$_2$(CO)(C))+(1×CO-(C)(N))+(1×N-(H)$_2$(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−258.99	−260.36	1.37	75BAR/PIL
$C_p°$ =		89.92		
Liquid phase				
$\Delta_f H°$ =		−320.65		
$C_p°$ =		157.94		

TABLE 33. Amides (28) — Continued

Propanamide; Propionamide (Continued) C_3H_7NO

(1×C–(H)$_3$(C))+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(N))+(1×N–(H)$_2$(CO))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	−338.20	−334.49	−3.71	75BAR/PIL
$C_p°$ =		112.87		
$S°$ =		139.42		
$\Delta_f S°$ =		−533.07		
$\Delta_f G°$ =		−175.56		
lnK_f =		70.82		

2-Methylpropanamide C_4H_9NO

(2×C–(H)$_3$(C))+(2×–CH$_3$ corr (tertiary))+(1×C–(H)(CO)(C)$_2$)+(1×CO–(C)(N))+(1×N–(H)$_2$(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−282.60	−285.55	2.95	89ABB/JIM
Liquid phase				
$\Delta_f H°$ =		−352.37		
$C_p°$ =		182.54		
Solid phase				
$\Delta_f H°$ =	−368.60	−367.84	−0.76	89ABB/JIM
$C_p°$ =		77.89		

2,2-Dimethylpropanamide $C_5H_{11}NO$

(3×C–(H)$_3$(C))+(3×–CH$_3$ corr (quaternary))+(1×C–(CO)(C)$_3$)+(1×CO–(C)(N))+(1×N–(H)$_2$(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−313.10	−312.79	−0.31	88ABB/JIM
Liquid phase				
$\Delta_f H°$ =		−378.75		
$C_p°$ =		209.60		
Solid phase				
$\Delta_f H°$ =	−399.70	−389.10	−10.60	89ABB/JIM
$C_p°$ =		111.75		

TABLE 33. Amides (28) — Continued

Butanamide; Butyramide C_4H_9NO

(1×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(N))+(1×N–(H)$_2$(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−279.20	−280.99	1.79	75BAR/PIL
$C_p°$ =		112.81		
Liquid phase				
$\Delta_f H°$ =		−346.38		
$C_p°$ =		188.36		
Solid phase				
$\Delta_f H°$ =	−365.53	−363.90	−1.63	75BAR/PIL
$C_p°$ =		134.79		
$S°$ =		162.43		
$\Delta_f S°$ =		−646.37		
$\Delta_f G°$ =		−171.18		
lnK_f =		69.05		

Pentanamide $C_5H_{11}NO$

(1×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(N))+(1×N–(H)$_2$(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−290.20	−301.62	11.42	59DAV/JON
$C_p°$ =		135.70		
Liquid phase				
$\Delta_f H°$ =		−372.11		
$C_p°$ =		218.78		
Solid phase				
$\Delta_f H°$ =	−379.49	−393.31	13.82	56YOU/KEI
$C_p°$ =		156.71		
$S°$ =		185.44		
$\Delta_f S°$ =		−759.67		
$\Delta_f G°$ =		−166.81		
lnK_f =		67.29		

Hexanamide $C_6H_{13}NO$

(1×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(N))+(1×N–(H)$_2$(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−324.20	−322.25	−1.95	73LEB/KAT2
$C_p°$ =		158.59		

TABLE 33. Amides (28) – Continued

Hexanamide (Continued) $C_6H_{13}NO$
(1×C–(H)$_3$(C)) + (3×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(N)) + (1×N–(H)$_2$(CO))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−397.90	−397.84	−0.06	73LEB/KAT2
$C_p°$ =		249.20		
Solid phase				
$\Delta_f H°$ =	−423.42	−422.72	−0.70	73LEB/KAT2
$C_p°$ =		178.63		
$S°$ =		208.45		
$\Delta_f S°$ =		−872.97		
$\Delta_f G°$ =		−162.44		
$\ln K_f$ =		65.53		

Octanamide $C_8H_{17}NO$
(1×C–(H)$_3$(C)) + (5×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(N)) + (1×N–(H)$_2$(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−362.80	−363.51	0.71	59DAV/JON
$C_p°$ =		204.37		
Liquid phase				
$\Delta_f H°$ =		−449.30		
$C_p°$ =		310.04		
Solid phase				
$\Delta_f H°$ =	−473.10	−481.54	8.44	56YOU/KEI
$C_p°$ =		222.47		
$S°$ =		254.47		
$\Delta_f S°$ =		−1099.57		
$\Delta_f G°$ =		−153.70		
$\ln K_f$ =		62.00		

N-Methylmethanamide; N-Methylformamide C_2H_5NO
(1×C–(H)$_3$(C)) + (1×N–(H)(C)(CO)) + (1×CO–(H)(N))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−182.93		
Liquid phase				
$\Delta_f H°$ =		−252.71		
$C_p°$ =	125.10	125.09	0.01	79VIS/SOM

TABLE 33. Amides (28) – Continued

N,N-Dimethylmethanamide; N,N-Dimethylformamide C_3H_7NO
(2×C–(H)$_3$(C)) + (1×CO–(H)(N)) + (1×N–(C)$_2$(CO)) + (2×–CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−191.70	−173.03	−18.67	61GEL
Liquid phase				
$\Delta_f H°$ =	−239.20	−230.00	−9.20	72VAS/ZHI
$C_p°$ =	152.00	151.99	0.01	74VIS/SOM

N-Ethylethanamide; N-Ethylacetamide C_4H_9NO
(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)(N)) + (1×N–(H)(C)(CO)) + (1×CO–(C)(N))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−262.36		
Liquid phase				
$\Delta_f H°$ =		−328.12		
$C_p°$ =	179.91	176.05	3.86	71KON/WAD

N-Propylethanamide; N-Propylacetamide $C_5H_{11}NO$
(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×N–(H)(C)(CO)) + (1×CO–(C)(N)) + (1×C–(H)$_2$(C)(N))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−282.99		
Liquid phase				
$\Delta_f H°$ =		−353.85		
$C_p°$ =	207.11	206.47	0.64	71KON/WAD

N-2-Propylethanamide; N-Isopropylacetamide $C_5H_{11}NO$
(3×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(N)) + (2×–CH$_3$ corr (tertiary)) + (1×N–(H)(C)(CO)) + (1×CO–(C)(N))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−297.54		
Liquid phase				
$\Delta_f H°$ =		−363.94		
$C_p°$ =	210.90	210.39	0.51	71KON/WAD

TABLE 33. Amides (28) – Continued

N-Butylethanamide; N-Butylacetamide $C_6H_{13}NO$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(N))+(1×N–(H)(C)(CO))+(1×CO–(C)(N))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−304.80	−303.62	−1.18	65WAD
Liquid phase				
$\Delta_fH°$ =	−380.90	−379.58	−1.32	62WAD
$C_p°$ =	236.00	236.89	−0.89	71KON/WAD

N-(2-Methyl-2-propyl)ethanamide; N-tert-Butylacetamide $C_6H_{13}NO$
(4×C–(H)$_3$(C))+(1×C–(C)$_3$(N))+(3×–CH$_3$ corr (quaternary))+(1×N–(H)(C)(CO))+(1×CO–(C)(N))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−331.97		
Liquid phase				
$\Delta_fH°$ =		−400.61		
$C_p°$ =		238.25		
Solid phase				
$\Delta_fH°$ =		−403.41		
$C_p°$ =	189.95	188.66	1.29	71KON/WAD

N-Methylpropanamide; N-Methylpropionamide C_4H_9NO
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(N))+(1×N–(H)(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−255.90		
Liquid phase				
$\Delta_fH°$ =		−321.46		
$C_p°$ =	179.08	174.92	4.16	71KON/WAD

TABLE 33. Amides (28) – Continued

N,N-Dimethylpropanamide; N,N-Dimethylpropionamide $C_5H_{11}NO$
(3×C–(H)$_3$(C))+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(N))+(1×N–(C)$_2$(CO))+(2×–CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−246.00		
Liquid phase				
$\Delta_fH°$ =		−298.75		
$C_p°$ =	209.20	201.82	7.38	71KON/WAD

N-Methylpentanamide $C_6H_{13}NO$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(N))+(1×N–(H)(C)(CO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−297.16		
Liquid phase				
$\Delta_fH°$ =		−372.92		
$C_p°$ =	228.90	235.76	−6.86	71KON/WAD

N-Butylpentanamide $C_9H_{19}NO$
(2×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(N))+(1×N–(H)(C)(CO))+(1×CO–(C)(N))+(1×C–(H)$_2$(CO)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−366.72		
Liquid phase				
$\Delta_fH°$ =		−455.18		
$C_p°$ =		327.02		
Solid phase				
$\Delta_fH°$ =	−465.10	−477.42	12.32	66SKU/BON
$C_p°$ =		269.42		

N-Butyldiacetamide; N-Butyldiacetylamine $C_8H_{15}NO_2$
(3×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(N))+(2×CO–(C)(N))+(1×N–(C)(CO)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−474.50	−474.50	0.00	65WAD
Liquid phase				
$\Delta_fH°$ =	−538.90	−538.89	−0.01	65WAD

TABLE 33. Amides (28) – Continued

Acetanilide; N-Phenylethanamide; N-Phenylacetamide C_8H_9NO
(1×C–(H)₃(C))+(1×CO–(C)(N))+(1×N–(H)(C_B)(CO))+(1×C_B–(N)(C_B)₂)+(5×C_B–(H)(C_B)₂)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−128.90	−128.61	−0.29	55AIH
Solid phase				
$\Delta_f H°$ =	−209.60	−202.44	−7.46	62WAD
$C_p°$ =	179.30	179.10	0.20	86NIL/WAD

Butanediamide; Succinamide $C_4H_8N_2O_2$
$(2\times N\text{–}(H)_2(CO))+(2\times CO\text{–}(C)(N))+(2\times C\text{–}(H)_2(CO)(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−436.20		
$C_p°$ =		128.38		
Liquid phase				
$\Delta_f H°$ =		−546.08		
$C_p°$ =		242.92		
Solid phase				
$\Delta_f H°$ =	−581.20	−575.50	−5.70	57TAM/LAM
$C_p°$ =		90.84		
$S°$ =		165.46		
$\Delta_f S°$ =		−776.33		
$\Delta_f G°$ =		−344.04		
$\ln K_f$ =		138.78		

Propanediamide; Malonamide $C_3H_6N_2O_2$
$(2\times N\text{–}(H)_2(CO))+(2\times CO\text{–}(C)(N))+(1\times C\text{–}(H)_2(CO)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−423.24		
Liquid phase				
$\Delta_f H°$ =		−520.85		
$C_p°$ =		199.90		
Solid phase				
$\Delta_f H°$ =	−546.10	−538.80	−7.30	55TAV/LAM

TABLE 33. Amides (28) – Continued

N,N-Dimethylethanamide; N,N-Dimethylacetamide C_4H_9NO
$(2\times C\text{–}(H)_3(N))+(1\times C\text{–}(H)_3(CO))+(1\times CO\text{–}(C)(N))+(1\times N\text{–}(C)_2(CO))+(2\times\text{–}CH_3\text{ corr (quaternary)})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−232.60	−224.16	−8.44	74GUT
Liquid phase				
$\Delta_f H°$ =	−278.30	−274.61	−3.69	72VAS/ZHI
$C_p°$ =		172.53		

N-Acetyl-N-butylacetamide $C_8H_{15}NO_2$
$(2\times C\text{–}(H)_3(CO))+(2\times CO\text{–}(C)(N))+(1\times N\text{–}(C)(CO)_2)+(1\times C\text{–}(H)_2(C)(N))+(2\times C\text{–}(H)_2(C)_2)+(1\times C\text{–}(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−474.50	−474.50	0.00	65WAD
Liquid phase				
$\Delta_f H°$ =	−538.90	−538.89	−0.01	65WAD

Benzamide C_7H_7NO
$(5\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(CO))+(1\times CO\text{–}(C_B)(N))+(1\times N\text{–}(H)_2(CO))$

	Literature	*Calculated*	*Residual*	*Reference*
Solid phase				
$\Delta_f H°$ =	−202.14	−202.20	0.06	90STE/CHI
$C_p°$ =	153.82	153.86	−0.04	90STE/CHI

1-Adamantyl carboxamide; Tricyclo[3.3.1.1^{3,7}]decane-1-carboxamide $C_{11}H_{17}NO$
$(4\times C\text{–}(H)(C)_3)+(5\times C\text{–}(H)_2(C)_2)+(1\times C\text{–}(H)(CO)(C)_2)+(1\times CO\text{–}(C)(N))+(1\times N\text{–}(H)_2(CO))+(1\times\text{Adamantane rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−319.00	−310.48	−8.52	89ABB/JIM
Solid phase				
$\Delta_f H°$ =	−427.20	−437.47	10.27	89ABB/JIM

TABLE 34. Ureas (24)

Urea CH_4N_2O

(2×N–(H)$_2$(CO) (amides, ureas))+(1×CO–(N)$_2$), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−235.51	−237.00	1.49	90KAB/MIR
$C_p°$ =	66.40	66.40	0.00	83FRE/GUS
$S°$ =	266.98	266.74	0.24	83FRE/GUS
$\Delta_f S°$ =		−294.17		
$\Delta_f G°$ =		−149.29		
$\ln K_f$ =		60.22		
Liquid phase				
$\Delta_f H°$ =	−320.20	−318.30	−1.90	72ZOR/HUR
Solid phase				
$\Delta_f H°$ =	−333.59	−333.60	0.01	90KAB/MIR
$C_p°$ =	93.08	93.00	0.08	86KOZ/DAL
$S°$ =	104.93	105.00	−0.07	86KOZ/DAL
$\Delta_f S°$ =		−455.90		
$\Delta_f G°$ =		−197.67		
$\ln K_f$ =		79.74		

Methylurea $C_2H_6N_2O$

(1×N–(H)$_2$(CO) (amides, ureas))+(1×CO–(N)$_2$)+
(1×N–(H)(C)(CO) (amides, ureas))+(1×C–(H)$_3$(N))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−233.48	−232.54	−0.94	90KAB/MIR
Liquid phase				
$\Delta_f H°$ =	−318.81	−319.11	0.30	72ZOR/HUR
Solid phase				
$\Delta_f H°$ =	−332.78	−324.89	−7.89	87SIM/KAB
$C_p°$ =		139.95		

N,N-Dimethylurea $C_3H_8N_2O$

(2×C–(H)$_3$(N))+(1×N–(C)$_2$(CO))+(1×CO–(N)$_2$)+
(1×N–(H)$_2$(CO) (amides, ureas))+
(2×–CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−219.96	−222.64	2.68	90KAB/MIR
Liquid phase				
$\Delta_f H°$ =	−296.09	−296.40	0.31	72ZOR/HUR
Solid phase				
$\Delta_f H°$ =	−319.06	−315.53	−3.53	87SIM/KAB

TABLE 34. Ureas (24) – Continued

Trimethylurea $C_4H_{10}N_2O$

(3×C–(H)$_3$(N))+(1×N–(H)(C)(CO) (amides, ureas))+
(1×CO–(N)$_2$)+(1×N–(C)$_2$(CO))+(2×–CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−218.18		
Liquid phase				
$\Delta_f H°$ =		−297.21		
Solid phase				
$\Delta_f H°$ =	−330.50	−306.82	−23.68	56TAV/LAM

Tetramethylurea $C_5H_{12}N_2O$

(4×C–(H)$_3$(N))+(2×N–(C)$_2$(CO))+(1×CO–(N)$_2$)+
(4×–CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−205.57	−208.28	2.71	90KAB/MIR
Liquid phase				
$\Delta_f H°$ =	−262.17	−274.50	12.33	87SIM/KAB
Solid phase				
$\Delta_f H°$ =	−276.27	−297.46	21.19	72ZOR/HUR

Ethylurea $C_3H_8N_2O$

(1×C–(H)$_3$(C))+(1×C–(H)$_2$(C)(N))+
(1×N–(H)(C)(CO) (amides, ureas))+(1×CO–(N)$_2$)+
(1×N–(H)$_2$(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−257.46	−260.84	3.38	90KAB/MIR
Liquid phase				
$\Delta_f H°$ =		−349.91		
Solid phase				
$\Delta_f H°$ =	−357.76	−358.89	1.13	87SIM/KAB
$C_p°$ =		161.87		

TABLE 34. Ureas (24) – Continued

N,N-Diethylurea $C_5H_{12}N_2O$

(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)(N)) + (1×N–(C)$_2$(CO)) + (1×CO–(N)$_2$) + (1×N–(H)$_2$(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−272.31	−270.12	−2.19	90KAB/MIR
Liquid phase				
$\Delta_fH°$ =		−349.22		
Solid phase				
$\Delta_fH°$ =	−372.21	−374.83	2.62	87SIM/KAB

Tetraethylurea $C_9H_{20}N_2O$

(4×C–(H)$_3$(C)) + (4×C–(H)$_2$(C)(N)) + (2×N–(C)$_2$(CO)) + (1×CO–(N)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−316.43	−303.24	−13.19	90KOZ/SIM
Liquid phase				
$\Delta_fH°$ =	−380.04	−380.14	0.10	90KOZ/SIM
Solid phase				
$\Delta_fH°$ =	−403.04	−416.06	13.02	90KOZ/SIM

N-Isopropylurea $C_4H_{10}N_2O$

(2×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(N)) + (2×–CH$_3$ corr (tertiary)) + (1×N–(H)(C)(CO) (amides, ureas)) + (1×CO–(N)$_2$) + (1×N–(H)$_2$(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−289.79	−296.02	6.23	90KAB/MIR
Liquid phase				
$\Delta_fH°$ =		−385.73		
Solid phase				
$\Delta_fH°$ =	−389.49	−390.21	0.72	87SIM/KAB

TABLE 34. Ureas (24) – Continued

N-*n*-Butylurea $C_5H_{12}N_2O$

(1×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(N)) + (1×N–(H)(C)(CO) (amides, ureas)) + (1×CO–(N)$_2$) + (1×N–(H)$_2$(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−313.58	−302.10	−11.48	90KAB/MIR
Liquid phase				
$\Delta_fH°$ =		−401.37		
Solid phase				
$\Delta_fH°$ =	−419.48	−417.71	−1.77	87SIM/KAB
$C_p°$ =		205.71		

N-*sec*-Butylurea $C_5H_{12}N_2O$

(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(N)) + (1×N–(H)(C)(CO) (amides, ureas)) + (1×–CH$_3$ corr (tertiary)) + (1×CO–(N)$_2$) + (1×N–(H)$_2$(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−307.03	−314.39	7.36	90KAB/MIR
Liquid phase				
$\Delta_fH°$ =		−409.28		
Solid phase				
$\Delta_fH°$ =	−413.06	−417.28	4.22	87SIM/KAB

N-*tert*-Butylurea $C_5H_{12}N_2O$

(3×C–(H)$_3$(C)) + (1×C–(C)$_3$(N)) + (3×–CH$_3$ corr (quaternary)) + (1×N–(H)(C)(CO) (amides, ureas)) + (1×CO–(N)$_2$) + (1×N–(H)$_2$(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−314.03	−330.45	16.42	90KAB/MIR
Liquid phase				
$\Delta_fH°$ =		−422.40		
Solid phase				
$\Delta_fH°$ =	−414.73	−430.42	15.69	87SIM/KAB
$C_p°$ =		190.71		

TABLE 34. Ureas (24) — Continued

N,N'-(Di-*tert*-butyl)urea $C_9H_{20}N_2O$

(6×C–(H)$_3$(C))+(2×C–(C)$_3$(N))+(6×–CH$_3$ corr (quat/quat))+(2×N–(H)(C)(CO) (amides, ureas))+(1×CO–(N)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−404.21	−400.38	−3.83	90KAB/MIR
Liquid phase				
$\Delta_f H^\circ$ =		−504.00		
Solid phase				
$\Delta_f H^\circ$ =	−499.81	−514.58	14.77	87SIM/KAB
C_p° =		288.42		

Phenylurea $C_7H_8N_2O$

(5×C$_B$–(H)(C$_B$)$_2$)+(1×C$_B$–(N)(C$_B$)$_2$)+(1×N–(H)(C$_B$)(CO))+(1×CO–(N)$_2$)+(1×N–(H)$_2$(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−127.09		
Solid phase				
$\Delta_f H^\circ$ =	−231.50	−229.45	−2.05	87KUL/KIP
C_p° =		181.15		

N,N'-Diphenylurea $C_{13}H_{12}N_2O$

(10×C$_B$–(H)(C$_B$)$_2$)+(2×C$_B$–(N)(C$_B$)$_2$)+(2×N–(H)(C$_B$)(CO))+(1×CO–(N)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−17.18		
Solid phase				
$\Delta_f H^\circ$ =	−116.83	−125.30	8.47	87SIM/KAB
C_p° =		269.30		

N,N-Diphenylurea $C_{13}H_{12}N_2O$

(10×C$_B$–(H)(C$_B$)$_2$)+(2×C$_B$–(N)(C$_B$)$_2$)+(1×N–(C$_B$)$_2$(CO))+(1×CO–(N)$_2$)+(1×N–(H)$_2$(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H^\circ$ =	−122.70	−122.70	0.00	52MED/THO

TABLE 34. Ureas (24) — Continued

N'-Methyl-N,N-diphenylurea $C_{14}H_{14}N_2O$

(10×C$_B$–(H)(C$_B$)$_2$)+(2×C$_B$–(N)(C$_B$)$_2$)+(1×C–(H)$_3$(N))+(1×N–(C$_B$)$_2$(CO))+(1×CO–(N)$_2$)+(1×N–(H)(C)(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H^\circ$ =	−106.80	−113.99	7.19	52MED/THO

N,N'-Dimethyl-N,N'-diphenylurea $C_{15}H_{16}N_2O$

(2×C–(H)$_3$(N))+(10×C$_B$–(H)(C$_B$)$_2$)+(2×C$_B$–(N))+(1×CO–(N)$_2$)+(2×N–(C)(C$_B$)(CO))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H^\circ$ =	−73.20	−67.78	−5.42	52MED/THO

N'-Ethyl-N,N-diphenylurea $C_{15}H_{16}N_2O$

(10×C$_B$–(H)(C$_B$)$_2$)+(2×C$_B$–(N)(C$_B$)$_2$)+(1×N–(C$_B$)$_2$(CO))+(1×CO–(N)$_2$)+(1×N–(H)(C)(CO) (amides, ureas))+(1×C–(H)$_2$(C)(N))+(1×C–(H)$_3$(C))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H^\circ$ =	−152.60	−147.99	−4.61	52MED/THO

N,N'-Diethyl-N,N'-diphenylurea $C_{17}H_{20}N_2O$

(10×C$_B$–(H)(C$_B$)$_2$)+(2×C$_B$–(N))+(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)(N))+(1×CO–(N)$_2$)+(2×N–(C)(C$_B$)(CO))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H^\circ$ =	−132.30	−135.78	3.48	43PRO/GIL

N'-(1-Naphthyl)-N,N-diphenylurea $C_{23}H_{18}N_2O$

(17×C$_B$–(H)(C$_B$)$_2$)+(3×C$_B$–(N))+(2×C$_{BF}$–(C$_{BF}$)(C$_B$)$_2$)+(1×N–(H)(C$_B$)(CO))+(1×CO–(N)$_2$)+(1×N–(C$_B$)$_2$(CO))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H^\circ$ =	64.00	26.11	37.89	55TAV/LAM

TABLE 34. Ureas (24) – Continued

Tetraphenylurea $C_{25}H_{20}N_2O$
(20 × C_B–(H)(C_B)$_2$) + (4 × C_B–(N)) + (2 × N–(C_B)$_2$(CO)) + (1 × CO–(N)$_2$)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	168.00	88.20	79.80	1897HAU

Acetylurea $C_3H_6N_2O_2$
(1 × C–(H)$_3$(CO)) + (1 × CO–(C)(N)) + (1 × N–(H)(CO)$_2$) + (1 × CO–(N)$_2$) + (1 × N–(H)$_2$(CO) (amides, ureas))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−441.16	−440.52	−0.64	88IMA/MUR
Solid phase				
$\Delta_f H°$ =	−544.21	−540.49	−3.72	88IMA/MUR
$C_p°$ =		127.98		

Methylene-bis-(N,N'-dimethylurea) $C_7H_{16}N_4O_2$
(4 × C–(H)$_3$(N)) + (4 × –CH_3 corr (quaternary)) + (2 × N–(C)$_2$(CO)) + (2 × CO–(N)$_2$) + (2 × N–(H)(C)(CO) (amides, ureas)) + (1 × C–(H)$_2$(N)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−381.84		
Solid phase				
$\Delta_f H°$ =	−547.70	−546.16	−1.54	90KAR/GUT

Trimethyl isocyanurate $C_6H_9N_3O_3$
(3 × CO–(N)$_2$) + (3 × C–(H)$_3$(N)) + (3 × N–(C)(CO)$_2$) + (1 × trimethyl cyanurate rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−589.70	−589.70	0.00	88IMA/MUR
Solid phase				
$\Delta_f H°$ =	−677.92	−677.92	0.00	88IMA/MUR

TABLE 35. Amino acids (38)

Aminoethanoic acid; Glycine $C_2H_5NO_2$
(1 × N–(H)$_2$(C)) + (1 × C–(H)$_2$(CO)(N)) + (1 × CO–(C)(O)) + (1 × O–(H)(CO)) + (1 × Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−375.30	−375.39	0.09	77NGA/SAB
Solid phase				
$\Delta_f H°$ =	−528.10	−528.10	0.00	37HUF/FOX
$C_p°$ =	99.20	99.00	0.20	60HUT/COL
$S°$ =	103.51	103.51	0.00	60HUT/COL
$\Delta_f S°$ =		−535.19		
$\Delta_f G°$ =		−368.53		
$\ln K_f$ =		148.66		

DL-2-Aminopropanoic acid; DL-Alanine $C_3H_7NO_2$
(1 × C–(H)$_3$(C)) + (1 × N–(H)$_2$(C)) + (1 × C–(H)(C)(CO)(N)) + (1 × CO–(C)(O)) + (1 × O–(H)(CO)) + (1 × Zwitterion energy; aliphatic) + (1 × –CH_3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−435.51		
Solid phase				
$\Delta_f H°$ =	−563.58	−557.88	−5.70	37HUF/FOX
$C_p°$ =	121.71	121.68	0.03	37HUF/ELL
$S°$ =	132.21	132.20	0.01	37HUF/ELL
$\Delta_f S°$ =		−642.81		
$\Delta_f G°$ =		−366.23		
$\ln K_f$ =		147.73		

N-Methylglycine; Sarcosine $C_3H_7NO_2$
(1 × C–(H)$_3$(C)) + (1 × N–(H)(C)$_2$) + (1 × C–(H)$_2$(CO)(N)) + (1 × CO–(C)(O)) + (1 × O–(H)(CO)) + (1 × Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−367.30	−369.35	2.05	78SAB/LAF
Solid phase				
$\Delta_f H°$ =	−513.30	−520.74	7.44	77SAB/LAF
$C_p°$ =	128.87	126.45	2.42	77SAB/LAF

TABLE 35. Amino acids (38) — Continued

4-Aminobutanoic acid $C_4H_9NO_2$

(1 × N–(H)$_2$(C)) + (1 × C–(H)$_2$(C)(N)) + (1 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)(O)) + (1 × O–(H)(CO)) + (1 × Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−443.06		
$C_p°$ =		135.40		
Liquid phase				
$\Delta_f H°$ =		−515.35		
$C_p°$ =		235.52		
$S°$ =		247.34		
$\Delta_f S°$ =		−663.98		
$\Delta_f G°$ =		−317.38		
lnK_f =		128.03		
Solid phase				
$\Delta_f H°$ =	−577.90	−588.46	10.56	55STR/SKU2
$C_p°$ =		142.84		
$S°$ =		150.26		
$\Delta_f S°$ =		−761.06		
$\Delta_f G°$ =		−361.55		
lnK_f =		145.85		

5-Aminopentanoic acid $C_5H_{11}NO_2$

(1 × N–(H)$_2$(C)) + (1 × C–(H)$_2$(C)(N)) + (2 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)(O)) + (1 × O–(H)(CO)) + (1 × Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−463.69		
$C_p°$ =		158.29		
Liquid phase				
$\Delta_f H°$ =		−541.08		
$C_p°$ =		265.94		
$S°$ =		279.72		
$\Delta_f S°$ =		−767.91		
$\Delta_f G°$ =		−312.13		
lnK_f =		125.91		
Solid phase				
$\Delta_f H°$ =	−604.10	−617.87	13.77	55STR/SKU2
$C_p°$ =		164.76		
$S°$ =		173.27		
$\Delta_f S°$ =		−874.36		
$\Delta_f G°$ =		−357.07		
lnK_f =		145.04		

7-Aminoheptanoic acid $C_7H_{15}NO_2$

(1 × N–(H)$_2$(C)) + (1 × C–(H)$_2$(C)(N)) + (4 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)(O)) + (1 × O–(H)(CO)) + (1 × Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−504.95		
$C_p°$ =		204.07		
Liquid phase				
$\Delta_f H°$ =		−592.54		
$C_p°$ =		326.78		
$S°$ =		344.48		
$\Delta_f S°$ =		−975.78		
$\Delta_f G°$ =		−301.61		
lnK_f =		121.67		
Solid phase				
$\Delta_f H°$ =	−667.40	−676.69	9.29	66SKU/BON
$C_p°$ =		208.60		
$S°$ =		219.29		
$\Delta_f S°$ =		−1100.97		
$\Delta_f G°$ =		−348.44		
lnK_f =		140.56		

9-Aminononanoic acid $C_9H_{19}NO_2$

(1 × N–(H)$_2$(C)) + (1 × C–(H)$_2$(C)(N)) + (6 × C–(H)$_2$(C)$_2$) + (1 × C–(H)$_2$(CO)(C)) + (1 × CO–(C)(O)) + (1 × O–(H)(CO)) + (1 × Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−546.21		
$C_p°$ =		249.85		
Liquid phase				
$\Delta_f H°$ =		−644.00		
$C_p°$ =		387.62		
$S°$ =		409.24		
$\Delta_f S°$ =		−1183.64		
$\Delta_f G°$ =		−291.10		
lnK_f =		117.43		
Solid phase				
$\Delta_f H°$ =	−727.80	−735.51	7.71	55STR/SKU2
$C_p°$ =		252.44		
$S°$ =		265.31		
$\Delta_f S°$ =		−1327.57		
$\Delta_f G°$ =		−339.70		
lnK_f =		137.03		

TABLE 35. Amino acids (38) – Continued

L-Valine $C_5H_{11}NO_2$

(2×C–(H)$_3$(C)) + (1×C–(H)(C)$_3$) + (2×–CH$_3$ corr (tertiary)) + (1×N–(H)$_2$(C)) + (1×C–(H)(C)(CO)(N)) + (1×CO–(C)(O)) + (1×O–(H)(CO)) + (1×Zwitterion energy; aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−481.20		
Solid phase				
$\Delta_f H°$ =	−617.90	−612.94	−4.96	57TSU/HUN
$C_p°$ =	168.82	140.32	28.50	63HUT/COL
$S°$ =	178.87	172.00	8.87	63HUT/COL
$\Delta_f S°$ =		−875.63		
$\Delta_f G°$ =		−351.87		
$\ln K_f$ =		141.94		

DL-Leucine $C_6H_{13}NO_2$

(2×C–(H)$_3$(C)) + (1×C–(H)(C)$_3$) + (2×–CH$_3$ corr (tertiary)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)(CO)(N)) + (1×N–(H)$_2$(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO)) + (1×Zwitterion energy; aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−501.83		
Solid phase				
$\Delta_f H°$ =	−640.60	−642.35	1.75	37HUF/FOX
$C_p°$ =	194.30	162.24	32.06	37HUF/ELL
$S°$ =	207.10	195.01	12.09	37HUF/ELL
$\Delta_f S°$ =		−988.93		
$\Delta_f G°$ =		−347.50		
$\ln K_f$ =		140.18		

DL-Isoleucine $C_6H_{13}NO_2$

(1×O–(H)(CO)) + (1×CO–(C)(O)) + (1×C–(H)(C)(CO)(N)) + (1×N–(H)$_2$(C)) + (1×C–(H)(C)$_3$) + (1×–CH$_3$ corr (tertiary)) + (1×C–(H)$_2$(C)$_2$) + (2×C–(H)$_3$(C)) + (1×Zwitterion energy; aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−499.57		
Solid phase				
$\Delta_f H°$ =	−635.30	−640.01	4.71	57TSU/HUN
$C_p°$ =		162.24		
$S°$ =		195.01		
$\Delta_f S°$ =		−988.93		
$\Delta_f G°$ =		−345.16		
$\ln K_f$ =		139.24		

TABLE 35. Amino acids (38) – Continued

2-Aminohexanoic acid; Norleucine $C_6H_{13}NO_2$

(1×C–(H)$_3$(C)) + (3×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)(CO)(N)) + (1×N–(H)$_2$(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO)) + (1×Zwitterion energy; aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−495.14		
Solid phase				
$\Delta_f H°$ =	−639.10	−643.77	4.67	55STR/SKU2
$C_p°$ =		187.44		
$S°$ =		210.81		
$\Delta_f S°$ =		−982.71		
$\Delta_f G°$ =		−350.87		
$\ln K_f$ =		141.50		

4-Aminohexanoic acid $C_6H_{13}NO_2$

(1×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(N)) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO)) + (1×N–(H)$_2$(C)) + (1×Zwitterion energy; aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−494.35		
$C_p°$ =		179.96		
Liquid phase				
$\Delta_f H°$ =		−572.54		
$C_p°$ =		300.28		
$S°$ =		310.64		
$\Delta_f S°$ =		−873.30		
$\Delta_f G°$ =		−312.16		
$\ln K_f$ =		125.92		
Solid phase				
$\Delta_f H°$ =	−646.18	−644.51	−1.67	55STR/SKU2

5-Aminohexanoic acid $C_6H_{13}NO_2$

(1×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(N)) + (1×–CH$_3$ corr (tertiary)) + (1×N–(H)$_2$(C)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO)) + (1×Zwitterion energy; aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−496.61		
$C_p°$ =		179.96		

TABLE 35. Amino acids (38) – Continued

5-Aminohexanoic acid (Continued) $C_6H_{13}NO_2$
(1×C–(H)₃(C))+(1×C–(H)(C)₂(N))+
(1×–CH₃ corr (tertiary))+(1×N–(H)₂(C))+(2×C–(H)₂(C)₂)+
(1×C–(H)₂(CO)(C))+(1×CO–(C)(O))+(1×O–(H)(CO))+
(1×Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		−574.72		
$C_p°$ =		300.28		
$S°$ =		310.64		
$\Delta_f S°$ =		−873.30		
$\Delta_f G°$ =		−314.34		
$\ln K_f$ =		126.80		
Solid phase				
$\Delta_f H°$ =	−643.29	−646.85	3.56	55STR/SKU2

DL-Serine; 3-Hydroxy-2-aminopropanoic acid $C_3H_7NO_3$
(1×O–(H)(CO))+(1×CO–(C)(O))+(1×C–(H)(C)(CO)(N))+
(1×N–(H)₂(C))+(1×C–(H)₂(O)(C))+(1×O–(H)(C))+
(1×Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−583.22		
Solid phase				
$\Delta_f H°$ =	−732.70	−737.96	5.26	78SAB/LAF2
$C_p°$ =	132.21	105.40	26.81	75SPI/WAD
$S°$ =		128.86		
$\Delta_f S°$ =		−748.67		
$\Delta_f G°$ =		−514.74		
$\ln K_f$ =		207.64		

3-Hydroxy-2-aminobutanoic acid; DL-Threonine $C_4H_9NO_3$
(1×C–(H)₃(C))+(1×C–(H)(O)(C)₂ (alcohols,peroxides))+
(1×–CH₃ corr (tertiary))+(1×O–(H)(C))+
(1×C–(H)(C)(CO)(N))+(1×N–(H)₂(C))+(1×CO–(C)(O))+
(1×O–(H)(CO))+(1×Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−620.94		
Solid phase				
$\Delta_f H°$ =	−758.80	−786.62	27.82	60POM/MIG
$C_p°$ =		155.70		
$S°$ =		167.77		
$\Delta_f S°$ =		−846.07		
$\Delta_f G°$ =		−534.36		
$\ln K_f$ =		215.56		

TABLE 35. Amino acids (38) – Continued

DL-Ornithine $C_5H_{12}N_2O_2$
(1×N–(H)₂(C) (second, amino acids))+(1×C–(H)₂(C)(N))+
(2×C–(H)₂(C)₂)+(1×C–(H)(C)(CO)(N))+(1×N–(H)₂(C))+
(1×CO–(C)(O))+(1×O–(H)(CO))+
(1×Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−441.30		
Solid phase				
$\Delta_f H°$ =	−652.60	−647.62	−4.98	60PON/MIG
$C_p°$ =	191.33	191.26	0.07	40HUF/FOX
$S°$ =	193.30	193.29	0.01	40HUF/FOX
$\Delta_f S°$ =		−1015.38		
$\Delta_f G°$ =		−344.88		
$\ln K_f$ =		139.12		

DL-Lysine $C_6H_{14}N_2O_2$
(1×O–(H)(CO))+(1×CO–(C)(O))+(1×N–(H)₂(C))+
(1×C–(H)(C)(CO)(N))+(3×C–(H)₂(C)₂)+(1×C–(H)₂(C)(N))+
(1×N–(H)₂(C) (second, amino acids))+
(1×Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−461.93		
Solid phase				
$\Delta_f H°$ =	−678.69	−677.03	−1.66	60PON/MIG
$C_p°$ =		213.18		
$S°$ =		216.30		
$\Delta_f S°$ =		−1128.68		
$\Delta_f G°$ =		−340.51		
$\ln K_f$ =		137.36		

L-Aspartic acid $C_4H_7NO_4$
(2×O–(H)(CO))+(2×CO–(C)(O))+(1×C–(H)(C)(CO)(N))+
(1×N–(H)₂(C))+(1×C–(H)₂(CO)(C))+
(1×Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−804.37		
Solid phase				
$\Delta_f H°$ =	−973.28	−972.45	−0.83	36HUF/ELL
$C_p°$ =	155.18	165.73	−10.55	63HUT/COL2
$S°$ =	170.12	154.15	15.97	63HUT/COL2
$\Delta_f S°$ =		−831.64		
$\Delta_f G°$ =		−724.50		
$\ln K_f$ =		292.26		

TABLE 35. Amino acids (38) — Continued

L-Glutamic acid $C_5H_9NO_4$

(2×O–(H)(CO)) + (2×CO–(C)(O)) + (1×C–$(H)_2(C)_2$) + (1×C–(H)(C)(CO)(N)) + (1×N–$(H)_2$(C)) + (1×Zwitterion energy; aliphatic) + (1×C–$(H)_2$(CO)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−825.00		
Solid phase				
Δ_fH° =	−1009.70	−1001.86	−7.84	52TSU/HUN
C_p° =	175.06	187.65	−12.59	63HUT/COL2
S° =	188.20	177.16	11.04	63HUT/COL2
Δ_fS° =		−944.95		
Δ_fG° =		−720.12		
$\ln K_f$ =		290.49		

L-Asparagine $C_4H_8N_2O_3$

(1×O–(H)(CO)) + (1×CO–(C)(O)) + (1×C–(H)(C)(CO)(N)) + (1×C–$(H)_2$(CO)(C)) + (1×CO–(C)(N)) + (1×N–$(H)_2$(CO) (amino acids)) + (1×N–$(H)_2$(C)) + (1×Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−609.09		
Solid phase				
Δ_fH° =	−788.70	−791.05	2.35	36HUF/ELL
C_p° =	159.80	161.03	−1.23	32HUF/BOR
S° =	174.50	173.27	1.23	32HUF/BOR
Δ_fS° =		−843.62		
Δ_fG° =		−539.53		
$\ln K_f$ =		217.64		

L-Glutamine $C_5H_{10}N_2O_3$

(1×O–(H)(CO)) + (1×CO–(C)(O)) + (1×C–(H)(C)(CO)(N)) + (1×C–$(H)_2$(CO)(C)) + (1×C–$(H)_2(C)_2$) + (1×CO–(C)(N)) + (1×N–$(H)_2$(CO) (amino acids)) + (1×N–$(H)_2$(C)) + (1×Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−629.72		
Solid phase				
Δ_fH° =	−825.50	−820.46	−5.04	57TSU/HUN
C_p° =	184.18	182.98	1.20	63HUT/COL2
S° =	195.06	196.28	−1.22	63HUT/COL2
Δ_fS° =		−956.92		
Δ_fG° =		−535.15		
$\ln K_f$ =		215.88		

TABLE 35. Amino acids (38) — Continued

DL-Phenylalanine $C_9H_{11}NO_2$

(5×C_B–(H)$(C_B)_2$) + (1×C_B–(C)$(C_B)_2$) + (1×C–$(H)_2$(C)(C_B)) + (1×C–(H)(C)(CO)(N)) + (1×N–$(H)_2$(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO)) + (1×Zwitterion energy, aromatic I)

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−319.64		
Solid phase				
Δ_fH° =	−459.80	−461.25	1.45	52BRE/DER
C_p° =	203.01	205.00	−1.99	63COL/HUT
S° =	213.64	211.06	2.58	63COL/HUT
Δ_fS° =		−859.53		
Δ_fG° =		−203.98		
$\ln K_f$ =		82.28		

L-Tyrosine $C_9H_{11}NO_3$

(1×O–(H)(C_B)) + (1×C_B–(O)$(C_B)_2$) + (4×C_B–(H)$(C_B)_2$) + (1×C_B–(C)$(C_B)_2$) + (1×C–$(H)_2$(C)(C_B)) + (1×C–(H)(C)(CO)(N)) + (1×N–$(H)_2$(C)) + (1×CO–(C)(O)) + (1×O–(H)(CO)) + (1×Zwitterion energy, aromatic I)

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−498.50		
Solid phase				
Δ_fH° =	−685.10	−666.03	−19.07	37HUF/FOX
C_p° =	216.44	213.83	2.61	63COL/HUT
S° =	214.01	218.52	−4.51	63COL/HUT
Δ_fS° =		−954.59		
Δ_fG° =		−381.42		
$\ln K_f$ =		153.86		

2-Aminobenzoic acid $C_7H_7NO_2$

(4×C_B–(H)$(C_B)_2$) + (1×N–$(H)_2(C_B)$) + (1×C_B–(N)$(C_B)_2$) + (1×O–(H)(CO)) + (1×CO–(O)(C_B)) + (1×C_B–(CO)$(C_B)_2$) + (1×Zwitterion energy, aromatic II) + (1×NH_2–COOH (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−296.00	−290.61	−5.39	74SAB/CHA
Liquid phase				
Δ_fH° =	−380.40	−380.00	−0.40	71LEB/GUT
C_p° =		258.70		

TABLE 35. Amino acids (38) – Continued

2-Aminobenzoic acid (Continued) $C_7H_7NO_2$

$(4\times C_B-(H)(C_B)_2)+(1\times N-(H)_2(C_B))+(1\times C_B-(N)(C_B)_2)+(1\times O-(H)(CO))+(1\times CO-(O)(C_B))+(1\times C_B-(CO)(C_B)_2)+$ (1 × Zwitterion energy, aromatic II) + (1 × NH_2–COOH (*ortho* corr))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−400.90	−401.73	0.83	71LEB/GUT
$C_p°$ =	165.27	165.27	0.00	26AND/LYN
$S°$ =		168.42		
$\Delta_fS°$ =		−629.55		
$\Delta_fG°$ =		−214.03		
$\ln K_f$ =		86.34		

3-Aminobenzoic acid $C_7H_7NO_2$

$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(N)(C_B)_2)+(1\times N-(H)_2(C_B))+(1\times C_B-(CO)(C_B)_2)+(1\times CO-(O)(C_B))+(1\times O-(H)(CO))+$ (1 × Zwitterion energy, aromatic II) + (1 × NH_2–COOH (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−283.60	−290.61	7.01	74SAB/CHA
Liquid phase				
$\Delta_fH°$ =	−389.80	−390.00	0.20	71LEB/GUT
$C_p°$ =		258.70		
Solid phase				
$\Delta_fH°$ =	−410.70	−411.73	1.03	71LEB/GUT
$C_p°$ =	162.76	162.76	0.00	26AND/LYN
$S°$ =		168.42		
$\Delta_fS°$ =		−629.55		
$\Delta_fG°$ =		−224.03		
$\ln K_f$ =		90.37		

4-Aminobenzoic acid $C_7H_7NO_2$

$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(N)(C_B)_2)+(1\times N-(H)_2(C_B))+(1\times C_B-(CO)(C_B)_2)+(1\times CO-(O)(C_B))+(1\times O-(H)(CO))+$ (1 × Zwitterion energy, aromatic II)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−296.70	−290.61	−6.09	74SAB/CHA
Liquid phase				
$\Delta_fH°$ =	−391.90	−392.00	0.10	71LEB/GUT
$C_p°$ =		258.70		

TABLE 35. Amino acids (38) – Continued

2-Aminobenzoic acid (Continued) $C_7H_7NO_2$

$(4\times C_B-(H)(C_B)_2)+(1\times N-(H)_2(C_B))+(1\times C_B-(N)(C_B)_2)+(1\times O-(H)(CO))+(1\times CO-(O)(C_B))+(1\times C_B-(CO)(C_B)_2)+$ (1 × Zwitterion energy, aromatic II) + (1 × NH_2–COOH (*ortho* corr))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−412.80	−415.73	2.93	77NAB/SAB
$C_p°$ =	177.82	169.98	7.84	26AND/LYN
$S°$ =		168.42		
$\Delta_fS°$ =		−629.55		
$\Delta_fG°$ =		−228.03		
$\ln K_f$		91.99		

N-Phenylglycine $C_8H_9NO_2$

$(5\times C_B-(H)(C_B)_2)+(1\times C_B-(N)(C_B)_2)+(1\times N-(H)(C)(C_B))+(1\times C-(H)_2(CO)(N))+(1\times CO-(C)(O))+(1\times O-(H)(CO))+$ (1 × Zwitterion energy, aromatic II)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−267.89		
Solid phase				
$\Delta_fH°$ =	−402.50	−398.75	−3.75	04FIS/WRE
$C_p°$ =	176.60	180.15	−3.55	80SAB/SKO

Hippuric acid; N-Benzoylglycine $C_9H_9NO_3$

$(5\times C_B-(H)(C_B)_2)+(1\times C_B-(CO)(C_B)_2)+(1\times CO-(C_B)(N))+(1\times N-(H)(C)(CO)$ (amino acids)$)+(1\times C-(H)_2(CO)(N))+(1\times CO-(C)(O))+(1\times O-(H)(CO))+$ (1 × Zwitterion energy, aromatic II)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−608.90	−609.15	0.25	61HUB/FRO
$C_p°$ =	214.35	214.56	−0.21	41HUF

Glycylglycine $C_4H_8N_2O_3$

$(1\times N-(H)_2(C))+(2\times C-(H)_2(CO)(N))+(1\times CO-(C)(N))+(1\times N-(H)(C)(CO)$ (amino acids)$)+(1\times CO-(C)(O))+(1\times O-(H)(CO))+$ (1 × Zwitterion energy; aliphatic)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−528.03		
Solid phase				
$\Delta_fH°$ =	−747.68	−748.15	0.17	92DIA/DOM
$C_p°$ =	163.97	163.22	0.75	69HUT/COL2

TABLE 35. Amino acids (38) — Continued

DL-Alanylglycine $C_5H_{10}N_2O_3$

(1×N–(H)$_2$(C))+(1×C–(H)(C)(CO)(N))+(1×C–(H)$_3$(C))+
(1×–CH$_3$ corr (tertiary))+(1×CO–(C)(N))+
(1×N–(H)(C)(CO) (amino acids))+(1×C–(H)$_2$(CO)(N))+
(1×CO–(C)(O))+(1×O–(H)(CO))+
(1×Zwitterion energy; aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		−588.15		
Solid phase				
$\Delta_fH°$ =	−777.80	−777.93	0.13	42HUF
$C_p°$ =	182.83	185.90	−3.07	41HUF

DL-Alanyl-DL-alanine $C_6H_{12}N_2O_3$

(1×N–(H)$_2$(C))+(2×C–(H)$_3$(C))+(2×–CH$_3$ corr (tertiary))+
(2×C–(H)(C)(CO)(N))+(1×CO–(C)(N))+
(1×N–(H)(C)(CO) (amino acids))+(1×CO–(C)(O))+
(1×O–(H)(CO))+(1×Zwitterion energy; aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		−648.27		
Solid phase				
$\Delta_fH°$ =	−807.32	−807.71	0.39	92DIA/DOM
$C_p°$ =		208.58		

DL-Leucylglycine $C_8H_{16}N_2O_3$

(2×C–(H)$_3$(C))+(1×C–(H)(C)$_3$)+(1×–CH$_3$ corr (tertiary))+
(1×C–(H)$_2$(C)$_2$)+(1×N–(H)$_2$(C))+(1×C–(H)(C)(CO)(N))+
(1×CO–(C)(N))+(1×N–(H)(C)(CO) (amino acids))+
(1×C–(H)$_2$(CO)(N))+(1×CO–(C)(O))+(1×O–(H)(CO))+
(1×Zwitterion energy; aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		−652.21		
Solid phase				
$\Delta_fH°$ =	−859.80	−860.06	0.26	42HUF
$C_p°$ =	256.34	226.46	29.88	41HUF

TABLE 35. Amino acids (38) — Continued

N-Glycyl-DL-valine $_7H_{14}N_2O_3$

(1×N–(H)$_2$(C))+(1×C–(H)$_2$(CO)(N))+(1×CO–(C)(N +
(1×N–(H)(C)(CO) (amino acids))+(1×C–(H)(C)(CO) I))+
(1×CO–(C)(O))+(1×O–(H)(CO))+(1×C–(H)(C)$_3$)+
(2×C–(H)$_3$(C))+(2×–CH$_3$ corr (tertiary))+
(1×Zwitterion energy; aliphatic)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		−633.84		
Solid phase				
$\Delta_fH°$ =	−835.00	−832.99	−2.01	62P /ALE
$C_p°$ =		204.54		

Hippurylglycine $H_{12}N_2O_4$

(5×C$_B$–(H)(C$_B$)$_2$)+(1×C$_B$–(CO)(C$_B$)$_2$)+(1×CO–(C$_B$)( )+
(2×N–(H)(C)(CO) (amino acids))+(2×C–(H)$_2$(CO)(N +
(1×CO–(C)(N))+(1×CO–(C)(O))+(1×O–(H)(CO))+
(1×Zwitterion energy, aromatic II)

	Literature	– Calculated	= Residual	Reference
Solid phase				
$\Delta_fH°$ =	−832.00	−829.20	−2.80	42HUF
$C_p°$ =	278.00	278.78	−0.78	41HUF

Glycylphenylalanine $C_{11}H_{14}N_2O_3$

(1×N–(H)$_2$(C))+(1×C–(H)$_2$(CO)(N))+(1×CO–(C)(N))+
(1×N–(H)(C)(CO) (amino acids))+(1×C–(H)(C)(CO)(N))+
(1×C–(H)$_2$(C)(C$_B$))+(5×C$_B$–(H)(C$_B$)$_2$)+(1×C$_B$–(C)(C$_B$)$_2$)+
(1×CO–(C)(O))+(1×O–(H)(CO))+
(1×Zwitterion energy, aromatic I)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		−472.28		
Solid phase				
$\Delta_fH°$ =	−684.50	−681.30	−3.20	62PON/ALE
$C_p°$ =		269.22		

TABLE 35. Amino acids (38) – Continued

Alanylphenylalanine $C_{12}H_{16}N_2O_3$
(1×N–(H)$_2$(C)) + (2×C–(H)(C)(CO)(N)) + (1×C–(H)$_3$(C)) + (1×–CH$_3$ corr (tertiary)) + (1×CO–(C)(N)) + (1×N–(H)(C)(CO) (amino acids)) + (1×C–(H)$_2$(C)(C$_B$)) + (5×C$_B$–(H)(C$_B$)$_2$) + (1×C$_B$–(C)(C$_B$)$_2$) + (1×CO–(C)(O)) + (1×O–(H)(CO)) + (1×Zwitterion energy, aromatic I)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−532.40		
Solid phase				
$\Delta_f H°$ =	−710.40	−711.08	0.68	62PON/ALE
$C_p°$ =		291.90		

Glycylalanylphenylalanine $C_{14}H_{19}N_3O_4$
(1×N–(H)$_2$(C)) + (1×C–(H)$_2$(CO)(N)) + (2×CO–(C)(N)) + (2×N–(H)(C)(CO) (amino acids)) + (2×C–(H)(C)(CO)(N)) + (1×C–(H)$_3$(C)) + (1×–CH$_3$ corr (tertiary)) + (1×CO–(C)(O)) + (1×O–(H)(CO)) + (1×C–(H)$_2$(C)(C$_B$)) + (5×C$_B$–(H)(C$_B$)$_2$) + (1×C$_B$–(C)(C$_B$)$_2$) + (1×Zwitterion energy, aromatic I)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−685.04		
Solid phase				
$\Delta_f H°$ =	−926.80	−931.13	4.33	62PON/ALE
$C_p°$ =		356.12		

Valylphenylalanine $C_{14}H_{20}N_2O_3$
(1×N–(H)$_2$(C)) + (2×C–(H)(C)(CO)(N)) + (2×C–(H)$_3$(C)) + (1×C–(H)(C)$_3$) + (1×–CH$_3$ corr (tertiary)) + (1×CO–(C)(N)) + (1×N–(H)(C)(CO) (amino acids)) + (1×C–(H)$_2$(C)(C$_B$)) + (5×C$_B$–(H)(C$_B$)$_2$) + (1×C$_B$–(C)(C$_B$)$_2$) + (1×CO–(C)(O)) + (1×O–(H)(CO)) + (1×Zwitterion energy, aromatic I)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−575.83		
Solid phase				
$\Delta_f H°$ =	−766.10	−763.80	−2.30	63PON/ALE
$C_p°$ =		310.54		

TABLE 36. Nitroso (9)

Dimethylnitrosoamine $C_2H_6N_2O$
(2×C–(H)$_3$(N)) + (2×–CH$_3$ corr (quaternary)) + (1×N–(C)$_2$(NO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−3.30	−3.64	0.34	67KOR/PEP
Liquid phase				
$\Delta_f H°$ =	−44.80	−45.00	0.20	67KOR/PEP

Nitrosobenzene C_6N_5NO
(5×C$_B$–(H)(C$_B$)$_2$) + (1×C$_B$–(NO)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		90.55		
Solid phase				
$\Delta_f H°$ =	−30.00	55.65	−85.65	30DRU/FLA

N-Nitrosopiperidine $C_5H_{10}N_2O$
(3×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(C)(N)) + (1×N–(C)$_2$(NO)) + (1×N-Nitrosopiperidine rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	16.60	16.71	−0.11	74GOL/PEP
Liquid phase				
$\Delta_f H°$ =	−31.10	−31.09	−0.01	74GOL/PEP

4-Nitroso-1-naphthol $C_{10}H_7NO_2$
(6×C$_B$–(H)(C$_B$)$_2$) + (2×C$_{BF}$–(C$_{BF}$)(C$_B$)$_2$) + (1×C$_B$–(O)) + (1×naphthalene 2 sub) + (1×O–(H)(C$_B$)) + (1×C$_B$–(NO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−20.50	−20.49	−0.01	68HAM/FAG
Solid phase				
$\Delta_f H°$ =	−107.90	−107.87	−0.03	68HAM/FAG

TABLE 36. Nitroso (9) – Continued

1,3,5-Cyclotrimethylenetrinitrosamine; R-salt $C_3H_6N_6O_6$
(3 × C–(H)$_2$(N)$_2$) + (3 × N–(C)$_2$(NO)) + (1 × R–salt rsc)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	282.30	282.30	0.00	49MED/THO

1,5-Dinitrosopentamethylenetetramine; 3,7-Dinitroso-1,3,5,7-tetraazabicyclo[3.3.1]nonane $C_5H_{10}N_6O_2$
(5 × C–(H)$_2$(N)$_2$) + (2 × N–(C)$_3$) + (2 × N–(C)$_2$(NO)) + (1 × DINO–PMTA rsc)

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	228.70	228.70	0.00	56MED/THO

Di-*n*-propyldiazene N-oxide $C_6H_{14}N_2O$
(2 × C–(H)$_3$(C)) + (2 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(C)(N_A)) + (1 × N_A–(C)) + (1 × N_A–(oxide)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−31.00	−16.88	−14.12	81BYS
Liquid phase				
$\Delta_fH°$ =	−82.70	−70.58	−12.12	81BYS

Di-*tert*-butyldiazene N-oxide $C_8H_{18}N_2O$
(6 × C–(H)$_3$(C)) + (2 × C–(C)$_3$(N_A)) + (1 × N_A–(C)) + (1 × N_A–(oxide)(C)) + (6 × –CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−107.60	−107.62	0.02	81BYS
Liquid phase				
$\Delta_fH°$ =	−153.50	−153.50	0.00	81BYS

1,4-Dicyanatobenzene; 1,4-Dicyanobenzene di-N-oxide $C_8H_4N_2O_2$
(4 × C_B–(H)(C_B)$_2$) + (2 × C_B–(CNO))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	410.50	410.50	0.00	92ACR/TUC
Solid phase				
$\Delta_fH°$ =	337.50	337.50	0.00	92ACR/TUC

TABLE 37. Nitro compounds (50)

Nitromethane CH_3NO_2
(1 × C–(H)$_3$(NO$_2$), Nitromethane), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−74.86	−74.86	0.00	54MCC/SCO
$C_p°$ =	57.32	57.32	0.00	69STU/WES
$S°$ =	275.01	275.01	0.00	69STU/WES
$\Delta_fS°$ =		−227.38		
$\Delta_fG°$ =		−7.07		
$\ln K_f$ =		2.85		
Liquid phase				
$\Delta_fH°$ =	−112.60	−112.60	0.00	73LEB/RYA
$C_p°$ =	105.98	105.98	0.00	47JON/GIA
$S°$ =	171.75	171.75	0.00	47JON/GIA
$\Delta_fS°$ =		−330.64		
$\Delta_fG°$ =		−14.02		
$\ln K_f$ =		5.66		

Dinitromethane $CH_2N_2O_4$
(1 × C–(H)$_2$(NO$_2$)$_2$, Dinitromethane)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−58.90	−58.90	0.00	71KNO/MIR
Liquid phase				
$\Delta_fH°$ =	−104.90	−104.90	0.00	71KNO/MIR

Trinitromethane CHN_3O_6
(1 × C–(H)(NO$_2$)$_3$, Trinitromethane)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−0.30	−0.30	0.00	67MIR/LEB
Liquid phase				
$\Delta_fH°$ =	−32.80	−32.80	0.00	67MIR/LEB
Solid phase				
$\Delta_fH°$ =	−48.00	−48.00	0.00	67MIR/LEB

Tetranitromethane CN_4O_8
(1 × C–(NO$_2$)$_4$, Tetranitromethane)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	82.30	82.30	0.00	75LEB/MIR

TABLE 37. Nitro compounds (50) — Continued

Tetranitromethane (Continued) CN_4O_8
($1\times C-(NO_2)_4$, Tetranitromethane)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	38.30	38.30	0.00	75LEB/MIR

Nitroethane $C_2H_5NO_2$
$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)(NO_2))$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−102.30	−102.76	0.46	49HOL/DOR
$C_p°$ =	78.20	78.87	−0.67	69STU/WES
$S°$ =	315.43	316.02	−0.59	69STU/WES
$\Delta_fS°$ =		−322.68		
$\Delta_fG°$ =		−6.55		
$\ln K_f$ =		2.64		
Liquid phase				
$\Delta_fH°$ =	−143.90	−141.11	−2.79	73LEB/RYA
$C_p°$ =	134.22	134.22	0.00	66LIU/ZIE

1-Nitropropane $C_3H_7NO_2$
$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(NO_2))$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−123.80	−123.39	−0.41	49HOL/DOR
$C_p°$ =	102.13	101.76	0.37	69STU/WES
$S°$ =	355.64	355.18	0.46	69STU/WES
$\Delta_fS°$ =		−419.83		
$\Delta_fG°$ =		1.78		
$\ln K_f$ =		−0.72		
Liquid phase				
$\Delta_fH°$ =	−167.20	−166.84	−0.36	73LEB/RYA
$C_p°$ =		164.64		

1-Nitrobutane $C_4H_9NO_2$
$(1\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(NO_2))$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−143.90	−144.02	0.12	49HOL/DOR
$C_p°$ =	124.89	124.65	0.24	69STU/WES
$S°$ =	394.47	394.34	0.13	69STU/WES
$\Delta_fS°$ =		−516.98		
$\Delta_fG°$ =		10.12		
$\ln K_f$ =		−4.08		

TABLE 37. Nitro compounds (50) — Continued

1-Nitrobutane (Continued) $C_4H_9NO_2$
$(1\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(NO_2))$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−192.51	−192.57	0.06	49HOL/DOR
$C_p°$ =		195.06		

1-Nitropentane $C_5H_{11}NO_2$
$(1\times C-(H)_3(C))+(3\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(NO_2))$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−164.65		
$C_p°$ =		147.54		
$S°$ =		433.50		
$\Delta_fS°$ =		−614.13		
$\Delta_fG°$ =		18.45		
$\ln K_f$ =		−7.44		
Liquid phase				
$\Delta_fH°$ =	−215.40	−218.30	2.90	73LEB/RYA
$C_p°$ =		225.48		

2-Nitropropane $C_3H_7NO_2$
$(2\times C-(H)_3(C))+(1\times C-(H)(C)_2(NO_2))+$
$(2\times -CH_3$ corr (tertiary)), $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−139.00	−142.04	3.04	49HOL/DOR
$C_p°$ =	101.50	101.04	0.46	69STU/WES
$S°$ =	347.69	345.93	1.76	69STU/WES
$\Delta_fS°$ =		−429.08		
$\Delta_fG°$ =		−14.11		
$\ln K_f$ =		5.69		
Liquid phase				
$\Delta_fH°$ =	−180.30	−182.08	1.78	58CAS/FLE

2-Nitrobutane $C_4H_9NO_2$
$(1\times C-(H)_2(C)_2)+(2\times C-(H)_3(C))+(1\times C-(H)(C)_2(NO_2))+$
$(1\times -CH_3$ corr (tertiary)), $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−163.60	−160.41	−3.19	49HOL/DOR
$C_p°$ =	123.47	123.93	−0.46	69STU/WES
$S°$ =	383.34	385.09	−1.75	69STU/WES
$\Delta_fS°$ =		−526.23		
$\Delta_fG°$ =		−3.51		
$\ln K_f$ =		1.42		

TABLE 37. Nitro compounds (50) — Continued

2-Nitrobutane (Continued) $C_4H_9NO_2$
(1×C-(H)$_2$(C)$_2$)+(2×C-(H)$_3$(C))+(1×C-(H)(C)$_2$(NO$_2$))+(1×-CH$_3$ corr (tertiary)), σ = 18

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−207.50	−205.63	−1.87	49HOL/DOR

2-Methyl-2-nitropropane $C_4H_9NO_2$
(3×C-(H)$_3$(C))+(1×C-(C)$_3$(NO$_2$))+(3×-CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−177.10	−177.11	0.01	70KNO/MIR
Liquid phase				
$\Delta_fH°$ =	−217.20	−217.20	0.00	70KNO/MIR
Solid phase				
$\Delta_fH°$ =	−229.80	−229.82	0.02	70KNO/MIR

1,1-Dinitroethane $C_2H_4N_2O_4$
(1×C-(H)$_3$(C))+(1×C-(H)(C)(NO$_2$)$_2$)+(1×-CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−81.32		
Liquid phase				
$\Delta_fH°$ =	−148.20	−138.59	−9.61	68LEB/RYA2

1,1-Dinitropropane $C_3H_6N_2O_4$
(1×C-(H)$_3$(C))+(1×C-(H)$_2$(C)$_2$)+(1×C-(H)(C)(NO$_2$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−100.70	−99.69	−1.01	49HOL/DOR
Liquid phase				
$\Delta_fH°$ =	−163.20	−162.14	−1.06	68LEB/RYA2

TABLE 37. Nitro compounds (50) — Continued

1,1-Dinitropentane $C_5H_{10}N_2O_4$
(1×C-(H)$_3$(C))+(3×C-(H)$_2$(C)$_2$)+(1×C-(H)(C)(NO$_2$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		140.95		
Liquid phase				
$\Delta_fH°$ =	−216.90	−213.60	−3.30	68LEB/RYA2

1,2-Dinitroethane $C_2H_4N_2O_4$
(2×C-(H)$_2$(C)(NO$_2$))+(1×NO$_2$-NO$_2$ (corr, aliph, adjacent))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−101.00		
C_p° =		106.28		
Liquid phase				
$\Delta_fH°$ =	−165.20	−167.00	1.80	68LEB/RYA2
C_p° =		195.48		
Solid phase				
$\Delta_fH°$ =	−178.80	−178.00	−0.80	68LEB/RYA2

1,3-Dinitropropane $C_3H_6N_2O_4$
(1×C-(H)$_2$(C)$_2$)+(2×C-(H)$_2$(C)(NO$_2$))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−141.63		
C_p° =		129.17		
Liquid phase				
$\Delta_fH°$ =	−215.50	−212.73	−2.77	71LEB/GUT
C_p° =		225.90		

1,4-Dinitrobutane $C_4H_8N_2O_4$
(2×C-(H)$_2$(C)$_2$)+(2×C-(H)$_2$(C)(NO$_2$))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−162.26		
C_p° =		152.06		

TABLE 37. Nitro compounds (50) – Continued

1,4-Dinitrobutane (Continued) $C_4H_8N_2O_4$
$(2\times C\text{–}(H)_2(C)_2)+(2\times C\text{–}(H)_2(C)(NO_2))$

	Literature	Calculated	Residual	Reference
Liquid phase				
Δ_fH° =	−237.50	−238.46	0.96	68LEB/RYA2
C_p° =		256.32		
Solid phase				
Δ_fH° =	−249.20	−256.82	7.62	68LEB/RYA2

2,2-Dinitropropane $C_3H_6N_2O_4$
$(2\times C\text{–}(H)_3(C))+(1\times C\text{–}(C)_2(NO_2)_2)+$
$(2\times\text{–}CH_3\text{ corr (quaternary)})$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−122.14		
Liquid phase				
Δ_fH° =	−181.20	−181.20	0.00	68LEB/RYA2
Solid phase				
Δ_fH° =	−192.50	−192.48	−0.02	68LEB/RYA2
C_p° =	206.27	206.28	−0.01	58BIL/NOL

Nitrobenzene $C_6H_5NO_2$
$(5\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(NO_2)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	67.50	67.60	−0.10	71KUS/WAD
Liquid phase				
Δ_fH° =	12.50	12.50	0.00	71LEB/KAT2
C_p° =	186.70	186.70	0.00	36PAR/TOD
S° =	224.30	224.30	0.00	36PAR/TOD
Δ_fS° =		−437.36		
Δ_fG° =		142.90		
$\ln K_f$ =		−57.64		

1,2-Dinitrobenzene $C_6H_4N_2O_4$
$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(NO_2)(C_B)_2)+$
$(1\times NO_2\text{–}NO_2$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		96.34		

1,2-Dinitrobenzene (Continued) $C_6H_4N_2O_4$
$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(NO_2)(C_B)_2)+$
$(1\times NO_2\text{–}NO_2$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Liquid phase				
Δ_fH° =	21.21	21.29	−0.08	71LEB/RYA
Solid phase				
Δ_fH° =	−1.80	1.72	−3.52	71LEB/RYA
C_p° =	186.20	186.20	0.00	26AND

1,3-Dinitrobenzene $C_6H_4N_2O_4$
$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(NO_2)(C_B)_2)+$
$(1\times NO_2\text{–}NO_2$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	53.80	63.34	−9.54	50NIT/SEK2
Liquid phase				
Δ_fH° =	−6.90	−10.46	3.56	71LEB/RYA
Solid phase				
Δ_fH° =	−27.40	−25.38	−2.02	71LEB/RYA
C_p° =	188.28	188.28	0.00	26AND

1,4-Dinitrobenzene $C_6H_4N_2O_4$
$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(NO_2)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		52.34		
Liquid phase				
Δ_fH° =	−14.40	−23.96	9.56	26AND/LYN
C_p° =		237.32		
S° =		275.38		
Δ_fS° =		−621.79		
Δ_fG° =		161.43		
$\ln K_f$ =		−65.12		
Solid phase				
Δ_fH° =	−38.70	−38.88	0.18	71LEB/RYA
C_p° =	192.00	182.44	9.56	26AND/LYN
S° =		311.92		
Δ_fS° =		−585.25		
Δ_fG° =		135.61		
$\ln K_f$ =		−54.70		

TABLE 37. Nitro compounds (50) – Continued

1,3,5-Trinitrobenzene $C_6H_3N_3O_6$

$(3 \times C_B\text{–}(H)(C_B)_2) + (3 \times C_B\text{–}(NO_2)(C_B)_2) + (3 \times NO_2\text{–}NO_2$ (*meta* corr))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	70.10	70.08	0.02	78CUN/PAL
Liquid phase				
$\Delta_f H°$ =	−20.50	−19.92	−0.58	71LEB/RYA
Solid phase				
$\Delta_f H°$ =	−37.20	−37.41	0.21	71LEB/RYA
$C_p°$ =		230.79		

1-Nitronaphthalene $C_{10}H_7NO_2$

$(7 \times C_B\text{–}(H)(C_B)_2) + (2 \times C_{BF}\text{–}(C_{BF})(C_B)_2) + (1 \times C_B\text{–}(NO_2)(C_B)_2) + (1 \times$ naphthalene 1 sub)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	149.70	135.42	14.28	50NIT/SEK2
Liquid phase				
$\Delta_f H°$ =		60.48		
$C_p°$ =		251.10		
$S°$ =		270.96		
$\Delta_f S°$ =		−544.23		
$\Delta_f G°$ =		222.74		
$\ln K_f$ =		−89.85		
Solid phase				
$\Delta_f H°$ =	42.60	41.41	1.19	37BAD
$C_p°$ =		196.47		
$S°$ =		257.71		
$\Delta_f S°$ =		−557.48		
$\Delta_f G°$ =		207.62		
$\ln K_f$ =		−83.75		

1-Methyl-2-nitrobenzene; 2-Nitrotoluene $C_7H_7NO_2$

$(1 \times C\text{–}(H)_3(C)) + (4 \times C_B\text{–}(H)(C_B)_2) + (1 \times C_B\text{–}(C)(C_B)_2) + (1 \times C_B\text{–}(NO_2)(C_B)_2) + (1 \times NO_2\text{–}CH_3$ (*ortho* corr))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		37.17		
Liquid phase				
$\Delta_f H°$ =	−9.70	−22.11	12.41	71LEN/VEL

TABLE 37. Nitro compounds (50) – Continued

1-Methyl-2-nitrobenzene; 2-Nitrotoluene C_7H_7NO

$(1 \times C\text{–}(H)_3(C)) + (4 \times C_B\text{–}(H)(C_B)_2) + (1 \times C_B\text{–}(C)(C_B)_2) + (1 \times C_B\text{–}(NO_2)(C_B)_2) + (1 \times NO_2\text{–}CH_3$ (*ortho* corr))

	Literature	– Calculated	= Residual	Reference
Solid phase				
$\Delta_f H°$ =		−35.22		

1-Methyl-3-nitrobenzene; 3-Nitrotoluene $C_7H_7NO_2$

$(1 \times C\text{–}(H)_3(C)) + (4 \times C_B\text{–}(H)(C_B)_2) + (1 \times C_B\text{–}(C)(C_B)_2) + (1 \times C_B\text{–}(NO_2)(C_B)_2) + (1 \times NO_2\text{–}CH_3$ (*meta* corr))

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−31.50	−28.11	−3.39	71LEN/VEL

1-Methyl-4-nitrobenzene; 4-Nitrotoluene $C_7H_7NO_2$

$(1 \times C\text{–}(H)_3(C)) + (4 \times C_B\text{–}(H)(C_B)_2) + (1 \times C_B\text{–}(C)(C_B)_2) + (1 \times C_B\text{–}(NO_2)(C_B)_2)$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	31.00	35.17	−4.17	70LEN/VEL
Liquid phase				
$\Delta_f H°$ =		−24.11		
$C_p°$ =		210.60		
$S°$ =		259.23		
$\Delta_f S°$ =		−538.74		
$\Delta_f G°$ =		136.52		
$\ln K_f$ =		−55.07		
Solid phase				
$\Delta_f H°$ =	−48.12	−39.22	−8.90	71LEN/VEL
$C_p°$ =	172.38	175.67	−3.29	79RIC/SAV
$S°$ =		252.65		
$\Delta_f S°$ =		−545.32		
$\Delta_f G°$ =		123.37		
$\ln K_f$ =		−49.77		

Nitromethylbenzene; Phenylnitromethane $C_7H_7NO_2$

$(5 \times C_B\text{–}(H)(C_B)_2) + (1 \times C_B\text{–}(C)(C_B)_2) + (1 \times C\text{–}(H)_2(C_B)(NO_2))$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	30.70	30.69	0.01	69PEP/LEB
Liquid phase				
$\Delta_f H°$ =	−22.80	−22.80	0.00	69PEP/LEB

TABLE 37. Nitro compounds (50) — Continued

Nitromethylbenzene; Phenylnitromethane (Continued) $C_7H_7NO_2$
$(5\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_2(C_B)(NO_2))$

	Literature	Calculated	Residual	Reference
Solid phase $\Delta_f H°$ =		−34.45		

2,4-Dinitrotoluene $C_7H_6N_2O_4$
$(1\times C-(H)_3(C))+(3\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(2\times C_B-(NO_2)(C_B)_2)+(1\times NO_2-CH_3$ (*ortho* corr)) + $(1\times NO_2-NO_2$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =	30.00	32.91	−2.91	77PEL
Liquid phase $\Delta_f H°$ =		−45.07		
Solid phase $\Delta_f H°$ =	−65.80	−60.75	−5.05	43PRO/GIL

2,6-Dinitrotoluene $C_7H_6N_2O_4$
$(1\times C-(H)_3(C))+(3\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(2\times C_B-(NO_2)(C_B)_2)+(2\times NO_2-CH_3$ (*ortho* corr)) + $(1\times NO_2-NO_2$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =	51.90	34.91	16.99	77PEL
Liquid phase $\Delta_f H°$ =		−43.07		
Solid phase $\Delta_f H°$ =	−46.40	−56.75	10.35	49MED/THO

2,4,6-Trinitrotoluene $C_7H_5N_3O_6$
$(1\times C-(H)_3(C))+(2\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(3\times C_B-(NO_2)(C_B)_2)+(3\times NO_2-NO_2$ (*meta* corr)) + $(2\times NO_2-CH_3$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =	32.20	41.65	−9.45	77PEL

TABLE 37. Nitro compounds (50) — Continued

2,4,6-Trinitrotoluene (Continued) $C_7H_5N_3O_6$
$(1\times C-(H)_3(C))+(2\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(3\times C_B-(NO_2)(C_B)_2)+(3\times NO_2-NO_2$ (*meta* corr)) + $(2\times NO_2-CH_3$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Liquid phase $\Delta_f H°$ =		−52.53		
Solid phase $\Delta_f H°$ =	−66.90	−68.78	1.88	39BUR/THO

2-Nitrophenol; o-Nitrophenol $C_6H_5NO_3$
$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times C_B-(NO_2)(C_B)_2)+(1\times O-(H)(C_B))+(1\times NO_2-OH$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =	−129.00	−101.26	−27.74	92RIB/REI
Liquid phase $\Delta_f H°$ =		−177.02		
Solid phase $\Delta_f H°$ =	−202.40	−191.63	−10.77	92RIB/REI

3-Nitrophenol; m-Nitrophenol $C_6H_5NO_3$
$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times C_B-(NO_2)(C_B)_2)+(1\times O-(H)(C_B))+(1\times NO_2-OH$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =	−105.50	−105.26	−0.24	92RIB/REI
Solid phase $\Delta_f H°$ =	−205.70	−204.63	−1.07	92RIB/REI

4-Nitrophenol; p-Nitrophenol $C_6H_5NO_3$
$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times C_B-(NO_2)(C_B)_2)+(1\times O-(H)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_f H°$ =	−112.10	−111.26	−0.84	92RIB/REI

TABLE 37. Nitro compounds (50) — Continued

4-Nitrophenol; p-Nitrophenol (Continued) $C_6H_5NO_3$
$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times C_B-(NO_2)(C_B)_2)+(1\times O-(H)(C_B))$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−193.02		
$C_p°$ =		248.37		
$S°$ =		228.73		
$\Delta_fS°$ =		−535.45		
$\Delta_fG°$ =		−33.37		
$\ln K_f$ =		13.46		
Solid phase				
$\Delta_fH°$ =	−212.40	−204.63	−7.77	92RIB/REI
$C_p°$ =		160.44		
$S°$ =		231.67		
$\Delta_fS°$ =		−532.51		
$\Delta_fG°$ =		−45.86		
$\ln K_f$ =		18.50		

2,4-Dinitrophenol $C_6H_4N_2O_5$
$(3\times C_B-(H)(C_B)_2)+(2\times C_B-(NO_2)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times O-(H)(C_B))+(1\times NO_2-NO_2$ (*meta* corr)$)+(1\times NO_2-OH$ (*ortho* corr)$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−128.10	−105.52	−22.58	58HOY/PEP
Liquid phase				
$\Delta_fH°$ =		−199.98		
Solid phase				
$\Delta_fH°$ =	−235.80	−217.16	−18.64	42BAD

2,6-Dinitrophenol $C_6H_4N_2O_4$
$(3\times C_B-(H)(C_B)_2)+(2\times C_B-(NO_2)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times O-(H)(C_B))+(1\times NO_2-NO_2$ (*meta* corr)$)+(2\times NO_2-OH$ (*ortho* corr)$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−97.80	−95.52	−2.28	58HOY/PEP
Liquid phase				
$\Delta_fH°$ =		−183.98		
Solid phase				
$\Delta_fH°$ =	−209.90	−204.16	−5.74	42BAD

TABLE 37. Nitro compounds (50) — Continued

2,4,6-Trinitrophenol; Picric acid $C_6H_3N_3O_7$
$(2\times C_B-(H)(C_B)_2)+(3\times C_B-(NO_2)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times O-(H)(C_B))+(3\times NO_2-NO_2$ (*meta* corr)$)+(2\times NO_2-OH$ (*ortho* corr)$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−88.78		
Liquid phase				
$\Delta_fH°$ =		−193.44		
Solid phase				
$\Delta_fH°$ =	−213.97	−216.19	2.22	60VOR/PRI

2-Nitroaniline $C_6H_6N_2O_2$
$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(NO_2)(C_B)_2)+(1\times C_B-(N)(C_B)_2)+(1\times N-(H)_2(C_B))+(1\times NH_2-NO_2$ (*ortho* corr)$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	63.80	67.74	−3.94	58HOY/PEP
Liquid phase				
$\Delta_fH°$ =	−9.40	−9.16	−0.24	71LEB/GUT
$C_p°$ =		241.63		
$S°$ =		242.71		
$\Delta_fS°$ =		−579.99		
$\Delta_fG°$ =		163.76		
$\ln K_f$ =		−66.06		
Solid phase				
$\Delta_fH°$ =	−26.10	−22.23	−3.87	71LEB/GUT
$C_p°$ =	164.40	170.48	−6.08	26AND/LYN
$S°$ =		233.89		
$\Delta_fS°$ =		−588.81		
$\Delta_fG°$ =		153.32		
$\ln K_f$ =		−61.85		

3-Nitroaniline $C_6H_6N_2O_2$
$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(NO_2)(C_B)_2)+(1\times N-(H)_2(C_B))+(1\times C_B-(N)(C_B)_2)+(1\times NH_2-NO_2$ (*meta* corr)$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	58.40	61.74	−3.34	73MAL/GIG2

TABLE 37. Nitro compounds (50) – Continued

3-Nitroaniline (Continued) $C_6H_6N_2O_2$

$(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(NO_2)(C_B)_2)+(1\times N\text{-}(H)_2(C_B))+(1\times C_B\text{-}(N)(C_B)_2)+(1\times NH_2\text{-}NO_2$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−14.40	−15.16	0.76	71LEB/GUT
$C_p°$ =		241.63		
$S°$ =		242.71		
$\Delta_fS°$ =		−579.99		
$\Delta_fG°$ =		157.76		
$\ln K_f$ =		−63.64		
Solid phase				
$\Delta_fH°$ =	−38.30	−28.23	−10.07	71LEB/GUT
$C_p°$ =	168.20	170.48	−2.28	26AND/LYN
$S°$ =		233.89		
$\Delta_fS°$ =		−588.81		
$\Delta_fG°$ =		147.32		
$\ln K_f$	−59.43			

4-Nitroaniline $C_6H_6N_2O_2$

$(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(NO_2)(C_B)_2)+(1\times C_B\text{-}(N)(C_B)_2)+(1\times N\text{-}(H)_2(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	58.80	71.74	−12.94	73MAL/GIG2
Liquid phase				
$\Delta_fH°$ =	−20.70	−5.16	−15.54	71LEB/GUT
$C_p°$ =		241.63		
$S°$ =		242.71		
$\Delta_fS°$ =		−579.99		
$\Delta_fG°$ =		167.76		
$\ln K_f$ =		−67.67		
Solid phase				
$\Delta_fH°$ =	−42.90	−18.23	−24.67	71LEB/GUT
$C_p°$ =	169.03	170.48	−1.45	26AND/LYN
$S°$ =		233.89		
$\Delta_fS°$ =		−588.81		
$\Delta_fG°$ =		157.32		
$\ln K_f$ =	−63.46			

2,3-Dinitroaniline $C_6H_5N_3O_4$

$(3\times C_B\text{-}(H)(C_B)_2)+(2\times C_B\text{-}(NO_2)(C_B)_2)+(1\times N\text{-}(H)_2(C_B))+(1\times C_B\text{-}(N)(C_B)_2)+(1\times NO_2\text{-}NO_2$ (*ortho* corr)) $+(1\times NH_2\text{-}NO_2$ (*ortho* corr)) $+(1\times NH_2\text{-}NO_2$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		86.48		

TABLE 37. Nitro compounds (50) – Continued

2,3-Dinitroaniline (Continued) $C_6H_5N_3O_4$

$(3\times C_B\text{-}(H)(C_B)_2)+(2\times C_B\text{-}(NO_2)(C_B)_2)+(1\times N\text{-}(H)_2(C_B))+(1\times C_B\text{-}(N)(C_B)_2)+(1\times NO_2\text{-}NO_2$ (*ortho* corr)) $+(1\times NH_2\text{-}NO_2$ (*ortho* corr)) $+(1\times NH_2\text{-}NO_2$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−10.37		
Solid phase				
$\Delta_fH°$ =	−11.70	−30.66	18.96	62ZAK/ALE
$C_p°$ =		205.07		

2,4-Dinitroaniline $C_6H_5N_3O_4$

$(3\times C_B\text{-}(H)(C_B)_2)+(2\times C_B\text{-}(NO_2)(C_B)_2)+(1\times N\text{-}(H)_2(C_B))+(1\times C_B\text{-}(N)(C_B)_2)+(1\times C\text{-}(C_B)(C)_3)+(1\times NO_2\text{-}NO_2$ (*meta* corr)) $+(1\times NH_2\text{-}NO_2$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		81.76		
Liquid phase				
$\Delta_fH°$ =		−13.42		
Solid phase				
$\Delta_fH°$ =	−65.60	−26.19	−39.41	62ZAK/ALE

2,5-Dinitroaniline $C_6H_5N_3O_4$

$(3\times C_B\text{-}(H)(C_B)_2)+(2\times C_B\text{-}(NO_2)(C_B)_2)+(1\times C_B\text{-}(N)(C_B)_2)+(1\times N\text{-}(H)_2(C_B))+(1\times NH_2\text{-}NO_2$ (*ortho* corr)) $+(1\times NH_2\text{-}NO_2$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		42.48		
Liquid phase				
$\Delta_fH°$ =		−55.62		
$C_p°$ =		292.25		
$S°$ =		293.79		
$\Delta_fS°$ =		−764.41		
$\Delta_fG°$ =		172.29		
$\ln K_f$ =		−69.50		
Solid phase				
$\Delta_fH°$ =	−44.30	−71.26	26.96	62ZAK/ALE
$C_p°$ =		201.31		
$S°$ =		321.60		
$\Delta_fS°$ =		−731.60		
$\Delta_fG°$ =		148.36		
$\ln K_f$ =	−59.85			

TABLE 37. Nitro compounds (50) — Continued

2,6-Dinitroaniline $C_6H_5N_3O_4$

$(3 \times C_B-(H)(C_B)_2) + (2 \times C_B-(NO_2)(C_B)_2) + (1 \times C_B-(N)(C_B)_2) + (1 \times N-(H)_2(C_B)) + (1 \times NO_2-NO_2$ (*meta* corr)) + $(2 \times NH_2-NO_2$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		59.48		
Liquid phase				
$\Delta_f H^\circ$ =		−36.12		
Solid phase				
$\Delta_f H^\circ$ =	−50.60	−51.76	1.16	62ZAK/ALE
C_p° =		207.15		

3,4-Dinitroaniline $C_6H_5N_3O_4$

$(3 \times C_B-(H)(C_B)_2) + (2 \times C_B-(NO_2)(C_B)_2) + (1 \times N-(H)_2(C_B)) + (1 \times C_B-(N)(C_B)_2) + (1 \times NH_2-NO_2$ (*meta* corr)) + $(1 \times NO_2-NO_2$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas Phas				
$\Delta_f H^\circ$ =		57.48		
Liquid phase				
$\Delta_f H^\circ$ =		−38.12		
Solid phase				
$\Delta_f H^\circ$ =	−32.60	−53.76	21.16	62ZAK/ALE
C_p° =		207.15		

3,5-Dinitroaniline $C_6H_5N_3O_4$

$(3 \times C_B-(H)(C_B)_2) + (2 \times C_B-(NO_2)(C_B)_2) + (1 \times C_B-(N)(C_B)_2) + (1 \times N-(H)_2(C_B)) + (1 \times NO_2-NO_2$ (*meta* corr)) + $(2 \times NH_2-NO_2$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		47.48		
Liquid phase				
$\Delta_f H^\circ$ =		−48.12		
Solid phase				
$\Delta_f H^\circ$ =	−38.90	−63.76	24.86	62ZAK/ALE
C_p° =		207.15		

TABLE 37. Nitro compounds (50) — Continued

2,4,6-Trinitroaniline; Picramide $C_6H_4N_4O_6$

$(2 \times C_B-(H)(C_B)_2) + (1 \times C_B-(N)(C_B)_2) + (3 \times C_B-(NO_2)(C_B)_2) + (1 \times N-(H)_2(C_B)) + (3 \times NO_2-NO_2$ (*meta* corr)) + $(2 \times NH_2-NO_2$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	41.70	66.22	−24.52	78CUN/PAL
Liquid phase				
$\Delta_f H^\circ$ =		−45.58		
Solid phase				
$\Delta_f H^\circ$ =	−83.60	−63.79	−19.81	49MED/TOM
C_p° =		249.66		

2-Nitrobenzoic acid $C_7H_5NO_4$

$(4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(NO_2)(C_B)_2) + (1 \times C_B-(CO)(C_B)_2) + (1 \times CO-(O)(C_B)) + (1 \times O-(H)(CO)) + (1 \times NO_2-COOH$ (*ortho* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−285.01		
Liquid phase				
$\Delta_f H^\circ$ =	−378.80	−380.80	2.00	71LEB/RYA
C_p° =		254.39		
Solid phase				
$\Delta_f H^\circ$ =	−398.48	−400.38	1.90	71LEB/RYA
C_p° =	191.63	176.94	14.69	26AND/LYN
S° =		255.45		
$\Delta_f S^\circ$ =		−616.99		
$\Delta_f G^\circ$ =		−216.42		
$\ln K_f$ =		87.30		

3-Nitrobenzoic acid $C_7H_5NO_4$

$(4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(NO_2)(C_B)_2) + (1 \times C_B-(CO)(C_B)_2) + (1 \times CO-(O)(C_B)) + (1 \times O-(H)(CO)) + (1 \times NO_2-COOH$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−296.01		
Liquid phase				
$\Delta_f H^\circ$ =	−394.70	−394.80	0.10	71LEB/RYA
C_p° =		254.39		

TABLE 37. Nitro compounds (50) – Continued

3-Nitrobenzoic acid (Continued) $C_6H_5NO_4$

$(4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(NO_2)(C_B)_2) + (1 \times C_B-(CO)(C_B)_2) + (1 \times CO-(O)(C_B)) + (1 \times O-(H)(CO)) + (1 \times NO_2-COOH$ (*meta* corr))

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H^\circ$ =	−414.01	−411.38	−2.63	71LEB/RYA
C_p° =	173.22	176.94	−3.72	26AND/LYN
S° =		255.45		
$\Delta_f S^\circ$ =		−611.25		
$\Delta_f G^\circ$ =		−229.13		
$\ln K_f$ =		92.43		

4-Nitrobenzoic acid $C_7H_5NO_4$

$(4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(NO_2)(C_B)_2) + (1 \times C_B-(CO)(C_B)_2) + (1 \times CO-(O)(C_B)) + (1 \times O-(H)(CO))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−310.01		
Liquid phase				
$\Delta_f H^\circ$ =	−392.20	−410.80	18.60	71LEB/RYA
C_p° =		254.39		
Solid phase				
$\Delta_f H^\circ$ =	−426.90	−425.38	−1.52	71LEB/RYA
C_p° =	180.33	176.94	3.39	26AND/LYN
S° =		255.45		
$\Delta_f S^\circ$ =		−616.99		
$\Delta_f G^\circ$ =		−241.42		
$\ln K_f$ =		97.39		

TABLE 38. Nitrites (3)

Methyl nitrite CH_3ONO

$(1 \times C-(H)_3(O)) + (1 \times O-(C)(NO))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−65.40	−66.49	1.09	62RAY/GER
C_p° =	63.22	63.22	0.00	69STU/WES
S° =	284.30	284.30	0.00	69STU/WES
$\Delta_f S^\circ$ =		−115.57		
$\Delta_f G^\circ$ =		−32.03		
$\ln K_f$ =		12.92		

Ethyl nitrite C_2H_5ONO

$(1 \times C-(H)_3(C)) + (1 \times C-(H)_2(O)(C)) + (1 \times O-(C)(NO))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−101.25	−99.39	−1.86	56GRA
C_p° =		83.55		
Liquid phase				
$\Delta_f H^\circ$ =	−127.60	−129.91	2.31	59GRA/WIL

***n*-Propyl nitrite** C_3H_7ONO

$(1 \times C-(H)_3(C)) + (1 \times C-(H)_2(C)_2) + (1 \times C-(H)_2(O)(C)) + (1 \times O-(C)(NO))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−125.94	−120.02	−5.92	59GRA/WIL
C_p° =		106.44		
Liquid phase				
$\Delta_f H^\circ$ =	−159.00	−155.64	−3.36	59GRA/WIL

TABLE 39. Nitrates (6)

Methyl nitrate CH_3ONO_2

(1×C–(H)$_3$(O))+(1×O–(C)(NO$_2$)), σ = 6

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−123.00	−121.97	−1.03	58RAY/OGG2
$C_p°$ =	76.48	77.19	−0.71	69STU/WES
$S°$ =	301.88	304.34	−2.46	69STU/WES
$\Delta_fS°$ =		−198.05		
$\Delta_fG°$ =		−62.92		
$\ln K_f$ =		25.38		
Liquid phase				
$\Delta_fH°$ =	−157.10	−156.57	−0.53	58RAY/OGG2
$C_p°$ =	157.19	132.88	24.31	53GRA/SMI
$S°$ =	216.98	210.80	6.18	53GRA/SMI
$\Delta_fS°$ =		−291.59		
$\Delta_fG°$ =		−69.63		
$\ln K_f$ =		28.09		

Ethyl nitrate $C_2H_5ONO_2$

(1×C–(H)$_3$(C))+(1×C–(H)$_2$(O)(C))+(1×O–(C)(NO$_2$)), σ = 6

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−154.10	−154.87	0.77	57GRA/PRA
$C_p°$ =	97.36	97.52	−0.16	69STU/WES
$S°$ =	348.32	347.77	0.55	69STU/WES
$\Delta_fS°$ =		−290.93		
$\Delta_fG°$ =		−68.13		
$\ln K_f$ =		27.48		
Liquid phase				
$\Delta_fH°$ =	−190.41	−192.37	1.96	57FAI/SKI
$C_p°$ =	170.30	166.52	3.78	54GRA/SMI
$S°$ =	247.20	243.39	3.81	54GRA/SMI
$\Delta_fS°$ =		−395.31		
$\Delta_fG°$ =		−74.51		
$\ln K_f$ =		30.06		

***n*-Propyl nitrate** $C_3H_7ONO_2$

(1×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(O)(C))+(1×O–(C)(NO$_2$)), σ = 6

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−173.89	−175.50	1.61	57GRA/PRA
$C_p°$ =	121.29	120.41	0.88	69STU/WES
$S°$ =	385.35	386.93	−1.58	69STU/WES
$\Delta_fS°$ =		−388.08		
$\Delta_fG°$ =		−59.79		
$\ln K_f$ =		24.12		

TABLE 39. Nitrates (6) – Continued

***n*-Propyl nitrate (Continued)** $C_3H_7ONO_2$

(1×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(O)(C))+(1×O–(C)(NO$_2$)), σ = 6

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−214.51	−218.10	3.59	57FAI/SKI
$C_p°$ =		196.94		
$S°$ =		275.77		
$\Delta_fS°$ =		−499.24		
$\Delta_fG°$ =		−69.25		
$\ln K_f$ =		27.94		

Isopropyl nitrate $C_3H_7ONO_2$

(2×C–(H)$_3$(C))+(1×C–(H)(O)(C)$_2$ (ethers,esters))+(1×O–(C)(NO$_2$))+(2×–CH$_3$ corr (tertiary)), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−191.00	−188.21	−2.79	57GRA/PRA
$C_p°$ =	120.67	120.70	−0.03	69STU/WES
$S°$ =	373.21	369.73	3.48	69STU/WES
$\Delta_fS°$ =		−405.28		
$\Delta_fG°$ =		−67.37		
$\ln K_f$ =		27.18		
Liquid phase				
$\Delta_fH°$ =	−229.70	−229.54	−0.16	57FAI/SKI
$C_p°$ =	191.10	194.92	−3.82	88LUS/RUB
$S°$ =	263.20	268.79	−5.59	88LUS/RUB
$\Delta_fS°$ =		−506.22		
$\Delta_fG°$ =		−78.61		
$\ln K_f$ =		31.71		

Ethylene glycol dinitrate; EGDN $C_2H_4N_2O_6$

(2×C–(H)$_2$(O)(C))+(2×O–(C)(NO$_2$))+(2×(ONO$_2$)–(ONO$_2$) (aliphatic corr))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−189.30	−195.02	5.72	77PEL
Liquid phase				
$\Delta_fH°$ =	−255.80	−257.72	1.92	34TOM/TAK

TABLE 39. Nitrates (6) – Continued

Glyceryl trinitrate; Nitroglycerine $C_3H_5N_3O_9$
(2×C–(H)$_2$(O)(C))+(3×O–(C)(NO$_2$))+
(1×C–(H)(O)(C)$_2$ (ethers,esters))+
(3×(ONO$_2$)–(ONO$_2$) (aliphatic corr))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	–279.70	–279.09	–0.61	88MIR/KOR
Liquid phase				
$\Delta_fH°$ =	–371.70	–371.78	0.08	88MIR/KOR

TABLE 40. Nitramines (10)

Nitrourea $CH_3N_3O_3$
(1×N–(H)$_2$(CO) (amides, ureas))+(1×CO–(N)$_2$)+
(1×N–(H)(CO)(NO$_2$))

	Literature	-Calculated	= Residual	Reference
Solid phase				
$\Delta_fH°$ =	–282.30	–282.35	0.05	49MED/THO

Methyldinitramine $CH_3N_3O_4$
(1×C–(H)$_3$(N))+(1×–CH$_3$ corr (quaternary))+
(1×N–(C)(NO$_2$)$_2$)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	53.50	53.48	0.02	87MIR/KOR
Liquid phase				
$\Delta_fH°$ =	1.50	1.50	0.00	87MIR/KOR

Methylenedinitramine; MEDINA $CH_4N_4O_4$
(1×C–(H)$_2$(N)$_2$)+(2×N–(H)(C)(NO$_2$))

	Literature	-Calculated	= Residual	Reference
Solid phase				
$\Delta_fH°$ =	–57.90	–59.00	1.10	54MUR/GOL

Dimethylnitramine $C_2H_6N_2O_2$
(2×C–(H)$_3$(N))+(2×–CH$_3$ corr (quaternary))+
(1×N–(C)$_2$(NO$_2$))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	–5.00	–5.64	0.64	71MAT/V'Y
Liquid phase				
$\Delta_fH°$ =		–54.00		
Solid phase				
$\Delta_fH°$ =	–74.90	–62.18	–12.72	71MAT/V'Y

Ethylenedinitramine; Haleite $C_2H_6N_4O_4$
(2×C–(H)$_2$(C)(N))+(2×N–(H)(C)(NO$_2$))

	Literature	-Calculated	= Residual	Reference
Solid phase				
$\Delta_fH°$ =	–104.60	–101.00	–3.60	73KRI/LIC
$C_p°$ =		175.30		

TABLE 40. Nitramines (10) – Continued

Diethylnitramine $C_4H_{10}N_2O_2$
(2 × C–(H)$_3$(C)) + (2 × C–(H)$_2$(C)(N)) + (1 × N–(C)$_2$(NO$_2$))

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	−53.10	−53.12	0.02	58CAS/FLE
Liquid phase $\Delta_f H°$ =	−106.20	−106.82	0.62	58CAS/FLE

N-Nitropiperidine $C_5H_{10}N_2O_2$
(3 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(C)(N)) + (1 × N–(C)$_2$(NO$_2$)) + (1 × N-Nitropiperidine rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	−44.40	−44.40	0.00	71MAT/V'Y
Liquid phase $\Delta_f H°$ =	−92.90	−92.90	0.00	71MAT/V'Y
Solid phase $\Delta_f H°$ =	−107.75	−107.75	0.00	87MES/TOD

1,3,5-Cyclotrimethylenetrinitramine; Hexogen; RDX $C_3H_6N_6O_6$
(3 × C–(H)$_2$(N)$_2$) + (3 × N–(C)$_2$(NO$_2$)) + (1 × RDX rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	205.30	206.00	−0.70	78CUN/PAL
Solid phase $\Delta_f H°$ =	71.00	72.00	−1.00	73KRI/LIC

TABLE 40. Nitramines (10) – Continued

1,3,5,7-Cyclotetramethylenetetranitramine; Octogen; HMX $C_4H_8N_8O_8$
(4 × C–(H)$_2$(N)$_2$) + (4 × N–(C)$_2$(NO$_2$)) + (1 × HMX rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	248.90	249.00	−0.10	78CUN/PAL
Solid phase $\Delta_f H°$ =	87.90	88.00	−0.10	73KRI/LIC

N-Methyl-N-nitro-(2,4,6-trinitro)aniline; Tetryl; Tetralite $C_7H_5N_5O_8$
(2 × C$_B$–(H)(C$_B$)$_2$) + (1 × C$_B$–(N)(C$_B$)$_2$) + (3 × C$_B$–(NO$_2$)(C$_B$)$_2$) + (1 × N–(C)(C$_B$)(NO$_2$)) + (1 × C–(H)$_3$(N))

	Literature	– Calculated	= Residual	Reference
Gas phase $\Delta_f H°$ =	162.80	162.71	0.09	78CUN/PAL
Liquid phase $\Delta_f H°$ =	52.00	52.31	−0.31	73KRI/LIC
Solid phase $\Delta_f H°$ =	29.00	29.07	−0.07	73KRI/LIC

TABLE 41. Cyclic CHNO (3)

Succinimide $C_4H_5NO_2$

(2×C–(H)$_2$(CO)(C)) + (2×CO–(C)(N)) + (1×N–(H)(CO)$_2$) + (1×succinimide rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−375.50	−375.50	0.00	90MEN/PIL
Solid phase				
$\Delta_f H°$ =	−459.10	−459.10	0.00	66COL/SKI

Glutarimide $C_5H_7NO_2$

(2×C–(H)$_2$(CO)(C)) + (1×C–(H)$_2$(C)$_2$) + (2×CO–(C)(N)) + (1×N–(H)(CO)$_2$) + (1×glutarimide rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−393.60	−393.60	0.00	90MEN/PIL
Solid phase				
$\Delta_f H°$ =	−487.70	−487.64	−0.06	90MEN/PIL

N,N-Bisuccinimide $C_8H_8N_2O_4$

(4×C–(H)$_2$(C)(CO)) + (4×CO–(C)(N)) + (2×N–(CO)$_2$(N)) + (2×succinimide rsc)

	Literature	-Calculated	= Residual	Reference
Solid phase				
$\Delta_f H°$ =	−709.36	−709.36	0.00	66COL/SKI

TABLE 42. Thiols (31)

Methanethiol CH_4S

(1×C–(H)$_3$(S)) + (1×S–(C)(H)), $\sigma = 3$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−22.97	−23.62	0.65	61GOO/LAC
$C_p°$ =	50.25	51.49	−1.24	69STU/WES
$S°$ =	255.06	255.86	−0.80	69STU/WES
$\Delta_f S°$ =		−43.08		
$\Delta_f G°$ =		−10.78		
$\ln K_f$ =		4.35		
Liquid phase				
$\Delta_f H°$ =	−46.70	−47.55	0.85	61GOO/LAC
$C_p°$ =		87.82		
$S°$ =		169.25		
$\Delta_f S°$ =		−129.69		
$\Delta_f G°$ =		−8.88		
$\ln K_f$ =		3.58		

Ethanethiol C_2H_6S

(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)(S)) + (1×S–(C)(H)), $\sigma = 3$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−46.11	−46.79	0.68	52MCC/SCO
$C_p°$ =	72.68	72.39	0.29	69STU/WES
$S°$ =	296.10	297.73	−1.63	69SYU/WES
$\Delta_f S°$ =		−137.52		
$\Delta_f G°$ =		−5.79		
$\ln K_f$ =		2.33		
Liquid phase				
$\Delta_f H°$ =	−73.60	−74.32	0.72	57MCC/HUB
$C_p°$ =	117.86	112.00	5.86	52MCC/SCO
$S°$ =	207.02	210.34	−3.32	52MCC/SCO
$\Delta_f S°$ =		−224.91		
$\Delta_f G°$ =		−7.26		
$\ln K_f$ =		2.93		

1-Propanethiol C_3H_8S

(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(S)) + (1×S–(C)(H)), $\sigma = 3$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−67.86	−67.42	−0.44	56PEN/SCO
$C_p°$ =	94.77	95.28	−0.51	69STU/WES
$S°$ =	336.39	336.89	−0.50	69STU/WES
$\Delta_f S°$ =		−234.67		
$\Delta_f G°$ =		2.55		
$\ln K_f$ =		−1.03		

TABLE 42. Thiols (31) — Continued

1-Propanethiol (Continued) C_3H_8S

(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(S)) + (1×S–(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−99.90	−100.05	0.15	54HUB/WAD
C_p^o =	144.56	142.42	2.14	56PEN/SCO
$S°$ =	242.50	242.72	−0.22	56PEN/SCO
$\Delta_fS°$ =		−328.84		
$\Delta_fG°$ =		−2.01		
$\ln K_f$ =		0.81		

1-Butanethiol $C_4H_{10}S$

(1×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(S)) + (1×S–(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−88.07	−88.05	−0.02	57SCO/FIN
C_p^o =	118.16	118.17	−0.01	69STU/WES
$S°$ =	375.22	376.05	−0.83	69STU/WES
$\Delta_fS°$ =		−331.82		
$\Delta_fG°$ =		10.88		
$\ln K_f$ =		−4.39		
Liquid phase				
$\Delta_fH°$ =	−124.70	−125.78	1.08	58HUB/GOO
C_p^o =	172.30	172.84	−0.54	57SCO/FIN
$S°$ =	275.98	275.10	0.88	57SCO/FIN
$\Delta_fS°$ =		−432.77		
$\Delta_fG°$ =		3.25		
$\ln K_f$ =		−1.31		

1-Pentanethiol $C_5H_{12}S$

(1×C–(H)$_3$(C)) + (3×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(S)) + (1×S–(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−110.10	−108.68	−1.42	65FIN/HOS
C_p^o =	141.21	141.06	0.15	69STU/WES
$S°$ =	415.29	415.21	0.08	69STU/WES
$\Delta_fS°$ =		−428.97		
$\Delta_fG°$ =		19.22		
$\ln K_f$ =		−7.75		
Liquid phase				
$\Delta_fH°$ =	−152.10	−151.51	−0.59	54HUB/CAT
C_p^o =	201.17	203.26	−2.09	52FINSCO
$S°$ =	310.37	307.48	2.89	52FIN/SCO
$\Delta_fS°$ =		−536.70		
$\Delta_fG°$ =		8.51		
$\ln K_f$ =		−3.43		

TABLE 42. Thiols (31) — Continued

1-Hexanethiol $C_6H_{14}S$

(1×C–(H)$_3$(C)) + (4×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(S)) + (1×S–(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−128.99	−129.31	0.32	66OSB/DOU
C_p^o =	164.05	163.95	0.10	69STU/WES
$S°$ =	454.30	454.37	−0.07	69STU/WES
$\Delta_fS°$ =		−526.13		
$\Delta_fG°$ =		27.55		
$\ln K_f$ =		−11.12		
Liquid phase				
$\Delta_fH°$ =	−175.70	−177.24	1.54	66GOO/DEP
C_p^o =	230.71	233.68	−2.97	70FIN/MCC
$S°$ =	343.21	339.86	3.35	70FIN/MCC
$\Delta_fS°$ =		−640.63		
$\Delta_fG°$ =		13.76		
$\ln K_f$ =		−5.55		

1-Heptanethiol $C_7H_{16}S$

(1×C–(H)$_3$(C)) + (5×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(S)) + (1×S–(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−150.00	−149.94	−0.06	66OSB/DOU
C_p^o =	186.94	186.84	0.10	69STU/WES
$S°$ =	493.25	493.53	−0.28	69STU/WES
$\Delta_fS°$ =		−623.28		
$\Delta_fG°$ =		35.89		
$\ln K_f$ =		−14.48		
Liquid phase				
$\Delta_fH°$ =	−200.50	−202.97	2.47	66GOO/DEP
C_p^o =	259.32	264.10	−4.78	70FIN/MCC
$S°$ =	375.35	372.24	3.11	70FIN/MCC
$\Delta_fS°$ =		−744.56		
$\Delta_fG°$ =		19.02		
$\ln K_f$ =		−7.67		

1-Octanethiol $C_8H_{18}S$

(1×C–(H)$_3$(C)) + (6×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(S)) + (1×S–(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−170.21	−170.57	0.36	69STU/WES
C_p^o =	209.79	209.73	0.06	69STU/WES
$S°$ =	532.20	532.69	−0.49	69STU/WES
$\Delta_fS°$ =		−720.43		
$\Delta_fG°$ =		44.23		
$\ln K_f$ =		−17.84		

TABLE 42. Thiols (31) — Continued

1-Octanethiol (Continued) $C_8H_{18}S$
(1×C-(H)$_3$(C))+(6×C-(H)$_2$(C)$_2$)+(1×C-(H)$_2$(C)(S))+(1×S-(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−228.70		
$C_p°$ =		294.52		
$S°$ =		404.62		
$\Delta_fS°$ =		−848.49		
$\Delta_fG°$ =		24.28		
$\ln K_f$ =		−9.79		

1-Nonanethiol $C_9H_{20}S$
(1×C-(H)$_3$(C))+(7×C-(H)$_2$(C)$_2$)+(1×C-(H)$_2$(C)(S))+(1×S-(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−190.83	−191.20	0.37	69STU/WES
$C_p°$ =	232.67	232.62	0.05	69STU/WES
$S°$ =	571.16	571.85	−0.69	69STU/WES
$\Delta_fS°$ =		−817.58		
$\Delta_fG°$ =		52.56		
$\ln K_f$ =		−21.20		
Liquid phase				
$\Delta_fH°$ =		−254.43		
$C_p°$ =		324.94		
$S°$ =		437.00		
$\Delta_fS°$ =		−952.42		
$\Delta_fG°$ =		29.54		
$\ln K_f$ =		−11.91		

1-Decanethiol $C_{10}H_{22}S$
(1×C-(H)$_3$(C))+(8×C-(H)$_2$(C)$_2$)+(1×C-(H)$_2$(C)(S))+(1×S-(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−211.46	−211.83	0.37	69STU/WES
$C_p°$ =	255.56	255.51	0.05	69STU/WES
$S°$ =	610.11	611.01	−0.90	69STU/WES
$\Delta_fS°$ =		−914.73		
$\Delta_fG°$ =		60.90		
$\ln K_f$ =		−24.57		
Liquid phase				
$\Delta_fH°$ =	−276.50	−280.16	3.66	66GOO/DEP
$C_p°$ =		355.36		
$S°$ =		469.38		
$\Delta_fS°$ =		−1056.35		
$\Delta_fG°$ =		34.79		
$\ln K_f$ =		−14.03		

TABLE 42. Thiols (31) — Continued

1-Hexadecanethiol $C_{16}H_{34}S$
(1×C-(H)$_3$(C))+(14×C-(H)$_2$(C)$_2$)+(1×C-(H)$_2$(C)(S))+(1×S-(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−335.10	−335.61	0.51	69STU/WES
$C_p°$ =	392.75	392.85	−0.10	69STU/WES
$S°$ =	843.79	845.97	−2.18	69STU/WES
$\Delta_fS°$ =		−1497.64		
$\Delta_fG°$ =		110.91		
$\ln K_f$ =		−44.74		
Liquid phase				
$\Delta_fH°$ =		−434.54		
$C_p°$ =		537.88		
$S°$ =		663.66		
$\Delta_fS°$ =		−1679.94		
$\Delta_fG°$ =		66.33		
$\ln K_f$ =		−26.76		

1-Eicosanethiol $C_{20}H_{42}S$
(1×C-(H)$_3$(C))+(18×C-(H)$_2$(C)$_2$)+(1×C-(H)$_2$(C)(S))+(1×S-(C)(H)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−417.56	−418.13	0.57	69STU/WES
$C_p°$ =	484.26	484.41	−0.15	69STU/WES
$S°$ =	999.60	1002.61	−3.01	69STU/WES
$\Delta_fS°$ =		−1886.24		
$\Delta_fG°$ =		144.25		
$\ln K_f$ =		−58.19		
Liquid phase				
$\Delta_fH°$ =		−537.46		
$C_p°$ =		659.56		
$S°$ =		793.18		
$\Delta_fS°$ =		−2095.67		
$\Delta_fG°$ =		87.36		
$\ln K_f$ =		−35.24		

1,2-Ethanedithiol $C_2H_6S_2$
(2×S-(C)(H))+(2×C-(H)$_2$(C)(S))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−9.70	−9.06	−0.64	62MAN/SUN
$C_p°$ =		93.32		

TABLE 42. Thiols (31) – Continued

1,2-Ethanedithiol (Continued) $C_2H_6S_2$

(2×S–(C)(H)) + (2×C–(H)$_2$(C)(S))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−54.40	−53.42	−0.98	62MAN/SUN
$C_p°$ =		151.04		
$S°$ =		254.08		
$\Delta_fS°$ =		−213.22		
$\Delta_fG°$ =		10.15		
$\ln K_f$ =		−4.10		

1,3-Propanedithiol $C_3H_8S_2$

(2×S–(C)(H)) + (1×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(C)(S))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−29.70	−29.69	−0.01	62MAN/SUN
$C_p°$ =		116.21		
Liquid phase				
$\Delta_fH°$ =	−79.40	−79.15	−0.25	62MAN/SUN
$C_p°$ =		181.46		
$S°$ =		286.46		
$\Delta_fS°$ =		−317.15		
$\Delta_fG°$ =		15.41		
$\ln K_f$ =		−6.22		

1,4-Butanedithiol $C_4H_{10}S_2$

(2×S–(C)(H)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(C)(S))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−50.40	−50.32	−0.08	62MAN/SUN
$C_p°$ =		139.10		
Liquid phase				
$\Delta_fH°$ =	−105.70	−104.88	−0.82	62MAN/SUN
$C_p°$ =		211.88		
$S°$ =		318.84		
$\Delta_fS°$ =		−421.08		
$\Delta_fG°$ =		20.67		
$\ln K_f$ =		−8.34		

1,5-Pentanedithiol $C_5H_{12}S_2$

(2×S–(C)(H)) + (3×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(C)(S))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−71.00	−70.95	−0.05	62MAN/SUN
$C_p°$ =		161.99		

TABLE 42. Thiols (31) – Continued

1,5-Pentanedithiol (Continued) $C_5H_{12}S_2$

(2×S–(C)(H)) + (3×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(C)(S))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−130.30	−130.61	0.31	62MAN/SUN
$C_p°$ =		242.30		
$S°$ =		351.22		
$\Delta_fS°$ =		−525.01		
$\Delta_fG°$ =		25.92		
$\ln K_f$ =		−10.46		

2-Propanethiol C_3H_8S

(1×S–(C)(H)) + (2×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(S)) + (2×–CH$_3$ corr (tertiary)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−76.23	−76.28	0.05	54MCC/FIN2
$C_p°$ =	95.98	97.51	−1.53	69STU/WES
$S°$ =	324.30	326.68	−2.38	69STU/WES
$\Delta_fS°$ =		−244.88		
$\Delta_fG°$ =		−3.27		
$\ln K_f$ =		1.32		
Liquid phase				
$\Delta_fH°$ =	−105.90	−105.59	−0.31	54HUB/WAD
$C_p°$ =	145.35	142.08	3.27	54MCC/FIN2
$S°$ =	233.55	235.94	−2.39	54MCC/FIN2
$\Delta_fS°$ =		−335.62		
$\Delta_fG°$ =		−5.53		
$\ln K_f$ =		2.23		

2-Butanethiol $C_4H_{10}S$

(1×S–(C)(H)) + (2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(S)) + (1×–CH$_3$ corr (tertiary)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−96.90	−94.65	−2.25	58MCC/FIN
$C_p°$ =	119.29	120.40	−1.11	69STU/WES
$S°$ =	366.73	365.84	0.89	69STU/WES
$\Delta_fS°$ =		−342.03		
$\Delta_fG°$ =		7.33		
$\ln K_f$ =		−2.96		
Liquid phase				
$\Delta_fH°$ =	−131.00	−129.14	−1.86	58HUB/GOO
$C_p°$ =	171.21	172.50	−1.29	58MCC/FIN
$S°$ =	266.35	268.32	−1.97	58MCC/FIN
$\Delta_fS°$ =		−439.55		
$\Delta_fG°$ =		1.91		
$\ln K_f$ =		−0.77		

TABLE 42. Thiols (31) – Continued

2-Methyl-1-propanethiol $C_4H_{10}S$

(1×S–(C)(H)) + (1×C–(H)$_2$(C)(S)) + (1×C–(H)(C)$_3$) + (2×–CH$_3$ corr (tertiary)) + (2×C–(H)$_3$(C)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−97.24	−94.74	−2.50	58HUB/GOO
$C_p°$ =	118.32	118.20	0.12	69STU/WES
$S°$ =	362.88	362.31	0.57	69STU/WES
$\Delta_fS°$ =		−345.56		
$\Delta_fG°$ =		8.29		
$\ln K_f$ =		−3.34		
Liquid phase				
$\Delta_fH°$ =	−132.00	−131.06	−0.94	58SCO/MCC
$C_p°$ =	171.88	169.86	2.02	58SCO/MCC
$S°$ =	266.35	269.75	−3.40	58SCO/MCC
$\Delta_fS°$ =		−438.12		
$\Delta_fG°$ =		−0.43		
$\ln K_f$ =		0.18		

2-Methyl-2-propanethiol $C_4H_{10}S$

(1×S–(C)(H)) + (3×C–(H)$_3$(C)) + (1×C–(C)$_3$(S)) + (3×–CH$_3$ corr (quaternary)), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−109.60	−108.30	−1.30	53MCC/SCO
$C_p°$ =	120.96	119.97	0.99	69STU/WES
$S°$ =	338.02	337.71	0.31	69STU/WES
$\Delta_fS°$ =		−370.16		
$\Delta_fG°$ =		2.06		
$\ln K_f$ =		−0.83		
Liquid phase				
$\Delta_fH°$ =	−140.50	−139.25	−1.25	58HUB/GOO
$C_p°$ =	175.06	169.66	5.40	53MCC/SCO
$S°$ =	246.44	248.99	−2.55	53MCC/SCO
$\Delta_fS°$ =		−458.88		
$\Delta_fG°$ =		−2.44		
$\ln K_f$ =		0.98		

2-Methyl-2-butanethiol $C_5H_{12}S$

(3×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×S–(C)(H)) + (1×C–(C)$_3$(S)) + (2×–CH$_3$ corr (quaternary)), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−127.03	−124.37	−2.66	62SCO/DOU
$C_p°$ =	143.51	142.86	0.65	69STU/WES
$S°$ =	386.94	376.87	10.07	69STU/WES
$\Delta_fS°$ =		−467.31		
$\Delta_fG°$ =		14.96		
$\ln K_f$ =		−6.03		

TABLE 42. Thiols (31) – Continued

2-Methyl-2-butanethiol (Continued) $C_5H_{12}S$

(3×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×S–(C)(H)) + (1×C–(C)$_3$(S)) + (2×–CH$_3$ corr (quaternary)), σ = 81

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−162.80	−160.59	−2.21	62SCO/DOU
$C_p°$ =	198.95	200.08	−1.13	74MES/FIN
$S°$ =	295.60	281.37	14.23	74MES/FIN
$\Delta_fS°$ =		−562.81		
$\Delta_fG°$ =		7.21		
$\ln K_f$ =		−2.91		

3-Methyl-1-butanethiol $C_5H_{12}S$

(1×S–(C)(H)) + (2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)(S)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_3$) + (2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−114.90	−115.37	0.47	72GOO2
$C_p°$ =		141.09		
Liquid phase				
$\Delta_fH°$ =	−154.30	−156.79	2.49	72GOO2
$C_p°$ =	200.33	200.28	0.05	74MES/FIN
$S°$ =	298.49	302.13	−3.64	74MES/FIN
$\Delta_fS°$ =		−542.05		
$\Delta_fG°$ =		4.82		
$\ln K_f$ =		−1.95		

Cyclopentanethiol $C_5H_{10}S$

(1×S–(C)(H)) + (1×C–(H)(C)$_2$(S)) + (4×C–(H)$_2$(C)$_2$) + (1×Cyclopentane (sub) rsc), σ = 1

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−47.91	−50.21	2.30	61BER/SCO
$C_p°$ =	107.91	109.74	−1.83	69STU/WES
$S°$ =	361.41	365.34	−3.93	69STU/WES
$\Delta_fS°$ =		−348.27		
$\Delta_fG°$ =		53.63		
$\ln K_f$ =		−21.63		
Liquid phase				
$\Delta_fH°$ =	−89.50	−85.34	−4.16	61BER/SCO
$C_p°$ =	165.23	167.48	−2.25	61BER/SCO
$S°$ =	256.86	255.51	1.35	61BER/SCO
$\Delta_fS°$ =		−458.10		
$\Delta_fG°$ =		51.24		
$\ln K_f$ =		−20.67		

TABLE 42. Thiols (31) – Continued

Cyclohexanethiol $C_6H_{12}S$
(1×S–(C)(H))+(1×C–(H)(C)$_2$(S))+(5×C–(H)$_2$(C)$_2$)+(1×Cyclohexane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−96.10	−90.78	−5.32	72GOO2
$C_p°$ =		137.68		
Liquid phase				
$\Delta_fH°$ =	−140.70	−136.72	−3.98	72GOO2
$C_p°$ =	192.63	195.01	−2.38	67MES/TOD
$S°$ =	258.57	256.34	2.23	67MES/TOD
$\Delta_fS°$ =		−593.58		
$\Delta_fG°$ =		40.26		
$\ln K_f$ =		−16.24		

3-Methyl-2-butanethiol $C_5H_{12}S$
(3×C–(H)$_3$(C))+(1×C–(H)(C)$_3$)+(2×–CH$_3$ corr (tertiary))+(1×S–(C)(H))+(1×C–(H)(C)$_2$(S))+(1×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−121.30	−121.97	0.67	72GOO2
$C_p°$ =		143.32		
Liquid phase				
$\Delta_fH°$ =	−158.80	−160.15	1.35	72GOO2
$C_p°$ =		199.94		
$S°$ =		295.35		
$\Delta_fS°$ =		−548.83		
$\Delta_fG°$ =		3.48		
$\ln K_f$ =		−1.41		

2,2-Dimethyl-1-propanethiol $C_5H_{12}S$
(3×C–(H)$_3$(C))+(1×C–(C)$_4$)+(3×–CH$_3$ corr (quaternary))+(1×C–(H)$_2$(C)(S))+(1×S–(C)(H))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−129.00	−125.79	−3.21	72GOO2
$C_p°$ =		140.38		
Liquid phase				
$\Delta_fH°$ =	−165.40	−164.72	−0.68	72GOO2
$C_p°$ =		195.20		
$S°$ =		278.29		
$\Delta_fS°$ =		−565.89		
$\Delta_fG°$ =		4.00		
$\ln K_f$ =		−1.61		

TABLE 42. Thiols (31) – Continued

2-Methyl-1-butanethiol $C_5H_{12}S$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+(1×–CH$_3$ corr (tertiary))+(1×C–(H)$_2$(C)(S))+(1×S–(C)(H))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−115.10	−113.11	−1.99	72GOO2
$C_p°$ =		141.09		
Liquid phase				
$\Delta_fH°$ =	−154.40	−154.61	0.21	72GOO2
$C_p°$ =		200.28		
$S°$ =		302.13		
$\Delta_fS°$ =		−542.05		
$\Delta_fG°$ =		7.00		
$\ln K_f$ =		−2.82		

2,3-Dimethyl-2-butanethiol $C_6H_{14}S$
(4×C–(H)$_3$(C))+(1×C–(H)(C)$_3$)+(2×–CH$_3$ corr (tertiary))+(1×S–(C)(H))+(1×C–(C)$_3$(S))+(1×–CH$_3$ corr (*tert/quat*))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−147.90	−144.37	−3.53	72GOO2
$C_p°$ =		165.78		
Liquid phase				
$\Delta_fH°$ =	−187.20	−184.59	−2.61	72GOO2
$C_p°$ =		227.52		
$S°$ =		308.40		
$\Delta_fS°$ =		−672.09		
$\Delta_fG°$ =		15.79		
$\ln K_f$ =		−6.37		

2-Methyl-2-pentanethiol $C_6H_{14}S$
(3×C–(H)$_3$(C))+(1×C–(C)$_3$(S))+(2×–CH$_3$ corr (quaternary))+(2×C–(H)$_2$(C)$_2$)+(1×S–(C)(H))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−148.30	−145.00	−3.30	72GOO2
$C_p°$ =		165.75		
Liquid phase				
$\Delta_fH°$ =	−188.30	−186.32	−1.98	72GOO2
$C_p°$ =		230.50		
$S°$ =		313.75		
$\Delta_fS°$ =		−666.74		
$\Delta_fG°$ =		12.47		
$\ln K_f$ =		−5.03		

TABLE 42. Thiols (31) — Continued

Benzenethiol C_6H_6S

(1×S–(C_B)(H))+(1×C_B–(S))+(5×C_B–(H)(C_B)$_2$), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	112.40	112.40	0.00	56SCO/MCC
$C_p°$ =	104.89	104.89	0.00	69STU/WES
$S°$ =	336.85	336.85	0.00	69STU/WES
$\Delta_fS°$ =		−121.36		
$\Delta_fG°$ =		148.58		
$\ln K_f$ =		−59.94		
Liquid phase				
$\Delta_fH°$ =	63.70	63.70	0.00	56SCO/MCC
$C_p°$ =	173.22	173.22	0.00	56SCO/MCC
$S°$ =	222.80	222.80	0.00	56SCO/MCC
$\Delta_fS°$ =		−235.41		
$\Delta_fG°$ =		133.89		
$\ln K_f$ =		−54.01		

Benzyl mercaptan C_7H_8S

(1×S–(C)(H))+(1×C–(H)$_2$(C_B)(S))+(1×C_B–(C)(C_B)$_2$)+(5×C_B–(H)(C_B)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	92.80	92.80	0.00	72GOO2
Liquid phase				
$\Delta_fH°$ =	36.20	36.20	0.00	72GOO2

TABLE 43. Sulfides (32)

Dimethyl sulfide C_2H_6S

(2×C–(H)$_3$(S))+(1×S–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−37.53	−37.53	0.00	57MCC/HUB
$C_p°$ =	74.10	74.10	0.00	69STU/WES
$S°$ =	285.80	285.80	0.00	69STU/WES
$\Delta_fS°$ =		−149.45		
$\Delta_fG°$ =		7.03		
$\ln K_f$ =		−2.84		
Liquid phase				
$\Delta_fH°$ =	−65.40	−65.40	0.00	57MCC/HUB
$C_p°$ =	118.11	118.11	0.00	42OSB/DOE
$S°$ =	196.40	196.40	0.00	42OSB/DOE
$\Delta_fS°$ =		−238.85		
$\Delta_fG°$ =		5.81		
$\ln K_f$ =		−2.34		

Ethyl methyl sulfide C_3H_8S

(1×C–(H)$_3$(C))+(1×C–(H)$_3$(S))+(1×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−59.62	−60.70	1.08	51SCO/FIN
$C_p°$ =	95.10	95.00	0.10	69STU/WES
$S°$ =	333.10	333.43	−0.33	69STU/WES
$\Delta_fS°$ =		−238.13		
$\Delta_fG°$ =		10.30		
$\ln K_f$ =		−4.15		
Liquid phase				
$\Delta_fH°$ =	−91.60	−92.17	0.57	54HUB/WAD
$C_p°$ =	144.64	142.29	2.35	51SCO/FIN
$S°$ =	239.00	237.49	1.51	51SCO/FIN
$\Delta_fS°$ =		−334.07		
$\Delta_fG°$ =		7.43		
$\ln K_f$ =		−3.00		

Diethyl sulfide $C_4H_{10}S$

(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−83.74	−83.87	0.13	52SCO/FIN2
$C_p°$ =	117.03	115.90	1.13	69STU/WES
$S°$ =	368.00	369.54	−1.54	69STU/WES
$\Delta_fS°$ =		−338.33		
$\Delta_fG°$ =		17.00		
$\ln K_f$ =		−6.86		

TABLE 43. Sulfides (32) – Continued

Diethyl sulfide (Continued) $C_4H_{10}S$

(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	–119.40	–118.94	–0.46	58HUB/GOO
$C_p°$ =	171.42	166.47	4.95	52SCO/FIN2
$S°$ =	269.28	278.58	–9.30	52SCO/FIN2
$\Delta_fS°$ =		–429.29		
$\Delta_fG°$ =		9.05		
$\ln K_f$ =		–3.65		

Isopropyl methyl sulfide $C_4H_{10}S$

(2×C–(H)$_3$(C))+(1×C–(H)$_3$(S))+(1×C–(H)(C)$_2$(S))+(1×S–(C)$_2$)+(2×–CH$_3$ corr (tertiary)), σ = 27

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	–90.42	–90.19	–0.23	55MCC/FIN
$C_p°$ =	117.15	120.12	–2.97	69STU/WES
$S°$ =	359.30	362.39	–3.09	69STU/WES
$\Delta_fS°$ =		–345.48		
$\Delta_fG°$ =		12.82		
$\ln K_f$ =		–5.17		
Liquid phase				
$\Delta_fH°$ =	–124.70	–123.44	–1.26	58HUB/GOO
$C_p°$ =	172.38	172.37	0.01	55MCC/FIN
$S°$ =	263.09	263.09	0.00	55MCC/FIN
$\Delta_fS°$ =		–444.78		
$\Delta_fG°$ =		9.17		
$\ln K_f$ =		–3.70		

Methyl propyl sulfide $C_4H_{10}S$

(1×C–(H)$_3$(C))+(1×C–(H)$_3$(S))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	–81.76	–81.33	–0.43	57SCO/FIN
$C_p°$ =	117.36	117.89	–0.53	69STU/WES
$S°$ =	371.70	372.59	–0.89	69STU/WES
$\Delta_fS°$ =		–335.28		
$\Delta_fG°$ =		18.63		
$\ln K_f$ =		–7.52		
Liquid phase				
$\Delta_fH°$ =	–118.50	–117.90	–0.60	58HUB/GOO
$C_p°$ =	171.63	172.71	–1.08	57SCO/FIN
$S°$ =	272.54	269.87	2.67	57SCO/FIN
$\Delta_fS°$ =		–438.00		
$\Delta_fG°$ =		12.69		
$\ln K_f$ =		–5.12		

Butyl methyl sulfide $C_5H_{12}S$

(1×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_3$(S))+(1×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	–102.17	–101.96	–0.21	61MCC/FIN
$C_p°$ =	140.75	140.78	–0.03	69STU/WES
$S°$ =	411.80	411.75	0.05	69STU/WES
$\Delta_fS°$ =		–432.43		
$\Delta_fG°$ =		26.97		
$\ln K_f$ =		–10.88		
Liquid phase				
$\Delta_fH°$ =	–142.90	–143.63	0.73	61MCC/FIN
$C_p°$ =	200.92	203.13	–2.21	61MCC/FIN
$S°$ =	307.48	302.25	5.23	61MCC/FIN
$\Delta_fS°$ =		–541.93		
$\Delta_fG°$ =		17.95		
$\ln K_f$ =		–7.24		

Ethyl propyl sulfide $C_5H_{12}S$

(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	–104.60	–104.50	–0.10	61MCC/FIN
$C_p°$ =	139.12	138.79	0.33	69STU/WES
$S°$ =	414.10	414.46	–0.36	69STU/WES
$\Delta_fS°$ =		–429.72		
$\Delta_fG°$ =		23.62		
$\ln K_f$ =		–9.53		
Liquid phase				
$\Delta_fH°$ =	–144.80	–144.67	–0.13	61MCC/FIN
$C_p°$ =	198.41	196.89	1.52	61MCC/FIN
$S°$ =	309.53	310.96	–1.43	61MCC/FIN
$\Delta_fS°$ =		–533.22		
$\Delta_fG°$ =		14.31		
$\ln K_f$ =		–5.77		

Butyl ethyl sulfide $C_6H_{14}S$

(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	–125.19	–125.13	–0.06	62MAC/MAY
$C_p°$ =	161.96	161.68	0.28	69STU/WES
$S°$ =	453.00	453.62	–0.62	69STU/WES
$\Delta_fS°$ =		–526.87		
$\Delta_fG°$ =		31.96		
$\ln K_f$ =		–12.89		

TABLE 43. Sulfides (32) – Continued

Butyl ethyl sulfide (Continued) $C_6H_{14}S$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−172.30	−170.40	−1.90	62MAC/MAY
$C_p°$ =		227.31		
$S°$ =		343.34		
$\Delta_fS°$ =		−637.15		
$\Delta_fG°$ =		19.57		
$\ln K_f$ =		−7.89		

Diisopropyl sulfide $C_6H_{14}S$
(4×C–(H)$_3$(C))+(2×C–(H)(C)$_2$(S))+(4×–CH$_3$ corr (tertiary))+(1×S–(C)$_2$), σ = 162

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−141.25	−142.85	1.60	62MAC/MAY
$C_p°$ =	169.24	166.14	3.10	69STU/WES
$S°$ =	415.47	427.45	−11.98	69STU/WES
$\Delta_fS°$ =		−553.04		
$\Delta_fG°$ =		22.04		
$\ln K_f$ =		−8.89		
Liquid phase				
$\Delta_fH°$ =	−181.60	−181.48	−0.12	62MAC/MAY
$C_p°$ =	232.00	226.63	5.37	67MES/TOD
$S°$ =	313.05	329.78	−16.73	67MES/TOD
$\Delta_fS°$ =		−650.71		
$\Delta_fG°$ =		12.53		
$\ln K_f$ =		−5.05		

Methyl pentyl sulfide $C_6H_{14}S$
(1×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(1×C–(H)$_3$(S))+(1×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−122.76	−122.59	−0.17	62MAC/MAY
$C_p°$ =	163.59	163.67	−0.08	69STU/WES
$S°$ =	450.74	450.91	−0.17	69STU/WES
$\Delta_fS°$ =		−529.58		
$\Delta_fG°$ =		35.30		
$\ln K_f$ =		−14.24		
Liquid phase				
$\Delta_fH°$ =	−167.10	−169.36	2.26	62MAC/MAY
$C_p°$ =		233.55		
$S°$ =		334.63		
$\Delta_fS°$ =		−645.86		
$\Delta_fG°$ =		23.20		
$\ln K_f$ =		−9.36		

TABLE 43. Sulfides (32) – Continued

Dipropyl sulfide $C_6H_{14}S$
(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−125.35	−125.13	−0.22	61MCC/FIN
$C_p°$ =	161.21	161.68	−0.47	69STU/WES
$S°$ =	448.36	447.86	0.50	69STU/WES
$\Delta_fS°$ =		−532.63		
$\Delta_fG°$ =		33.67		
$\ln K_f$ =		−13.58		
Liquid phase				
$\Delta_fH°$ =	−169.90	−170.40	0.50	61MCC/FIN
$C_p°$ =	225.48	227.31	−1.83	61MCC/FIN
$S°$ =	338.28	343.34	−5.06	61MCC/FIN
$\Delta_fS°$ =		−637.15		
$\Delta_fG°$ =		19.57		
$\ln K_f$ =		−7.89		

Butyl propyl sulfide $C_7H_{16}S$
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−145.94	−145.76	−0.18	69STU/WES
$C_p°$ =	184.05	184.57	−0.52	69STU/WES
$S°$ =	493.95	492.78	1.17	69STU/WES
$\Delta_fS°$ =		−624.02		
$\Delta_fG°$ =		40.29		
$\ln K_f$ =		−16.25		
Liquid phase				
$\Delta_fH°$ =		−196.13		
$C_p°$ =		257.73		
$S°$ =		375.72		
$\Delta_fS°$ =		−741.08		
$\Delta_fG°$ =		24.82		
$\ln K_f$ =		−10.01		

Ethyl pentyl sulfide $C_7H_{16}S$
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−145.81	−145.76	−0.05	69STU/WES
$C_p°$ =	184.84	184.57	0.27	69STU/WES
$S°$ =	491.95	492.78	−0.83	69STU/WES
$\Delta_fS°$ =		−624.02		
$\Delta_fG°$ =		40.29		
$\ln K_f$ =		−16.25		

TABLE 43. Sulfides (32) – Continued

Ethyl pentyl sulfide (Continued) $C_7H_{16}S$
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−196.13		
$C_p°$ =		257.73		
$S°$ =		375.72		
$\Delta_fS°$ =		−741.08		
$\Delta_fG°$ =		24.82		
$\ln K_f$ =		−10.01		

Diisobutyl sulfide $C_8H_{18}S$
(4×C–(H)$_3$(C))+(2×C–(H)(C)$_3$)+(4×–CH$_3$ corr (tertiary))+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−179.50	−179.77	0.27	62MAC/MAY
$C_p°$ =		207.52		
Liquid phase				
$\Delta_fH°$ =	−229.20	−232.42	3.22	62MAC/MAY
$C_p°$ =		282.19		
$S°$ =		397.40		
$\Delta_fS°$ =		−855.71		
$\Delta_fG°$ =		22.71		
$\ln K_f$ =		−9.16		

Diisopentyl sulfide $C_{10}H_{22}S$
(4×C–(H)$_3$(C))+(2×C–(H)(C)$_3$)+(4×–CH$_3$ corr (tertiary))+(2×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−221.50	−221.03	−0.47	62MAC/MAY
$C_p°$ =		253.30		
Liquid phase				
$\Delta_fH°$ =	−281.80	−283.88	2.08	62MAC/MAY
$C_p°$ =		343.03		
$S°$ =		462.16		
$\Delta_fS°$ =		−1063.57		
$\Delta_fG°$ =		33.22		
$\ln K_f$ =		−13.40		

TABLE 43. Sulfides (32) – Continued

Di-*tert*-butyl sulfide $C_8H_{18}S$
(6×C–(H)$_3$(C))+(2×C–(C)$_3$(S))+(6×–CH$_3$ corr (quat/quat))+(1×S–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−188.90	−183.37	−5.53	62MAC/MAY
$C_p°$ =		211.06		
Liquid phase				
$\Delta_fH°$ =	−232.60	−226.30	−6.30	62MAC/MAY
$C_p°$ =		281.79		
$S°$ =		355.88		
$\Delta_fS°$ =		−897.23		
$\Delta_fG°$ =		41.21		
$\ln K_f$ =		−16.62		

Hexyl methyl sulfide $C_7H_{16}S$
(1×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(S))+(1×S–(C)$_2$)+(1×C–(H)$_3$(S)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−145.27	−143.22	−2.05	62MAC/MAY
$C_p°$ =	186.48	186.56	−0.08	69STU/WES
$S°$ =	489.70	490.07	−0.37	69STU/WES
$\Delta_fS°$ =		−626.73		
$\Delta_fG°$ =		43.64		
$\ln K_f$ =		−17.60		
Liquid phase				
$\Delta_fH°$ =	−190.46	−195.09	4.63	62MAC/MAY
$C_p°$ =		263.97		
$S°$ =		367.01		
$\Delta_fS°$ =		−749.79		
$\Delta_fG°$ =		28.46		
$\ln K_f$ =		−11.48		

Dibutyl sulfide $C_8H_{18}S$
(2×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−167.32	−166.39	−0.93	61MCC/FIN
$C_p°$ =	206.94	207.46	−0.52	69STU/WES
$S°$ =	526.52	526.18	0.34	69STU/WES
$\Delta_fS°$ =		−726.93		
$\Delta_fG°$ =		50.35		
$\ln K_f$ =		−20.31		

TABLE 43. Sulfides (32) — Continued

Dibutyl sulfide (Continued) $C_8H_{18}S$
(2×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−220.70	−221.86	1.16	61MCC/FIN
$C_p°$ =	284.34	288.15	−3.81	61MCC/FIN
$S°$ =	405.09	408.10	−3.01	61MCC/FIN
$\Delta_fS°$ =		−845.01		
$\Delta_fG°$ =		30.08		
$\ln K_f$ =		−12.13		

Ethyl hexyl sulfide $C_8H_{18}S$
(2×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−166.40	−166.39	−0.01	69STU/WES
$C_p°$ =	207.69	207.46	0.23	69STU/WES
$S°$ =	530.91	531.94	−1.03	69STU/WES
$\Delta_fS°$ =		−721.17		
$\Delta_fG°$ =		48.63		
$\ln K_f$ =		−19.62		
Liquid phase				
$\Delta_fH°$ =		−221.86		
$C_p°$ =		288.15		
$S°$ =		408.10		
$\Delta_fS°$ =		−845.01		
$\Delta_fG°$ =		30.08		
$\ln K_f$ =		−12.13		

Heptyl methyl sulfide $C_8H_{18}S$
(1×C–(H)$_3$(C))+(5×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(S))+(1×S–(C)$_2$)+(1×C–(H)$_3$(S)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−163.97	−163.85	−0.12	69STU/WES
$C_p°$ =	209.33	209.45	−0.12	69STU/WES
$S°$ =	528.65	529.23	−0.58	69STU/WES
$\Delta_fS°$ =		−723.88		
$\Delta_fG°$ =		51.98		
$\ln K_f$ =		−20.97		
Liquid phase				
$\Delta_fH°$ =		−220.82		
$C_p°$ =		294.39		
$S°$ =		399.39		
$\Delta_fS°$ =		−853.72		
$\Delta_fG°$ =		33.72		
$\ln K_f$ =		−13.60		

TABLE 43. Sulfides (32) — Continued

Dipentyl sulfide $C_{10}H_{22}S$
(2×C–(H)$_3$(C))+(6×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−208.53	−207.65	−0.88	62MAC/MAY
$C_p°$ =	252.67	253.24	−0.57	69STU/WES
$S°$ =	604.38	604.50	−0.12	69STU/WES
$\Delta_fS°$ =		−921.24		
$\Delta_fG°$ =		67.02		
$\ln K_f$ =		−27.03		
Liquid phase				
$\Delta_fH°$ =	−266.40	−273.32	6.92	62MAC/MAY
$C_p°$ =		348.99		
$S°$ =		472.86		
$\Delta_fS°$ =		−1052.88		
$\Delta_fG°$ =		40.59		
$\ln K_f$ =		−16.38		

Butyl heptyl sulfide $C_{11}H_{24}S$
(2×C–(H)$_3$(C))+(7×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−229.16	−228.28	−0.88	69STU/WES
$C_p°$ =	275.56	276.13	−0.57	69STU/WES
$S°$ =	649.11	649.42	−0.31	69STU/WES
$\Delta_fS°$ =		−1012.62		
$\Delta_fG°$ =		73.63		
$\ln K_f$ =		−29.70		
Liquid phase				
$\Delta_fH°$ =		−299.05		
$C_p°$ =		379.41		
$S°$ =		505.24		
$\Delta_fS°$ =		−1156.81		
$\Delta_fG°$ =		45.85		
$\ln K_f$ =		−18.50		

Dihexyl sulfide $C_{12}H_{26}S$
(2×C–(H)$_3$(C))+(8×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(1×S–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−249.74	−248.91	−0.83	69STU/WES
$C_p°$ =	298.40	299.02	−0.62	69STU/WES
$S°$ =	682.28	682.82	−0.54	69STU/WES
$\Delta_fS°$ =		−1115.54		
$\Delta_fG°$ =		83.69		
$\ln K_f$ =		−33.76		

TABLE 43. Sulfides (32) — Continued

Dihexyl sulfide (Continued) $C_{12}H_{26}S$

(2×C-(H)$_3$(C))+(8×C-(H)$_2$(C)$_2$)+(2×C-(H)$_2$(C)(S))+(1×S-(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−324.78		
$C_p°$ =		409.83		
$S°$ =		537.62		
$\Delta_fS°$ =		−1260.74		
$\Delta_fG°$ =		51.11		
$\ln K_f$ =		−20.62		

Butyl nonyl sulfide $C_{13}H_{28}S$

(2×C-(H)$_3$(C))+(9×C-(H)$_2$(C)$_2$)+(2×C-(H)$_2$(C)(S))+(1×S-(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−270.37	−269.54	−0.83	69STU/WES
$C_p°$ =	321.29	321.91	−0.62	69STU/WES
$S°$ =	727.01	727.74	−0.73	69STU/WES
$\Delta_fS°$ =		−1206.93		
$\Delta_fG°$ =		90.31		
$\ln K_f$ =		−36.43		
Liquid phase				
$\Delta_fH°$ =		−350.51		
$C_p°$ =		440.25		
$S°$ =		570.00		
$\Delta_fS°$ =		−1364.67		
$\Delta_fG°$ =		56.37		
$\ln K_f$ =		−22.74		

Butyl pentadecyl sulfide $C_{19}H_{40}S$

(2×C-(H)$_3$(C))+(15×C-(H)$_2$(C)$_2$)+(2×C-(H)$_2$(C)(S))+(1×S-(C)$_2$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−394.05	−393.32	−0.73	69STU/WES
$C_p°$ =	458.48	459.25	−0.77	69STU/WES
$S°$ =	960.69	962.70	−2.01	69STU/WES
$\Delta_fS°$ =		−1789.83		
$\Delta_fG°$ =		140.32		
$\ln K_f$ =		−56.60		
Liquid phase				
$\Delta_fH°$ =		−504.89		
$C_p°$ =		622.77		
$S°$ =		764.28		
$\Delta_fS°$ =		−1988.25		
$\Delta_fG°$ =		87.91		
$\ln K_f$ =		−35.46		

TABLE 43. Sulfides (32) — Continued

***tert*-Butyl methyl sulfide** $C_5H_{12}S$

(3×C-(H)$_3$(C))+(1×C-(H)$_3$(S))+(1×S-(C)$_2$)+(1×C-(C)$_3$(S))+(3×-CH$_3$ corr (quaternary)), σ = 243

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−121.04	−122.21	1.17	62SCO/GOO
$C_p°$ =	145.02	142.58	2.44	69STU/WES
$S°$ =	373.25	373.42	−0.17	69STU/WES
$\Delta_fS°$ =		−470.76		
$\Delta_fG°$ =		18.15		
$\ln K_f$ =		−7.32		
Liquid phase				
$\Delta_fH°$ =	−157.10	−157.10	0.00	62SCO/GOO
$C_p°$ =	199.95	199.95	0.00	62SCO/GOO
$S°$ =	276.14	276.14	0.00	62SCO/GOO
$\Delta_fS°$ =		−568.04		
$\Delta_fG°$ =		12.26		
$\ln K_f$ =		−4.95		

3-Ethyl-1-propene sulfide; 4-Thia-1-hexene $C_5H_{10}S$

(1×C-(H)$_3$(C))+(1×C-(H)$_2$(C)(S))+(1×S-(C)$_2$)+(1×C-(H)$_2$(C$_d$)(S))+(1×C$_d$-(H)(C))+(1×C$_d$-(H)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	17.80	18.27	−0.47	62MAC/MAY2
Liquid phase				
$\Delta_fH°$ =	−21.50	−24.20	2.70	62MAC/MAY2

Isopropyl ethyl sulfide $C_5H_{12}S$

(3×C-(H)$_3$(C))+(1×C-(H)$_2$(C)(S))+(1×S-(C)$_2$)+(1×C-(H)(C)$_2$(S))+(2×-CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−117.20	−113.36	−3.84	62MAC/MAY
$C_p°$ =		141.02		
Liquid phase				
$\Delta_fH°$ =	−156.10	−150.21	−5.89	62MAC/MAY
$C_p°$ =		196.55		
$S°$ =		304.18		
$\Delta_fS°$ =		−540.00		
$\Delta_fG°$ =		10.79		
$\ln K_f$ =		−4.35		

TABLE 43. Sulfides (32) – Continued

tert-Butyl ethyl sulfide $C_6H_{14}S$

(4 × C–(H)$_3$(C)) + (1 × C–(H)$_2$(C)(S)) + (1 × S–(C)$_2$) + (1 × C–(C)$_3$(S)) + (3 × –CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−148.00	−145.38	−2.62	62MAC/MAY
$C_p°$ =		163.48		
Liquid phase				
$\Delta_f H°$ =	−187.30	−183.87	−3.43	62MAC/MAY
$C_p°$ =		224.13		
$S°$ =		317.23		
$\Delta_f S°$ =		−663.26		
$\Delta_f G°$ =		13.88		
$\ln K_f$ =		−5.60		

Allyl tert-butyl sulfide $C_7H_{14}S$

(3 × C–(H)$_3$(C)) + (1 × C–(C)$_3$(S)) + (3 × –CH$_3$ corr (quaternary)) + (1 × S–(C)$_2$) + (1 × C–(H)$_2$(C$_d$)(S)) + (1 × C$_d$–(H)$_2$) + (1 × C$_d$–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−46.70	−43.24	−3.46	62MAC/MAY
Liquid phase				
$\Delta_f H°$ =	−91.00	−89.13	−1.87	62MAC/MAY

Diphenyl sulfide $C_{12}H_{10}S$

(2 × C$_B$–(S)) + (10 × C$_B$–(H)(C$_B$)$_2$) + (1 × S-(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	231.20	231.20	0.00	62MAC/MAY2
$C_p°$ =		187.86		
Liquid phase				
$\Delta_f H°$ =	163.40	163.40	0.00	62MAC/MAY2
$C_p°$ =	271.12	271.12	0.00	31SMI/AND2

Methyl phenyl sulfide C_7H_8S

(1 × C–(H)$_3$(S)) + (1 × S–(C$_B$)(C)) + (1 × C$_B$–(S)) + (5 × C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	97.30	98.25	−0.95	72GOO2

TABLE 43. Sulfides (32) – Continued

Methyl phenyl sulfide (Continued) C_7H_8S

(1 × C–(H)$_3$(S)) + (1 × S–(C$_B$)(C)) + (1 × C$_B$–(S)) + (5 × C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	43.00	45.78	−2.78	72GOO2
$C_p°$ =	206.02	206.02	0.00	74MES/FIN
$S°$ =	252.50	252.50	0.00	74MES/FIN
$\Delta_f S°$ =		−342.02		
$\Delta_f G°$ =		147.75		
$\ln K_f$ =		−59.60		

Ethyl phenyl sulfide $C_8H_{10}S$

(1 × C–(H)$_3$(C)) + (1 × C–(H)$_2$(C)(S)) + (1 × S–(C$_B$)(C)) + (1 × C$_B$–(S)) + (5 × C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	77.00	75.08	1.92	62MAC/MAY3
Liquid phase				
$\Delta_f H°$ =	21.80	19.01	2.79	62MAC/MAY3
$C_p°$ =		230.20		
$S°$ =		293.59		
$\Delta_f S°$ =		−437.24		
$\Delta_f G°$ =		149.37		
$\ln K_f$ =		−60.26		

TABLE 44. Disulfides (8)

Dimethyl disulfide $C_2H_6S_2$

(2×C–(H)$_3$(S))+(2×S–(C)(S)), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−24.41	−29.28	4.87	58HUB/DOU
C_p° =	94.31	97.96	−3.65	69STU/WES
$S°$ =	336.64	331.61	5.03	69STU/WES
$\Delta_fS°$ =		−135.69		
$\Delta_fG°$ =		11.18		
$\ln K_f$ =		−4.51		
Liquid Phase				
$\Delta_fH°$ =	−62.60	−66.50	3.90	58HUB/DOU
C_p° =	146.11	154.38	−8.27	50SCO/FIN
$S°$ =	235.29	228.28	7.01	50SCO/FIN
$\Delta_fS°$ =		−239.02		
$\Delta_fG°$ =		4.76		
$\ln K_f$ =		−1.92		

Diethyl disulfide $C_4H_{10}S_2$

(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)(S))+(2×S–(C)(S)), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−74.64	−75.62	0.98	58HUB/DOU
C_p° =	141.34	139.76	1.58	69STU/WES
$S°$ =	414.51	415.35	−0.84	69STU/WES
$\Delta_fS°$ =		−324.58		
$\Delta_fG°$ =		21.15		
$\ln K_f$ =		−8.53		
Liquid Phase				
$\Delta_fH°$ =	−120.10	−120.04	−0.06	58HUB/DOU
C_p° =	204.01	202.74	1.27	52SCO/FIN
$S°$ =	305.01	310.46	−5.45	52SCO/FIN
$\Delta_fS°$ =		−429.46		
$\Delta_fG°$ =		8.00		
$\ln K_f$ =		−3.23		

Dipropyl disulfide $C_6H_{14}S_2$

(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(2×S–(C)(S)), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−117.19	−116.88	−0.31	58HUB/DOU
C_p° =	185.35	185.54	−0.19	69STU/WES
$S°$ =	494.97	493.67	1.30	69STU/WES
$\Delta_fS°$ =		−518.88		
$\Delta_fG°$ =		37.82		
$\ln K_f$ =		−15.26		

TABLE 44. Disulfides (8) – Continued

Dipropyl disulfide (Continued) $C_6H_{14}S_2$

(2×C–(H)$_3$(C))+(2×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(2×S–(C)(S)), σ = 18

	Literature	Calculated	Residual	Reference
Liquid Phase				
$\Delta_fH°$ =	−171.50	−171.50	0.00	58HUB/DOU
C_p° =	262.46	263.58	−1.12	58HUB/DOU
$S°$ =	373.55	375.22	−1.67	58HUB/DOU
$\Delta_fS°$ =		−637.33		
$\Delta_fG°$ =		18.52		
$\ln K_f$ =		−7.47		

Dibutyl disulfide $C_8H_{18}S_2$

(2×C–(H)$_3$(C))+(4×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(2×S–(C)(S)), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−158.41	−158.14	−0.27	64MAC/MCC
C_p° =	231.08	231.32	−0.24	69STU/WES
$S°$ =	572.83	571.99	0.84	69STU/WES
$\Delta_fS°$ =		−713.18		
$\Delta_fG°$ =		54.49		
$\ln K_f$ =		−21.98		
Liquid Phase				
$\Delta_fH°$ =	−222.90	−222.96	0.06	64MAC/MCC
C_p° =		324.42		
$S°$ =		439.98		
$\Delta_fS°$ =		−845.19		
$\Delta_fG°$ =		29.03		
$\ln K_f$ =		−11.71		

Dipentyl disulfide $C_{10}H_{22}S_2$

(2×C–(H)$_3$(C))+(6×C–(H)$_2$(C)$_2$)+(2×C–(H)$_2$(C)(S))+(2×S–(C)(S)), σ = 18

	Literature	Calculated	Residual	Reference
Gas Phase				
$\Delta_fH°$ =	−199.62	−199.40	−0.22	69STU/WES
C_p° =	276.81	277.10	−0.29	69STU/WES
$S°$ =	650.74	650.31	0.43	69STU/WES
$\Delta_fS°$ =		−907.48		
$\Delta_fG°$ =		71.17		
$\ln K_f$ =		−28.71		
Liquid Phase				
$\Delta_fH°$ =		−274.42		
C_p° =		385.26		
$S°$ =		504.74		
$\Delta_fS°$ =		−1053.05		
$\Delta_fG°$ =		39.55		
$\ln K_f$ =		−15.95		

TABLE 44. Disulfides (8) – Continued

Dihexyl disulfide $C_{12}H_{26}S_2$

$(2\times C\text{–}(H)_3(C))+(8\times C\text{–}(H)_2(C)_2)+(2\times C\text{–}(H)_2(C)(S))+(2\times S\text{–}(C)(S))$, $\sigma = 18$

	Literature	– Calculated	= Residual	Reference
Gas Phase				
Δ_fH° =	–240.83	–240.66	–0.17	69STU/WES
C_p° =	322.54	322.88	–0.34	69STU/WES
S° =	728.64	728.63	0.01	69STU/WES
Δ_fS° =		–1101.78		
Δ_fG° =		87.84		
$\ln K_f$ =		–35.43		
Liquid Phase				
Δ_fH° =		–325.88		
C_p° =		446.10		
S° =		569.50		
Δ_fS° =		–1260.91		
Δ_fG° =		50.06		
$\ln K_f$ =		–20.19		

Didecyl disulfide $C_{20}H_{42}S_2$

$(2\times C\text{–}(H)_3(C))+(16\times C\text{–}(H)_2(C)_2)+(2\times C\text{–}(H)_2(C)(S))+(2\times S\text{–}(C)(S))$, $\sigma = 18$

	Literature	– Calculated	= Residual	Reference
Gas Phase				
Δ_fH° =	–405.72	–405.70	–0.02	69STU/WES
C_p° =	505.51	506.00	–0.49	69STU/WES
S° =	1040.23	1041.91	–1.68	69STU/WES
Δ_fS° =		–1878.99		
Δ_fG° =		154.52		
$\ln K_f$ =		–62.33		
Liquid Phase				
Δ_fH° =		–531.72		
C_p° =		689.46		
S° =		828.54		
Δ_fS° =		–2092.36		
Δ_fG° =		92.12		
$\ln K_f$ =		–37.16		

Diphenyl disulfide $C_{12}H_{10}S_2$

$(10\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(S))+(2\times S\text{–}(C_B)(S))$

	Literature	– Calculated	= Residual	Reference
Gas Phase				
Δ_fH° =	243.50	243.50	0.00	62MAC/MAY2
Solid Phase				
Δ_fH° =	148.50	148.50	0.00	62MAC/MAY2

TABLE 45. Sulfoxides (6)

Dimethyl sulfoxide C_2H_6OS

$(2\times C\text{–}(H)_3(SO))+(1\times SO\text{–}(C)_2)$, $\sigma = 18$

	Literature	– Calculated	= Residual	Reference
Gas phase				
Δ_fH° =	–151.30	–151.30	0.00	48DOU
C_p° =	88.95	88.61	0.34	62MAC/OHA
S° =	306.27	306.34	–0.07	62MAC/OHA
Δ_fS° =		–231.43		
Δ_fG° =		–82.30		
$\ln K_f$ =		33.20		
Liquid phase				
Δ_fH° =	–204.20	–204.20	0.00	46DOU
C_p° =	153.18	153.18	0.00	70CLE/WES
S° =	188.78	188.78	0.00	70CLE/WES
Δ_fS° =		–348.99		
Δ_fG° =		–100.15		
$\ln K_f$ =		40.40		

Diethyl sulfoxide $C_4H_{10}OS$

$(2\times C\text{–}(H)_3(C))+(2\times C\text{–}(H)_2(C)(SO))+(1\times SO\text{–}(C)_2)$

	Literature	– Calculated	= Residual	Reference
Gas phase				
Δ_fH° =	–205.60	–209.62	4.02	61MAC/OHA4
Liquid phase				
Δ_fH° =	268.00	277.96	9.96	61MAC/OHA4

Allyl ethyl sulfoxide $C_5H_{10}OS$

$(1\times C\text{–}(H)_3(C))+(1\times C\text{–}(H)_2(C)(SO))+(1\times SO\text{–}(C)_2)+(1\times C\text{–}(H)_2(C_d)(SO))+(1\times C_d\text{–}(H)(C))+(1\times C_d\text{–}(H)_2)$

	Literature	– Calculated	= Residual	Reference
Gas phase				
Δ_fH° =	–103.70	–103.12	–0.58	61MAC/OHA4
Liquid phase				
Δ_fH° =	–173.30	–173.30	0.00	61MAC/OHA4

Dipropyl sulfoxide $C_6H_{14}OS$

$(2\times C\text{–}(H)_3(C))+(2\times C\text{–}(H)_2(C)_2)+(2\times C\text{–}(H)_2(C)(SO))+(1\times SO\text{–}(C)_2)$

	Literature	– Calculated	= Residual	Reference
Gas phase				
Δ_fH° =	–254.90	–250.88	–4.02	61MAC/OHA4

TABLE 45. Sulfoxides (6) — Continued

Dipropyl sulfoxide $C_6H_{14}OS$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(C)(SO)) + (1×SO–(C)$_2$)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =	−329.40	−329.42	0.02	61MAC/OHA4

***tert*-Butyl ethyl sulfoxide** $C_6H_{14}OS$
(4×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)(SO)) + (1×SO–(C)$_2$) + (1×C–(C)$_3$(SO)) + (3×–CH$_3$ corr (quaternary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−274.10	−274.10	0.00	61MAC/OHA4
Liquid phase				
$\Delta_f H°$ =	−348.50	−348.50	0.00	61MAC/OHA4

Diphenyl sulfoxide $C_{12}H_{10}OS$
(10×C$_B$–(H)(C$_B$)$_2$) + (2×C$_B$–(SO)) + (1×SO–(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	106.80	106.80	0.00	61MAC/OHA4

TABLE 46. Sulfones (38)

Dimethyl sulfone $C_2H_6O_2S$
(2×C–(H)$_3$(SO$_2$)) + (1×SO$_2$–(C)$_2$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−373.10	−373.10	0.00	70MAC/STE
$C_p°$ =	100.00	100.00	0.00	62MAC/OHA
$S°$ =	317.98	317.98	0.00	62MAC/OHA
$\Delta_f S°$ =		−322.31		
$\Delta_f G°$ =		−277.00		
$\ln K_f$ =		111.74		
Liquid phase				
$\Delta_f H°$ =	−436.36	−436.36	0.00	
Solid phase				
$\Delta_f H°$ =	−450.10	−450.10	0.00	61BUS/MAC
$C_p°$ =	125.35	125.35	0.00	70CLE/WES
$S°$ =	145.48	145.48	0.00	70CLE/WES
$\Delta_f S°$ =		−494.81		
$\Delta_f G°$ =		−302.57		
$\ln K_f$ =		122.06		

Ethyl methyl sulfone $C_3H_8O_2S$
(1×C–(H)$_3$(C)) + (1×C–(H)$_3$(SO$_2$)) + (1×C–(H)$_2$(C)(SO$_2$)) + (1×SO$_2$–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−408.36	−400.13	−8.23	70MAC/STE
Liquid phase				
$\Delta_f H°$ =		−470.12		
Solid phase				
$\Delta_f H°$ =	−486.06	−486.06	0.00	61BUS/MAC

Divinyl sulfone $C_4H_6O_2S$
(2×C$_d$–(H)$_2$) + (2×C$_d$–(H)(SO$_2$)) + (1×SO$_2$–(C$_d$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−150.90	−150.90	0.00	69MAC/MCN

TABLE 46. Sulfones (38) — Continued

Allyl methyl sulfone $C_4H_8O_2S$
$(1\times C_d-(H)_2)+(1\times C_d-(H)(C))+(1\times C-(H)_2(C_d)(SO_2))+(1\times SO_2-(C)_2)+(1\times C-(H)_3(SO_2))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−305.60	−297.69	−7.91	70MAC/STE
Liquid phase $\Delta_fH°$ =	−384.70	−385.00	0.30	70MAC/STE

Diethyl sulfone $C_4H_{10}O_2S$
$(2\times C-(H)_3(C))+(2\times C-(H)_2(C)(SO_2))+(1\times SO_2-(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−428.86	−427.16	−1.70	70MAC/STE
Liquid phase $\Delta_fH°$ =		−503.88		
Solid phase $\Delta_fH°$ =	−515.20	−522.02	6.82	61MAC/OHA

Isopropyl methyl sulfone $C_4H_{10}O_2S$
$(1\times C-(H)_3(SO_2))+(1\times SO_2-(C)_2)+(1\times C-(H)(C)_2(SO_2))+(2\times -CH_3 \text{ corr (tertiary)})+(2\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−434.00	−433.88	−0.12	61BUS/MAC

Allyl ethyl sulfone $C_5H_{10}O_2S$
$(1\times C_d-(H)_2)+(1\times C_d-(H)(C))+(1\times C-(H)_2(C_d)(SO_2))+(1\times SO_2-(C)_2)+(1\times C-(H)_2(C)(SO_2))+(1\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−322.17	−324.72	2.55	70MAC/STE
Liquid phase $\Delta_fH°$ =	−405.64	−418.76	13.12	61MAC/OHA

TABLE 46. Sulfones (38) — Continued

Butyl methyl sulfone $C_5H_{12}O_2S$
$(1\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(SO_2))+(1\times SO_2-(C)_2)+(1\times C-(H)_3(SO_2))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−459.40	−441.39	−18.01	70MAC/STE
Liquid phase $\Delta_fH°$ =	−535.55	−521.58	−13.97	61MAC/OHA

***tert*-Butyl methyl sulfone** $C_5H_{12}O_2S$
$(1\times C-(H)_3(SO_2))+(1\times SO_2-(C)_2)+(1\times C-(C)_3(SO_2))+(3\times C-(H)_3(C))+(3\times -CH_3 \text{ corr (quaternary)})$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−473.20	−469.78	−3.42	70MAC/STE
Solid phase $\Delta_fH°$ =	−555.68	−552.85	−2.83	61BUS/MAC

***tert*-Butyl ethyl sulfone** $C_6H_{14}O_2S$
$(4\times C-(H)_3(C))+(1\times C-(H)_2(C)(SO_2))+(1\times SO_2-(C)_2)+(1\times C-(C)_3(SO_2))+(3\times -CH_3 \text{ corr (quaternary)})$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−491.40	−496.81	5.41	61MAC/OHA
Liquid phase $\Delta_fH°$ =	−578.00	−578.51	0.51	61MAC/OHA

Di-*tert*-butyl sulfone $C_8H_{18}O_2S$
$(6\times C-(H)_3(C))+(1\times SO_2-(C)_2)+(2\times C-(C)_3(SO_2))+(6\times -CH_3 \text{ corr } (\textit{quat/quat}))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−546.00	−542.94	−3.06	70MAC/STE
Solid phase $\Delta_fH°$ =	−640.07	−642.94	2.87	61MAC/OHA

TABLE 46. Sulfones (38) – Continued

Dipropyl sulfone $C_6H_{14}O_2S$

(2 × C–(H)$_3$(C)) + (2 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(C)(SO$_2$)) + (1 × SO$_2$–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−467.77	−468.42	0.65	70MAC/STE
Liquid phase $\Delta_fH°$ =	−547.85	−555.34	7.49	61MAC/OHA

Dibutyl sulfone $C_8H_{18}O_2S$

(2 × C–(H)$_3$(C)) + (4 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(C)(SO$_2$)) + (1 × SO$_2$–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−509.60	−509.68	0.08	70MAC/STE
Liquid phase $\Delta_fH°$ =		−606.80		
Solid phase $\Delta_fH°$ =	−609.86	−639.66	29.80	61BUS/MAC

Diisobutyl sulfone $C_8H_{18}O_2S$

(4 × C–(H)$_3$(C)) + (2 × C–(H)(C)$_3$) + (4 × –CH$_3$ corr (tertiary)) + (2 × C–(H)$_2$(C)(SO$_2$)) + (1 × SO$_2$–(C)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−535.15	−523.06	−12.09	70MAC/STE
Liquid phase $\Delta_fH°$ =	−624.84	−617.36	−7.48	61MAC/OHA

Methyl phenyl sulfone $C_7H_8O_2S$

(1 × C–(H)$_3$(SO$_2$)) + (1 × SO$_2$–(C)(C$_B$)) + (1 × C$_B$–(SO$_2$)(C$_B$)$_2$) + (5 × C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−253.40	−246.83	−6.57	61MAC/OHA2

TABLE 46. Sulfones (38) – Continued

Phenyl vinyl sulfone $C_8H_8O_2S$

(1 × C$_d$–(H)$_2$) + (1 × C$_d$–(H)(SO$_2$)) + (1 × SO$_2$–(C$_d$)(C$_B$)) + (1 × C$_B$–(SO$_2$)(C$_B$)$_2$) + (5 × C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−129.00	−129.12	0.12	69MAC/MCN

Methyl p-tolyl sulfone $C_8H_{10}O_2S$

(1 × C–(H)$_3$(C)) + (1 × C$_B$–(C)(C$_B$)$_2$) + (4 × C$_B$–(H)(C$_B$)$_2$) + (1 × C$_B$–(SO$_2$)(C$_B$)$_2$) + (1 × SO$_2$–(C)(C$_B$)) + (1 × C–(H)$_3$(SO$_2$))

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−273.10	−279.26	6.16	61MAC/OHA

Benzyl methyl sulfone $C_8H_{10}O_2S$

(1 × C–(H)$_3$(SO$_2$)) + (1 × SO$_2$–(C)$_2$) + (1 × C–(H)$_2$(C$_B$)(SO$_2$)) + (1 × C$_B$–(C)(C$_B$)$_2$) + (5 × C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−272.10	−267.95	−4.15	61BUS/MAC

1-(Propynylsulfonyl)benzene $C_9H_8O_2S$

(1 × C–(H)$_3$(C)) + (1 × C$_t$–(C)) + (1 × C$_t$–(SO$_2$)) + (1 × SO$_2$–(C$_t$)(C$_B$)) + (1 × C$_B$–(SO$_2$)(C$_B$)$_2$) + (5 × C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	43.20	38.17	5.03	69MAC/STE3

2-(Propynylsulfonyl)benzene $C_9H_8O_2S$

(1 × C$_t$–(H)) + (1 × C$_t$–(C)) + (1 × C–(H)$_2$(C$_t$)(SO$_2$)) + (1 × SO$_2$–(C)(C$_B$)) + (1 × C$_B$–(SO$_2$)(C$_B$)$_2$) + (5 × C$_B$–(H)(C$_B$)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	36.20	40.39	−4.19	69MAC/STE3

TABLE 46. Sulfones (38) – Continued

Allenyl phenyl sulfone $C_9H_8O_2S$

$(1\times C_d\text{-}(H)_2)+(1\times C_a)+(1\times C_d\text{-}(H)(SO_2))+(1\times SO_2\text{-}(C_d)(C_B))+(1\times C_B\text{-}(SO_2)(C_B)_2)+(5\times C_B\text{-}(H)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	1.80	13.55	−11.75	70MAC/STE

p-Tolyl vinyl sulfone $C_9H_{10}O_2S$

$(1\times C\text{-}(H)_3(C))+(1\times C_B\text{-}(C)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(SO_2)(C_B)_2)+(1\times SO_2\text{-}(C_d)(C_B))+(1\times C_d\text{-}(H)(SO_2))+(1\times C_d\text{-}(H)_2)$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−162.30	−161.55	−0.75	69MAC/MCN

1-Methyl-4-(1-propynylsulfonyl)benzene $C_{10}H_{10}O_2S$

$(1\times C\text{-}(H)_3(C))+(1\times C_B\text{-}(C)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(SO_2)(C_B)_2)+(1\times SO_2\text{-}(C_t)(C_B))+(1\times C_t\text{-}(SO_2))+(1\times C_t\text{-}(C))+(1\times C\text{-}(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	10.10	5.74	4.36	69MAC/STE3

1-Methyl-4-(2-propynylsulfonyl)benzene $C_{10}H_{10}O_2S$

$(1\times C\text{-}(H)_3(C))+(1\times C_B\text{-}(C)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(SO_2)(C_B)_2)+(1\times SO_2\text{-}(C)(C_B))+(1\times C\text{-}(H)_2(C_t)(SO_2))+(1\times C_t\text{-}(C))+(1\times C_t\text{-}(H))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	0.70	7.96	−7.26	69MAC/STE3

1-Methyl-4-(1,2-propadienylsulfonyl)benzene $C_{10}H_{10}O_2S$

$(1\times C\text{-}(H)_3(C))+(1\times C_B\text{-}(C)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(SO_2)(C_B)_2)+(1\times SO_2\text{-}(C_d)(C_B))+(1\times C_d\text{-}(H)(SO_2))+(1\times C_a)+(1\times C_d\text{-}(H)_2)$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−32.60	−18.88	−13.72	69MAC/STE3

(E)-1-Methyl-4-(1-propenylsulfonyl)benzene $C_{10}H_{12}O_2S$

$(1\times C\text{-}(H)_3(C))+(1\times C_B\text{-}(C)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(SO_2)(C_B)_2)+(1\times SO_2\text{-}(C_d)(C_B))+(1\times C_d\text{-}(H)(SO_2))+(1\times C_d\text{-}(H)(C))+(1\times C\text{-}(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−208.90	−193.81	−15.09	69MAC/MCN

1-Methyl-4-(2-propenylsulfonyl)benzene $C_{10}H_{12}O_2S$

$(1\times C\text{-}(H)_3(C))+(1\times C_B\text{-}(C)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(SO_2)(C_B)_2)+(1\times SO_2\text{-}(C)(C_B))+(1\times C\text{-}(H)_2(C_d)(SO_2))+(1\times C_d\text{-}(H)(C))+(1\times C_d\text{-}(H)_2)$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−203.30	−203.85	0.55	69MAC/MCN

1-Methyl-4-(1-methylethenylsulfonyl)benzene $C_{10}H_{12}O_2S$

$(1\times C\text{-}(H)_3(C))+(1\times C_B\text{-}(C)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(SO_2)(C_B)_2)+(1\times SO_2\text{-}(C_d)(C_B))+(1\times C_d\text{-}(C)(SO_2))+(1\times C_d\text{-}(H)_2)+(1\times C\text{-}(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−196.70	−191.38	−5.32	69MAC/MCN

1-Methyl-4-(3-butenylsulfonyl)benzene $C_{11}H_{14}O_2S$

$(1\times C\text{-}(H)_3(C))+(1\times C_B\text{-}(C)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(SO_2)(C_B)_2)+(1\times SO_2\text{-}(C)(C_B))+(1\times C\text{-}(H)_2(C)(SO_2))+(1\times C\text{-}(H)_2(C)(C_d))+(1\times C_d\text{-}(H)(C))+(1\times C_d\text{-}(H)_2)$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−226.00	−222.27	−3.73	69MAC/MCN

1-Methyl-4-(2-butenylsulfonyl)benzene $C_{11}H_{14}O_2S$

$(1\times C\text{-}(H)_3(C))+(1\times C_B\text{-}(C)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(SO_2)(C_B)_2)+(1\times SO_2\text{-}(C)(C_B))+(1\times C\text{-}(H)_2(C_d)(SO_2))+(2\times C_d\text{-}(H)(C))+(1\times C\text{-}(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−240.80	−236.11	−4.69	69MAC/MCN

TABLE 46. Sulfones (38) — Continued

1-Methyl-4-(1-butenylsulfonyl)benzene $C_{11}H_{14}O_2S$
$(1\times C-(H)_3(C))+(1\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times C_B-(SO_2)(C_B)_2)+(1\times SO_2-(C_d)(C_B))+(1\times C_d-(H)(SO_2))+(1\times C_d-(H)(C))+(1\times C-(H)_2(C)(C_d))+(1\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−229.80	−214.69	−15.11	69MAC/MCN

1-Methyl-4-(2-methyl-2-propenylsulfonyl)benzene $C_{11}H_{14}O_2S$
$(1\times C-(H)_3(C))+(1\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times C_B-(SO_2)(C_B)_2)+(1\times SO_2-(C)(C_B))+(1\times C-(H)_2(C_d)(SO_2))+(1\times C_d-(C)_2)+(1\times C_d-(H)_2)+(1\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−241.50	−238.29	−3.21	69MAC/MCN

Diphenyl sulfone $C_{12}H_{10}O_2S$
$(10\times C_B-(H)(C_B)_2)+(2\times C_B-(SO_2)(C_B)_2)+(1\times SO_2-(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−118.70	−118.70	0.00	70COX/PIL
Solid phase $\Delta_fH°$ =	−225.00	−225.00	0.00	61MAC/OHA2

***trans*-Phenyl β-styryl sulfone** $C_{14}H_{12}O_2S$
$(10\times C_B-(H)(C_B)_2)+(1\times C_B-(SO_2)(C_B)_2)+(1\times SO_2-(C_d)(C_B))+(1\times C_d-(H)(SO_2))+(1\times C_d-(H)(C_B))+(1\times C_B-(C_d)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−35.00	−33.94	−1.06	69MAC/MCN

Dibenzyl sulfone $C_{14}H_{14}O_2S$
$(10\times C_B-(H)(C_B)_2)+(2\times C_B-(C)(C_B)_2)+(2\times C-(H)_2(C_B)(SO_2))+(1\times SO_2-(C)_2)$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−157.10	−162.80	5.70	61MAC/OHA

TABLE 46. Sulfones (38) — Continued

***cis*-β-Styryl p-tolyl sulfone** $C_{15}H_{14}O_2S$
$(1\times C-(H)_3(C))+(1\times C_B-(C)(C_B)_2)+(9\times C_B-(H)(C_B)_2)+(1\times C_B-(SO_2)(C_B)_2)+(1\times SO_2-(C_d)(C_B))+(1\times C_d-(H)(SO_2))+(1\times C_d-(H)(C_B))+(1\times C_B-(C_d)(C_B)_2)+(1\times cis\text{(unsat) corr})$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−60.00	−61.52	1.52	69MAC/MCN

***trans*-β-Styryl p-tolyl sulfone** $C_{15}H_{14}O_2S$
$(1\times C-(H)_3(C))+(9\times C_B-(H)(C_B)_2)+(1\times C_B-(SO_2)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times SO_2-(C_d)(C_B))+(1\times C_d-(H)(SO_2))+(1\times C_d-(H)(C_B))+(1\times C_B-(C_d)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−69.60	−66.37	−3.23	69MAC/MCN

Diphenyl disulfone $C_{12}H_{10}O_4S_2$
$(10\times C_B-(H)(C_B)_2)+(2\times C_B-(SO_2)(C_B)_2)+(2\times SO_2-(SO_2)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase $\Delta_fH°$ =	−481.30	−481.30	0.00	64MAC/OHA
Solid phase $\Delta_fH°$ =	−643.10	−643.10	0.00	64MAC/OHA

TABLE 47. Sulfites (5)

Dimethyl sulfite $C_2H_6O_3S$
(2×C–(H)$_3$(C)) + (2×O–(C)(SO)) + (1×SO–(O)$_2$)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−483.40	−482.72	−0.68	69MAC/STE

Ethyl methyl sulfite $C_3H_8O_3S$
(2×C–(H)$_3$(C)) + (2×O–(C)(SO)) + (1×SO–(O)$_2$) + (1×C–(H)$_2$(O)(C))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−524.00	−515.62	−8.38	69MAC/STE

Diethyl sulfite $C_4H_{10}O_3S$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(O)(C)) + (2×O–(C)(SO)) + (1×SO–(O)$_2$)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−552.20	−548.52	−3.68	69MAC/STE

Dipropyl sulfite $C_6H_{14}O_3S$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(O)(C)) + (2×O–(C)(SO)) + (1×SO–(O)$_2$)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−588.30	−589.78	1.48	69MAC/STE

Dibutyl sulfite $C_8H_{18}O_3S$
(2×C–(H)$_3$(C)) + (4×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(O)(C)) + (2×O–(C)(SO)) + (1×SO–(O)$_2$)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−625.30	−631.04	5.74	69MAC/STE

TABLE 48. Sulfates (4)

Dimethyl sulfate $C_2H_6O_4S$
(2×C–(H)$_3$(C)) + (2×O–(C)(SO$_2$)) + (1×SO$_2$–(O)$_2$)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−687.00	−684.62	−2.38	69MAC/STE

Diethyl sulfate $C_4H_{10}O_4S$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(O)(C)) + (2×O–(C)(SO$_2$)) + (1×SO$_2$–(O)$_2$)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−756.30	−750.42	−5.88	69MAC/STE

Dipropyl sulfate $C_6H_{14}O_4S$
(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(O)(C)) + (2×O–(C)(SO$_2$)) + (1×SO$_2$–(O)$_2$)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−792.00	−791.68	−0.32	69MAC/STE

Dibutyl sulfate $C_8H_{18}O_4S$
(2×C–(H)$_3$(C)) + (4×C–(H)$_2$(C)$_2$) + (2×C–(H)$_2$(O)(C)) + (2×O–(C)(SO$_2$)) + (1×SO$_2$–(O)$_2$)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−828.90	−832.94	4.04	69MAC/STE

TABLE 49. Cyclic CHS (13)

Thiacyclopropane C_2H_4S

(1 × S–(C)₂) + (2 × C–(H)₂(C)(S)) + (1 × Thiacyclopropane rsc), $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	82.22	82.22	0.00	52GUT/SCO2
C_p° =	53.68	53.68	0.00	69STU/WES
S° =	255.27	255.27	0.00	69STU/WES
Δ_fS° =		−49.41		
Δ_fG° =		96.95		
$\ln K_f$ =		−39.11		
Liquid phase				
Δ_fH° =	51.60	51.60	0.00	63SUN

Thiacyclobutane C_3H_6S

(1 × C–(H)₂(C)₂) + (2 × C–(H)₂(C)(S)) + (1 × S–(C)₂) + (1 × Thiacyclobutane rsc), $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	61.00	61.00	0.00	53SCO/FIN
C_p° =	69.33	69.33	0.00	69STU/WES
S° =	285.22	285.22	0.00	69STU/WES
Δ_fS° =		−155.77		
Δ_fG° =		107.44		
$\ln K_f$ =		−43.34		
Liquid phase				
Δ_fH° =	25.10	25.10	0.00	54HUB/KAT
C_p° =	113.39	113.39	0.00	53SCO/FIN
S° =	184.93	184.93	0.00	53SCO/FIN
Δ_fS° =		−256.06		
Δ_fG° =		101.44		
$\ln K_f$ =		−40.92		

Thiacyclopentane C_4H_8S

(2 × C–(H)₂(C)₂) + (2 × C–(H)₂(C)(S)) + (1 × S–(C)₂) + (1 × Thiacyclopentane rsc), $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−34.20	−34.20	0.00	52HUB/FIN
C_p° =	90.88	90.88	0.00	69STU/WES
S° =	309.36	309.36	0.00	69STU/WES
Δ_fS° =		−267.94		
Δ_fG° =		45.69		
$\ln K_f$ =		−18.43		

TABLE 49. Cyclic CHS (13) – Continued

Thiacyclopentane (Continued) C_4H_8S

(2 × C–(H)₂(C)₂) + (2 × C–(H)₂(C)(S)) + (1 × S–(C)₂) + (1 × Thiacyclopentane rsc), $\sigma = 2$

	Literature	Calculated	Residual	Reference
Liquid phase				
Δ_fH° =	−73.10	−73.10	0.00	54HUB/KAT
C_p° =	140.16	140.16	0.00	52HUB/FIN
S° =	207.82	207.82	0.00	52HUB/FIN
Δ_fS° =		−369.48		
Δ_fG° =		37.06		
$\ln K_f$ =		−14.95		

Thiacyclohexane C_5H_{10}

(3 × C–(H)₂(C)₂) + (2 × C–(H)₂(C)(S)) + (1 × S–(C)₂) + (1 × Thiacyclohexane rsc), $\sigma = 1$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−63.26	−63.26	0.00	54MCC/FIN
C_p° =	108.20	108.20	0.00	69STU/WES
S° =	323.26	323.26	0.00	69STU/WES
Δ_fS° =		−390.35		
Δ_fG° =		53.12		
$\ln K_f$ =		−21.43		
Liquid phase				
Δ_fH° =	−106.00	−106.00	0.00	54MCC/FIN
C_p° =	163.30	163.30	0.00	54MCC/FIN
S° =	218.24	218.24	0.00	54MCC/FIN
Δ_fS° =		−495.37		
Δ_fG° =		41.69		
$\ln K_f$ =		−16.82		

Thiacycloheptane $C_6H_{12}S$

(4 × C–(H)₂(C)₂) + (2 × C–(H)₂(C)(S)) + (1 × S–(C)₂) + (1 × Thiacycloheptane rsc), $\sigma = 1$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−61.34	−61.34	0.00	69STU/WES
C_p° =	124.60	124.60	0.00	69STU/WES
S° =	361.92	361.92	0.00	69STU/WES
Δ_fS° =		−488.00		
Δ_fG° =		84.16		
$\ln K_f$ =		−33.95		
Liquid phase				
Δ_fH° =	−112.80	−112.80	0.00	69STU/WES

TABLE 49. Cyclic CHS (13) – Continued

Thiophene C_4H_4S

$(4\times C_B-(H)(C_B)_2)+(1\times S-(C_B)_2)+(1\times \text{Thiophene rsc}), \sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	114.30	114.30	0.00	49WAD/KNO
$C_p°$ =	72.89	72.89	0.00	69STU/WES
$S°$ =	278.86	278.86	0.00	69STU/WES
$\Delta_fS°$ =		−37.30		
$\Delta_fG°$ =		125.42		
$\ln K_f$ =		−50.59		

2-Methylthiophene C_5H_6S

$(3\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_3(C))+(1\times S-(C_B)_2)+(1\times \text{Thiophene rsc}), \sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	83.68	81.87	1.81	69STU/WES
$C_p°$ =	95.40	94.76	0.64	69STU/WES
$S°$ =	320.58	318.89	1.69	69STU/WES
$\Delta_fS°$ =		−133.58		
$\Delta_fG°$ =		121.70		
$\ln K_f$ =		−49.09		

3-Methylthiophene C_5H_6S

$(3\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_3(C))+(1\times S-(C_B)_2)+(1\times \text{Thiophene rsc}), \sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	82.80	81.87	0.93	69STU/WES
$C_p°$ =	94.85	94.76	0.09	69STU/WES
$S°$ =	321.29	318.89	2.40	69STU/WES
$\Delta_fS°$ =		−133.58		
$\Delta_fG°$ =		121.70		
$\ln K_f$ =		−49.09		

2-Methyl thiolane $C_5H_{10}S$

$(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(S))+(1\times C-(H)(C)_2(S))+(1\times C-(H)_3(C))+(1\times S-(C)_2)+(1\times \text{Thiacyclopentane rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−64.20	−59.17	−5.03	72GOO2
$C_p°$ =		116.00		

TABLE 49. Cyclic CHS (13) – Continued

2-Methyl thiolane (Continued) $C_5H_{10}S$

$(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(C)(S))+(1\times C-(H)(C)_2(S))+(1\times C-(H)_3(C))+(1\times S-(C)_2)+(1\times \text{Thiacyclopentane rsc})$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−105.40	−100.01	−5.39	72GOO2
$C_p°$ =	171.80	170.24	1.56	74MES/FIN
$S°$ =	245.31	233.42	11.89	74MES/FIN
$\Delta_fS°$ =		−480.19		
$\Delta_fG°$ =		43.16		
$\ln K_f$ =		−17.41		

3-Methyl thiolane $C_5H_{10}S$

$(1\times C-(H)_2(C)_2)+(1\times C-(H)_3(C))+(1\times C-(H)(C)_3)+(2\times C-(H)_2(C)(S))+(1\times S-(C)_2)+(1\times \text{Thiacyclopentane rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−60.50	−57.00	−3.50	72GOO2
$C_p°$ =		113.80		
Liquid phase				
$\Delta_fH°$ =	−102.70	−99.75	−2.95	72GOO2
$C_p°$ =	171.80	167.60	4.20	74MES/FIN
$S°$ =	241.00	234.85	6.15	74MES/FIN
$\Delta_fS°$ =		−478.76		
$\Delta_fG°$ =		42.99		
$\ln K_f$ =		−17.34		

Cyclopentyl methyl sulfide $C_6H_{12}S$

$(1\times C-(H)_3(S))+(1\times S-(C)_2)+(4\times C-(H)_2(C)_2)+(1\times C-(H)(C)_2(S))+(1\times \text{Cyclopentane (sub) rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−64.70	−64.12	−0.58	72GOO2
$C_p°$ =		132.35		
Liquid phase				
$\Delta_fH°$ =	−109.80	−103.19	−6.61	72GOO2
$C_p°$ =	192.92	197.77	−4.85	74MES/TOD
$S°$ =	285.47	282.66	2.81	74MES/TOD
$\Delta_fS°$ =		−567.26		
$\Delta_fG°$ =		65.94		
$\ln K_f$ =		−26.60		

TABLE 49. Cyclic CHS (13) — Continued

2,3-Dihydrothiophene C_4H_6S
(1 × S–(C)(C_d)) + (1 × C_d–(H)(S)) + (1 × C_d–(H)(C)) + (1 × C–$(H)_2$(C)(C_d)) + (1 × C–$(H)_2$(C)(S)) + (1 × 2,3-Dihydrothiophene rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	90.70	90.70	0.00	62DAV/SUN

2,5-Dihydrothiophene C_4H_6S
(1 × S–$(C)_2$) + (2 × C–$(H)_2$(C_d)(S)) + (2 × C_d–(H)(C)) + (1 × 2,5-Dihydrothiophene rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	86.90	86.90	0.00	62DAV/SUN
Liquid phase				
$\Delta_f H°$ =	47.00	47.00	0.00	62DAV/SUN

TABLE 50. Fluorides (46)

Fluoromethane; Methyl fluoride CH_3F
(1 × C–$(H)_3$(F), methyl fluoride), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−247.00	−247.00	0.00	85LIA/KAR
$C_p°$ =	37.49	37.49	0.00	69STU/WES
$S°$ =	222.80	222.80	0.00	69STU/WES
$\Delta_f S°$ =		−80.14		
$\Delta_f G°$ =		−223.11		
$\ln K_f$ =		90.00		

Fluoroethane C_2H_5F
(1 × C–$(H)_3$(C)) + (1 × C–$(H)_2$(C)(F)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−261.50	−263.38	1.88	69STU/WES
$C_p°$ =	59.04	59.39	−0.35	69STU/WES
$S°$ =	264.93	264.99	−0.06	69STU/WES
$\Delta_f S°$ =		−174.26		
$\Delta_f G°$ =		−211.42		
$\ln K_f$ =		85.29		

1-Fluoropropane C_3H_7F
(1 × C–$(H)_3$(C)) + (1 × C–$(H)_2$$(C)_2$) + (1 × C–$(H)_2$(C)(F)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−285.90	−284.01	−1.89	56LAC/KIA2
$C_p°$ =	82.63	82.28	0.35	69STU/WES
$S°$ =	304.22	304.15	0.07	69STU/WES
$\Delta_f S°$ =		−271.41		
$\Delta_f G°$ =		−203.09		
$\ln K_f$ =		81.92		

2-Fluoropropane C_3H_7F
(2 × C–$(H)_3$(C)) + (1 × C–(H)$(C)_2$(F)) + (2 × –CH_3 corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−293.50	−293.50	0.00	56LAC/KIA2
$C_p°$ =	82.01	82.01	0.00	69STU/WES

TABLE 50. Fluorides (46) — Continued

1,1-Difluoroethane $C_2H_4F_2$
(1×C–(H)$_3$(C))+(1×C–(H)(C)(F)$_2$), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−497.00	−497.00	0.00	68KOL/SHT
$C_p°$ =	67.95	67.95	0.00	69STU/WES
$S°$ =	282.51	282.51	0.00	69STU/WES
$\Delta_f S°$ =		−192.80		
$\Delta_f G°$ =		−439.52		
$\ln K_f$ =		177.30		

1,1,1-Trifluoroethane $C_2H_3F_3$
(1×C–(H)$_3$(C))+(1×C–(C)(F)$_3$), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−744.60	−716.07	−28.53	65KOL/MAR
$C_p°$ =	78.45	78.72	−0.27	69STU/WES
$S°$ =	287.27	287.27	0.00	69STU/WES
$\Delta_f S°$ =		−224.09		
$\Delta_f G°$ =		−649.26		
$\ln K_f$ =		261.91		

1,1,2-Trifluoroethane $C_2H_3F_3$
(1×C–(H)(C)(F)$_2$)+(1×C–(H)$_2$(C)(F)), σ = 1

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−730.70	−675.86	−54.84	56LAC/KIA
$C_p°$ =		75.88		
$S°$ =		311.12		
$\Delta_f S°$ =		−200.24		
$\Delta_f G°$ =		−616.16		
$\ln K_f$ =		248.55		

Hexafluoroethane C_2F_6
(2×C–(C)(F)$_3$), σ = 18

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−1343.10	−1347.62	4.52	66SIN
$C_p°$ =	106.40	105.98	0.42	69STU/WES
$S°$ =	322.08	332.41	−10.33	69STU/WES
$\Delta_f S°$ =		−287.12		
$\Delta_f G°$ =		−1262.02		
$\ln K_f$ =		509.09		

Hexadecafluoroheptane C_7F_{16}
(2×C–(C)(F)$_3$)+(5×C–(C)$_2$(F)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−3383.60	−3404.57	20.97	51OLI/GRI
$C_p°$ =		313.08		
Liquid phase				
$\Delta_f H°$ =	−3420.00	−3419.99	−0.01	59GOO/DOU

Tetrafluoroethylene C_2F_4
(2×C_d–(F)$_2$), σ = 4

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−659.80	−659.80	0.00	56SCO/GOO
$C_p°$ =	80.50	78.86	1.64	69STU/WES
$S°$ =	299.95	299.73	0.22	69STU/WES
$\Delta_f S°$ =		−117.11		
$\Delta_f G°$ =		−624.88		
$\ln K_f$ =		252.07		

Fluoroethylene C_2H_3F
(1×C_d–(H)(F))+(1×C_d–(H)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−138.80	−138.80	0.00	70KOL/PAP
$C_p°$ =		49.83		

1,1-Difluoroethylene $C_2H_2F_2$
(1×C_d–(H)$_2$)+(1×C_d–(F)$_2$), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−334.00	−303.58	−30.42	56NEU/MAR
$C_p°$ =	59.16	60.81	−1.65	69STU/WES
$S°$ =	265.18	265.39	−0.21	69STU/WES
$\Delta_f S°$ =		−79.35		
$\Delta_f G°$ =		−279.92		
$\ln K_f$ =		112.92		

TABLE 50. Fluorides (46) — Continued

Trifluoroethylene C_2HF_3

$(1\times C_d\text{–}(H)(F)) + (1\times C_d\text{–}(F)_2)$, $\sigma = 1$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−490.40	−495.02	4.62	62KOL/MAR
C_p° =	69.20	67.88	1.32	69STU/WES
S° =	292.62	292.87	−0.25	69STU/WES
Δ_fS° =		−87.92		
Δ_fG° =		−468.81		
$\ln K_f$ =		189.11		

3,3,3-Trifluoropropene $C_3H_3F_3$

$(1\times C_d\text{–}(H)_2) + (1\times C_d\text{–}(H)(C)) + (1\times C\text{–}(C)(F)_3)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−614.20	−611.17	−3.03	67KOL/MAR
C_p° =		93.11		

Hexafluorobenzene C_6F_6

$(6\times C_B\text{–}(F)(C_B)_2) + (6\times ortho$ corr-(F)(F)), $\sigma = 12$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−955.60	−962.16	6.56	65COU/GRE
C_p° =	156.61	156.60	0.01	69STU/WES
S° =	383.21	384.46	−1.25	69STU/WES
Δ_fS° =		−258.03		
Δ_fG° =		−885.23		
$\ln K_f$ =		357.10		
Liquid phase				
Δ_fH° =	−991.30	−997.20	5.90	69COX/GUN
C_p° =	221.58	222.54	−0.96	65COU/GRE
S° =	280.79	325.14	−44.35	65COU/GRE
Δ_fS° =		−317.35		
Δ_fG° =		−902.58		
$\ln K_f$ =		364.10		

Pentafluoro(trifluoromethyl)benzene C_7F_8

$(5\times C_B\text{–}(F)(C_B)_2) + (1\times C_B\text{–}(C)(C_B)_2) + (1\times C\text{–}(C_B)(F)_3) +$
$(2\times ortho$ corr-(F)(CF3)) + $(4\times ortho$ corr-(F)(F))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−1268.60	−1268.85	0.25	73KRE/PRI
C_p° =		192.55		
Liquid phase				
Δ_fH° =	−1310.20	−1309.50	−0.70	73KRE/PRI

TABLE 50. Fluorides (46) — Continued

Decafluorobiphenyl $C_{12}F_{10}$

$(10\times C_B\text{–}(F)(C_B)_2) + (2\times C_B\text{–}(C_B)_3) + (8\times ortho$ corr-(F)(F)) +
$(2\times ortho$ corr-(F)(F′))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−1263.20	−1586.08	322.88	79PRI/SAP2
C_p° =		287.24		
Liquid phase				
Δ_fH° =		−1661.58		
C_p° =		405.04		
Solid phase				
Δ_fH° =	−1348.10	−1685.94	337.84	79PRI/SAP2
C_p° =		317.06		
S° =		385.90		
Δ_fS° =		−696.39		
Δ_fG° =		−1478.31		
$\ln K_f$ =		596.34		

Fluorobenzene C_6H_5F

$(1\times C_B\text{–}(F)(C_B)_2) + (5\times C_B\text{–}(H)(C_B)_2)$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−116.00	−112.21	−3.79	56SCO/MCC
C_p° =	94.43	94.15	0.28	69STU/WES
S° =	302.63	303.31	−0.68	69STU/WES
Δ_fS° =		−158.90		
Δ_fG° =		−64.83		
$\ln K_f$ =		26.15		
Liquid phase				
Δ_fH° =	−150.60	−150.40	−0.20	56SCO/GOO
C_p° =	146.36	150.49	−4.13	56SCO/MCC
S° =	205.94	198.54	7.40	56SCO/MCC
Δ_fS° =		−263.67		
Δ_fG° =		−71.79		
$\ln K_f$ =		28.96		

1-Fluoro-4-methylbenzene; p-Fluorotoluene C_7H_7F

$(1\times C_B\text{–}(F)(C_B)_2) + (4\times C_B\text{–}(H)(C_B)_2) + (1\times C_B\text{–}(C)(C_B)_2) +$
$(1\times C\text{–}(H)_3(C))$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−147.50	−144.64	−2.86	62SCO/MES
C_p° =	116.15	116.02	0.13	69STU/WES
S° =	339.53	337.57	1.96	69STU/WES
Δ_fS° =		−260.95		
Δ_fG° =		−66.84		
$\ln K_f$ =		26.96		

TABLE 50. Fluorides (46) — Continued

1-Fluoro-4-methylbenzene; p-Fluorotoluene (Continued) C_7H_7F

$(1\times C_B-(F)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_3(C))$, $\sigma = 6$

	Literature	Calculated	Residual	Reference
Liquid phase				
Δ_fH° =	−186.90	−187.01	0.11	62GOO/LAC
C_p° =		174.39		
S° =		233.47		
Δ_fS° =		−365.05		
Δ_fG° =		−78.17		
$\ln K_f$ =		31.53		

1,2-Difluorobenzene $C_6H_4F_2$

$(4\times C_B-(H)(C_B)_2)+(2\times C_B-(F)(C_B)_2)+(1\times$ *ortho* corr-(F)(F)), $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−293.80	−286.38	−7.42	63SCO/MES
C_p° =	106.52	106.64	−0.12	69STU/WES
S° =	320.03	322.52	−2.49	69STU/WES
Δ_fS° =		−175.75		
Δ_fG° =		−233.98		
$\ln K_f$ =		94.39		
Liquid phase				
Δ_fH° =	−330.16	−324.76	−5.40	62GOO/LAC
C_p° =	159.03	164.90	−5.87	63SCO/MES
S° =	222.59	223.86	−1.27	63SCO/MES
Δ_fS° =		−274.40		
Δ_fG° =		−242.95		
$\ln K_f$ =		98.00		

1,3-Difluorobenzene $C_6H_4F_2$

$(4\times C_B-(H)(C_B)_2)+(2\times C_B-(F)(C_B)_2)+(1\times$ *meta* corr-(F)(F)), $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−309.20	−307.28	−1.92	62GOO/LAC
C_p° =	106.27	106.64	−0.37	69STU/WES
S° =	320.37	322.52	−2.15	69STU/WES
Δ_fS° =		−175.75		
Δ_fG° =		−254.88		
$\ln K_f$ =		102.82		
Liquid phase				
Δ_fH° =	−344.13	−343.76	−0.37	62GOO/LAC
C_p° =	159.12	164.90	−5.78	70MES/FIN
S° =	223.84	223.86	−0.02	70MES/FIN
Δ_fS° =		−274.40		
Δ_fG° =		−261.95		
$\ln K_f$ =		105.67		

TABLE 50. Fluorides (46) — Continued

1,4-Difluorobenzene $C_6H_4F_2$

$(4\times C_B-(H)(C_B)_2)+(2\times C_B-(F)(C_B)_2)$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−306.70	−307.28	0.58	62GOO/LAC
C_p° =	106.90	106.64	0.26	69STU/WES
S° =	315.60	322.52	−6.92	69STU/WES
Δ_fS° =		−175.75		
Δ_fG° =		−254.88		
$\ln K_f$ =		102.82		
Liquid phase				
Δ_fH° =	−342.42	−349.76	7.34	62GOO/LAC
C_p° =	160.70	164.90	−4.20	50UEB/ORT
S° =		223.86		
Δ_fS° =		−274.40		
Δ_fG° =		−267.95		
$\ln K_f$ =		108.09		

2,2′-Difluorobiphenyl $C_{12}H_8F_2$

$(8\times C_B-(H)(C_B)_2)+(2\times C_B-(F)(C_B)_2)+(2\times C_B-(C_B)_3)+(1\times$ *ortho* corr-(F)(F′))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−200.80	−200.72	−0.08	64SMI/GOR
C_p° =		187.32		
Liquid phase				
Δ_fH° =		−274.70		
C_p° =		289.76		
Solid phase				
Δ_fH° =	−295.80	−293.70	−2.10	64SMI/GOR
C_p° =		221.70		
S° =		249.58		
Δ_fS° =		−544.27		
Δ_fG° =		−131.43		
$\ln K_f$ =		53.02		

4,4′-Difluorobiphenyl $C_{12}H_8F_2$

$(8\times C_B-(H)(C_B)_2)+(2\times C_B-(F)(C_B)_2)+(2\times C_B-(C_B)_3)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−205.30	−208.72	3.42	64SMI/GOR
C_p° =		187.32		
Liquid phase				
Δ_fH° =		−282.70		
C_p° =		289.76		

TABLE 50. Fluorides (46) — Continued

4,4′-Difluorobiphenyl (Continued) $C_{12}H_8F_2$
$(8\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(F)(C_B)_2)+(2\times C_B\text{–}(C_B)_3)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_f H°$ =	−296.50	−301.70	5.20	64SMI/GOR
$C_p°$ =		221.70		
$S°$ =		249.58		
$\Delta_f S°$ =		−544.27		
$\Delta_f G°$ =		−139.43		
$\ln K_f$ =		56.24		

(Trifluoromethyl)benzene $C_7H_5F_3$
$(5\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(C)(C_B)_2)+(1\times C\text{–}(C_B)(F)_3)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−599.10	−599.10	0.00	59SCO/DOU
$C_p°$ =		130.10		
Liquid phase				
$\Delta_f H°$ =	−636.70	−636.70	0.00	64GOO/LAC

1,2,4,5-Tetrafluorobenzene $C_6H_2F_4$
$(2\times C_B\text{–}(H)(C_B)_2)+(4\times C_B\text{–}(F)(C_B)_2)+(2\times$ *ortho* corr-(F)(F)$)+$
$(2\times$ *meta* corr-(F)(F)$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−655.62		
$C_p°$ =		131.62		
Liquid phase				
$\Delta_f H°$ =	−683.70	−686.48	2.78	78HAR/HEA
$C_p°$ =	192.21	193.72	−1.51	73AND/MAR
$S°$ =	250.41	274.50	−24.09	73AND/MAR
$\Delta_f S°$ =		−295.88		
$\Delta_f G°$ =		−598.26		
$\ln K_f$ =		241.34		

1,2,3,4-Tetrafluorobenzene $C_6H_2F_4$
$(2\times C_B\text{–}(H)(C_B)_2)+(4\times C_B\text{–}(F)(C_B)_2)+(3\times$ *ortho* corr-(F)(F)$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−634.72		
$C_p°$ =		131.62		

TABLE 50. Fluorides (46) — Continued

4,4′-Difluorobiphenyl (Continued) $C_{12}H_8F_2$
$(8\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(F)(C_B)_2)+(2\times C_B\text{–}(C_B)_3)$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H°$ =		−673.48		
$C_p°$ =	189.91	193.72	−3.81	73AND/MAR
$S°$ =	256.10	274.50	−18.40	73AND/MAR
$\Delta_f S°$ =		−295.88		
$\Delta_f G°$ =		−585.26		
$\ln K_f$ =		236.09		

1,2,3,5-Tetrafluorobenzene $C_6H_2F_4$
$(2\times C_B\text{–}(H)(C_B)_2)+(4\times C_B\text{–}(F)(C_B)_2)+(2\times$ *ortho* corr-(F)(F)$)+$
$(2\times$ *meta* corr-(F)(F)$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−655.62		
$C_p°$ =		131.62		
Liquid phase				
$\Delta_f H°$ =		−686.48		
$C_p°$ =	190.29	193.72	−3.43	73AND/MAR
$S°$ =	257.32	274.50	−17.18	73AND/MAR
$\Delta_f S°$ =		−295.88		
$\Delta_f G°$ =		−598.26		
$\ln K_f$ =		241.34		

1-Fluoro-3-(trifluoromethyl)benzene $C_7H_4F_4$
$(4\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(F)(C_B)_2)+(1\times C_B\text{–}(C)(C_B)_2)+$
$(1\times C\text{–}(C_B)(F)_3)+(1\times$ *meta* corr-(F)(CF3)$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−792.20	−792.17	−0.03	59GOO/DOU
$C_p°$ =		142.59		
Liquid phase				
$\Delta_f H°$ =	−830.20	−830.06	−0.14	59GOO/DOU

Pentafluorobenzene C_6HF_5
$(1\times C_B\text{–}(H)(C_B)_2)+(5\times C_B\text{–}(F)(C_B)_2)+(4\times$ *ortho* corr-(F)(F)$)+$
$(1\times$ *meta* corr-(F)(F)$)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−807.50	−808.89	1.39	68COU/HAL
$C_p°$ =		144.11		

TABLE 50. Fluorides (46) — Continued

Pentafluorobenzene (Continued) C_6HF_5
(1 × C_B–(H)(C_B)$_2$) + (5 × C_B–(F)(C_B)$_2$) + (4 × *ortho* corr-(F)(F)) + (1 × *meta* corr-(F)(F))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−841.80	−841.84	0.04	69COX/GUN
$C_p°$ =	204.68	208.13	−3.45	68COU/HAL
$S°$ =	275.89	299.82	−23.93	68COU/HAL
$\Delta_fS°$ =		−306.61		
$\Delta_fG°$ =		−750.42		
$\ln K_f$ =		302.72		

2,3,4,5,6-Pentafluorotoluene $C_7H_3F_5$
(1 × C–(H)$_3$(C)) + (1 × C_B–(C)(C_B)$_2$) + (5 × C_B–(F)(C_B)$_2$) + (4 × *ortho* corr-(F)(F)) + (2 × *ortho* corr-(alk)(X))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−842.90	−836.30	−6.60	69COX/GUN
$C_p°$ =		165.98		
Liquid phase				
$\Delta_fH°$ =	−883.80	−871.85	−11.95	69COX/GUN
$C_p°$ =		232.03		
$S°$ =		334.75		
$\Delta_fS°$ =		−407.99		
$\Delta_fG°$ =		−750.21		
$\ln K_f$ =		302.63		

Dodecafluorocyclohexane C_6F_{12}
(6 × C–(C)$_2$(F)$_2$) + (1 × Cyclohexane (sub) rsc)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−2370.40	−2468.73	98.33	79PRI/SAP
$C_p°$ =		225.70		
Liquid phase				
$\Delta_fH°$ =	−2406.30	−2404.28	−2.02	79PRI/SAP
Solid phase				
$\Delta_fH°$ =		−2562.32		

TABLE 50. Fluorides (46) — Continued

Acetyl fluoride C_2H_3FO
(1 × C–(H)$_3$(CO)) + (1 × CO–(C)(F))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−422.10	−422.10	0.00	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−467.20	−467.20	0.00	49CAR/SKI

2,2,2-Trifluoroethanol $C_2H_3F_3O$
(1 × C–(C)(F)$_3$) + (1 × C–(H)$_2$(O)(C)) + (1 × O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−888.40	−866.04	−22.36	73ROC/SYM
$C_p°$ =		91.48		
Liquid phase				
$\Delta_fH°$ =	−932.40	−936.37	3.97	71KOL/IVA
$C_p°$ =		151.46		
$S°$ =		212.04		
$\Delta_fS°$ =		−401.84		
$\Delta_fG°$ =		−816.56		
$\ln K_f$ =		329.40		

3,3,3-Trifluoro-1-propanol $C_3H_5F_3O$
(1 × O–(H)(C)) + (1 × C–(H)$_2$(O)(C)) + (1 × C–(H)$_2$(C)$_2$) + (1 × C–(C)(F)$_3$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−886.67		
$C_p°$ =		114.37		
Liquid phase				
$\Delta_fH°$ =	−969.60	−962.10	−7.50	69KOL/IVA
$C_p°$ =		181.88		
$S°$ =		244.42		
$\Delta_fS°$ =		−505.77		
$\Delta_fG°$ =		−811.30		
$\ln K_f$ =		327.27		

TABLE 50. Fluorides (46) — Continued

2,2,3,3-Tetrafluoro-1-propanol $C_3H_4F_4$

(1×C–(H)(C)(F)₂)+(1×C–(C)₂(F)₂)+(1×C–(H)₂(O)(C))+(1×O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−1061.30	−1058.36	−2.94	73ROC/SYM
$C_p°$ =		122.13		
Liquid phase				
$\Delta_fH°$ =	−1114.90	−1114.90	0.00	69KOL/IVA

2,2,3,3,3-Pentafluoro-1-propanol $C_3H_3F_5O$

(1×O–(H)(C))+(1×C–(H)₂(O)(C))+(1×C–(C)₂(F)₂)+(1×C–(C)(F)₃)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−1310.30	−1277.43	−32.87	73ROC/SYM
$C_p°$ =		132.90		
Liquid phase				
$\Delta_fH°$ =	−1354.70	−1336.74	−17.96	69KOL/IVA

Pentafluorophenol C_6HF_5O

(1×O–(H)(C_B))+(1×C_B–(O)(C_B)₂)+(5×C_B–(F)(C_B)₂)+(4×*ortho* corr-(F)(F))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−956.80	−987.75	30.95	69COX/GUN
$C_p°$ =		164.52		
Liquid phase				
$\Delta_fH°$ =	−1007.70	−1053.36	45.66	68AND/COU
$C_p°$ =		269.80		
$S°$ =		304.25		
$\Delta_fS°$ =		−404.70		
$\Delta_fG°$ =		−932.70		
$\ln K_f$ =		376.24		
Solid phase				
$\Delta_fH°$ =	−1024.10	−1066.25	42.15	69COX/GUN
$C_p°$ =		189.21		
$S°$ =		229.16		
$\Delta_fS°$ =		−479.79		
$\Delta_fG°$ =		−923.20		
$\ln K_f$ =		372.41		

TABLE 50. Fluorides (46) — Continued

2,2,3,3,4,4,4-Heptafluoro-1-butanol $C_4H_3F_7O$

(1×O–(H)(C))+(1×C–(H)₂(O)(C))+(2×C–(C)₂(F)₂)+(1×C–(C)(F)₃)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−1688.82		
$C_p°$ =		174.32		
Liquid phase				
$\Delta_fH°$ =	−1781.90	−1737.11	−44.79	71KOL/IVA2

2,2,3,3,4,4,5,5-Octafluoro-1,6-hexanediol $C_6H_6F_8O_2$

(2×O–(H)(C))+(2×C–(H)₂(O)(C))+(4×C–(C)₂(F)₂)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−2084.20	−2030.02	−54.18	74KOL/SLA
$C_p°$ =		242.66		
Liquid phase				
$\Delta_fH°$ =		−2056.08		
Solid phase				
$\Delta_fH°$ =	−2173.40	−2180.40	7.00	74KOL/SLA

Pentafluorobenzoic acid $C_7HF_5O_2$

(1×O–(H)(CO))+(1×CO–(O)(C_B))+(5×C_B–(F)(C_B)₂)+(4×*ortho* corr-(F)(F))+(1×C_B–(CO)(C_B)₂)+(2×*ortho* corr-(F)(COOH))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−1147.90	−1146.50	−1.40	69COX/GUN
Liquid phase				
$\Delta_fH°$ =		−1271.14		
$C_p°$ =		275.82		
Solid phase				
$\Delta_fH°$ =	−1239.60	−1247.00	7.40	69COX/GUN
$C_p°$ =		205.71		
$S°$ =		252.94		
$\Delta_fS°$ =		−564.27		
$\Delta_fG°$ =		−1078.76		
$\ln K_f$ =		435.17		

TABLE 50. Fluorides (46) — Continued

2-Fluorobenzoic acid $C_7H_5FO_2$

(1 × C_B–(F)(C_B)$_2$) + (4 × C_B–(H)(C_B)$_2$) + (1 × O–(H)(CO)) + (1 × CO–(O)(C_B)) + (1 × C_B–(CO)(C_B)$_2$) + (1 × *ortho* corr-(F)(COOH))

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−469.82		
Liquid phase				
$\Delta_f H°$ =		−573.70		
$C_p°$ =		218.18		
Solid phase				
$\Delta_f H°$ =	−567.60	−566.88	−0.72	56SCO/GOO
$C_p°$ =		158.03		
$S°$ =		184.78		
$\Delta_f S°$ =		−488.21		
$\Delta_f G°$ =		−421.32		
$\ln K_f$ =		169.96		

3-Fluorobenzoic acid $C_7H_5FO_2$

(4 × C_B–(H)(C_B)$_2$) + (1 × C_B–(F)(C_B)$_2$) + (1 × O–(H)(CO)) + (1 × CO–(O)(C_B)) + (1 × C_B–(CO)(C_B)$_2$)

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−489.82		
Liquid phase				
$\Delta_f H°$ =		−573.70		
$C_p°$ =		218.18		
Solid phase				
$\Delta_f H°$ =	−582.00	−586.88	4.88	56SCO/GOO
$C_p°$ =		158.03		
$S°$ =		184.78		
$\Delta_f S°$ =		−488.21		
$\Delta_f G°$ =		−441.32		
$\ln K_f$ =		178.03		

4-Fluorobenzoic acid $C_7H_5FO_2$

(4 × C_B–(H)(C_B)$_2$) + (1 × C_B–(F)(C_B)$_2$) + (1 × O–(H)(CO)) + (1 × CO–(O)(C_B)) + (1 × C_B–(CO)(C_B)$_2$)

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−494.50	−489.82	−4.68	69COX/GUN
Liquid phase				
$\Delta_f H°$ =		−573.70		
$C_p°$ =		218.18		

TABLE 50. Fluorides (46) — Continued

4-Fluorobenzoic acid (Continued) $C_7H_5FO_2$

(4 × C_B–(H)(C_B)$_2$) + (1 × C_B–(F)(C_B)$_2$) + (1 × O–(H)(CO)) + (1 × CO–(O)(C_B)) + (1 × C_B–(CO)(C_B)$_2$)

	Literature	− Calculated	= Residual	Reference
Solid phase				
$\Delta_f H°$ =	−568.60	−586.88	18.28	56SCO/GOO
$C_p°$ =		158.03		
$S°$ =		184.78		
$\Delta_f S°$ =		−488.21		
$\Delta_f G°$ =		−441.32		
$\ln K_f$ =		178.03		

Bis-(3,3,3-trifluoropropyl)ether $C_6H_8F_6O$

(2 × C–(C)(F)$_3$) + (2 × C–(H)$_2$(C)$_2$) + (2 × C–(H)$_2$(O)(C)) + (1 × O–(C)$_2$)

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−1604.30	−1556.10	−48.20	74SLA/KOL
$C_p°$ =		210.96		
Liquid phase				
$\Delta_f H°$ =	−1645.30	−1652.03	6.73	74SLA/KOL
$C_p°$ =		298.75		
$S°$ =		427.84		
$\Delta_f S°$ =		−839.45		
$\Delta_f G°$ =		−1401.75		
$\ln K_f$ =		565.46		

Octafluoropropane; Perfluoropropane C_3F_8

(2 × C–(C)(F)$_3$) + (1 × C–(C)$_2$(F)$_2$)

	Literature	− Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−1760.12	−1759.01	−1.11	67KOL/TAL
$C_p°$ =		147.40		

TABLE 51. Chlorides (116)

Chloromethane; Methyl chloride CH_3Cl
(1×C-(H)$_3$(Cl), methyl chloride), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−81.90	−81.90	0.00	71FLE/PIL
$C_p°$ =	40.75	40.75	0.00	69STU/WES
$S°$ =	234.37	234.47	−0.10	69STU/WES
$\Delta_f S°$ =		−78.62		
$\Delta_f G°$ =		−58.46		
$\ln K_f$ =		23.58		

Chloroethane C_2H_5Cl
(1×C-(H)$_3$(C))+(1×C-(H)$_2$(C)(Cl)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−112.26	−111.71	−0.55	71FLE/PIL
$C_p°$ =	62.72	63.26	−0.54	69STU/WES
$S°$ =	275.85	277.43	−1.58	69STU/WES
$\Delta_f S°$ =		−171.97		
$\Delta_f G°$ =		−60.44		
$\ln K_f$ =		24.38		
Liquid phase				
$\Delta_f H°$ =	−136.90	−134.51	−2.39	48GOR/GIA
$C_p°$ =	103.30	100.24	3.06	48GOR/GIA
$S°$ =	186.27	187.57	−1.30	48GOR/GIA
$\Delta_f S°$ =		−261.82		
$\Delta_f G°$ =		−56.45		
$\ln K_f$ =		22.77		

1-Chloropropane C_3H_7Cl
(1×C-(H)$_3$(C))+(1×C-(H)$_2$(C)$_2$)+(1×C-(H)$_2$(C)(Cl)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−132.51	−132.34	−0.17	71FLE/PIL
$C_p°$ =	84.68	86.15	−1.47	69STU/WES
$S°$ =	319.11	316.59	2.52	69STU/WES
$\Delta_f S°$ =		−269.12		
$\Delta_f G°$ =		−52.10		
$\ln K_f$ =		21.02		
Liquid phase				
$\Delta_f H°$ =	−160.40	−160.24	−0.16	77MAN/SEL
$C_p°$ =	131.38	130.66	0.72	1881REI
$S°$ =		219.95		
$\Delta_f S°$ =		−365.75		
$\Delta_f G°$ =		−51.19		
$\ln K_f$ =		20.65		

TABLE 51. Chlorides (116) – Continued

1-Chlorobutane C_4H_9Cl
(1×C-(H)$_3$(C))+(2×C-(H)$_2$(C)$_2$)+(1×C-(H)$_2$(C)(Cl)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−154.60	−152.97	−1.63	68WAD
$C_p°$ =	107.57	109.04	−1.47	69STU/WES
$S°$ =	358.07	355.75	2.32	69STU/WES
$\Delta_f S°$ =		−366.27		
$\Delta_f G°$ =		−43.77		
$\ln K_f$ =		17.66		
Liquid phase				
$\Delta_f H°$ =	−188.10	−185.97	−2.13	75STR/SUN
$C_p°$ =	159.64	161.08	−1.44	85LAI/WIL
$S°$ =		252.33		
$\Delta_f S°$ =		−469.69		
$\Delta_f G°$ =		−45.93		
$\ln K_f$ =		18.53		

1-Chloropentane $C_5H_{11}Cl$
(1×C-(H)$_3$(C))+(3×C-(H)$_2$(C)$_2$)+(1×C-(H)$_2$(C)(Cl)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−175.20	−173.60	−1.60	68WAD
$C_p°$ =	130.46	131.93	−1.47	69STU/WES
$S°$ =	397.02	394.91	2.11	69STU/WES
$\Delta_f S°$ =		−463.42		
$\Delta_f G°$ =		−35.43		
$\ln K_f$ =		14.29		
Liquid phase				
$\Delta_f H°$ =	−213.44	−211.70	−1.74	75STR/SUN
$C_p°$ =		191.50		
$S°$ =		284.71		
$\Delta_f S°$ =		−573.62		
$\Delta_f G°$ =		−40.68		
$\ln K_f$ =		16.41		

1-Chlorooctane $C_8H_{17}Cl$
(1×C-(H)$_3$(C))+(6×C-(H)$_2$(C)$_2$)+(1×C-(H)$_2$(C)(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−238.88	−235.49	−3.39	68WAD
$C_p°$ =		200.60		
Liquid phase				
$\Delta_f H°$ =	−291.30	−288.89	−2.41	75STR/SUN
$C_p°$ =		282.76		
$S°$ =		381.85		
$\Delta_f S°$ =		−885.41		
$\Delta_f G°$ =		−24.91		
$\ln K_f$ =		10.05		

TABLE 51. Chlorides (116) – Continued

1-Chlorododecane $C_{12}H_{25}Cl$
(1×C–(H)$_3$(C))+(10×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−321.98	−318.01	−3.97	75STR/SUN
$C_p°$ =		292.16		
Liquid phase				
$\Delta_f H°$ =	−392.31	−391.81	−0.50	75STR/SUN
$C_p°$ =		404.44		
$S°$ =		511.37		
$\Delta_f S°$ =		−1301.13		
$\Delta_f G°$ =		−3.88		
$\ln K_f$ =		1.56		

1-Chlorooctadecane $C_{18}H_{37}Cl$
(1×C–(H)$_3$(C))+(16×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−446.04	−441.79	−4.25	75STR/SUN
$C_p°$ =		429.50		
Liquid phase				
$\Delta_f H°$ =	−544.20	−546.19	1.99	75STR/SUN
$C_p°$ =		586.96		
$S°$ =		705.65		
$\Delta_f S°$ =		−1924.72		
$\Delta_f G°$ =		27.67		
$\ln K_f$ =		−11.16		

1-Chloro-3-methylbutane $C_5H_{11}Cl$
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+
(2×–CH$_3$ corr (tertiary))+(1×C–(H)$_2$(C)(Cl)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−180.33	−180.29	−0.04	69STU/WES
$C_p°$ =	133.89	131.96	1.93	69STU/WES
$S°$ =	399.82	381.17	18.65	69STU/WES
$\Delta_f S°$ =		−477.16		
$\Delta_f G°$ =		−38.03		
$\ln K_f$ =		15.34		
Liquid phase				
$\Delta_f H°$ =	−216.98	−216.98	0.00	69STU/WES
$C_p°$ =	179.50	188.52	−9.02	48KUR
$S°$ =		279.36		
$\Delta_f S°$ =		−578.97		
$\Delta_f G°$ =		−44.36		
$\ln K_f$ =		17.89		

TABLE 51. Chlorides (116) – Continued

1-Chloro-2-methylpropane C_4H_9Cl
(2×C–(H)$_3$(C))+(1×C–(H)(C)$_3$)+(2×–CH$_3$ corr (tertiary))+
(1×C–(H)$_2$(C)(Cl)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−159.40	−159.66	0.26	68WAD
$C_p°$ =	108.49	109.07	−0.58	69STU/WES
$S°$ =	353.80	342.01	11.79	69STU/WES
$\Delta_f S°$ =		−380.00		
$\Delta_f G°$ =		−46.36		
$\ln K_f$ =		18.70		
Liquid phase				
$\Delta_f H°$ =	−191.10	−191.25	0.15	53SMI/BJE
$C_p°$ =	158.57	158.10	0.47	48KUR
$S°$ =		246.98		
$\Delta_f S°$ =		−475.04		
$\Delta_f G°$ =		−49.62		
$\ln K_f$ =		20.02		

2-Chloropropane C_3H_7Cl
(2×C–(H)$_3$(C))+(1×C–(H)(C)$_2$(Cl))+
(2×–CH$_3$ corr (tertiary)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−144.90	−144.65	−0.25	71FLE/PIL
$C_p°$ =	87.32	86.46	0.86	69STU/WES
$S°$ =	304.18	307.71	−3.53	69STU/WES
$\Delta_f S°$ =		−277.99		
$\Delta_f G°$ =		−61.77		
$\ln K_f$ =		24.92		
Liquid phase				
$\Delta_f H°$ =	−172.10	−170.75	−1.35	31MAT/FEH
$C_p°$ =		138.98		

2-Chlorobutane C_4H_9Cl
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_2$(Cl)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−161.20	−160.76	−0.44	68WAD
$C_p°$ =	108.49	109.35	−0.86	69STU/WES
$S°$ =	350.41	346.87	3.54	69STU/WES
$\Delta_f S°$ =		−375.14		
$\Delta_f G°$ =		−48.91		
$\ln K_f$ =		19.73		
Liquid phase				
$\Delta_f H°$ =	−192.80	−192.12	−0.68	53SMI/BJE
$C_p°$ =		169.40		

TABLE 51. Chlorides (116) — Continued

2-Chlorohexane $C_6H_{13}Cl$

(2×C–(H)$_3$(C)) + (3×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_2$(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−203.30	−202.02	−1.28	68WAD
$C_p°$ =		155.13		
Liquid phase				
$\Delta_fH°$ =	−246.10	−243.58	−2.52	56KIR
$C_p°$ =		230.24		

2-Chloro-3-methylbutane $C_5H_{11}Cl$

(3×C–(H)$_3$(C)) + (1×C–(H)(C)$_3$) + (2×–CH$_3$ corr (tertiary)) + (1×C–(H)(C)$_2$(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−185.10	−188.08	2.98	68WAD
$C_p°$ =		132.27		
Liquid phase				
$\Delta_fH°$ =	−226.60	−223.13	−3.47	73ESI/KAB
$C_p°$ =		196.84		

2-Chloro-2-methylpropane C_4H_9Cl

(3×C–(H)$_3$(C)) + (3×–CH$_3$ corr (quaternary)) + (1×C–(C)$_3$(Cl)), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−182.40	−184.16	1.76	64LEV/AND
$C_p°$ =	114.22	106.82	7.40	69STU/WES
$S°$ =	322.17	321.16	1.01	69STU/WES
$\Delta_fS°$ =		−400.85		
$\Delta_fG°$ =		−64.65		
$\ln K_f$ =		26.08		
Liquid phase				
$\Delta_fH°$ =	−211.40	−212.78	1.38	68WAD

TABLE 51. Chlorides (116) — Continued

2-Chloro-2-methylbutane $C_5H_{11}Cl$

(3×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (2×–CH$_3$ corr (quaternary)) + (1×C–(C)$_3$(Cl)), σ = 27

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−202.20	−200.23	−1.97	31MAT/FEH
$C_p°$ =	131.59	129.71	1.88	69STU/WES
$S°$ =	368.44	369.46	−1.02	69STU/WES
$\Delta_fS°$ =		−488.87		
$\Delta_fG°$ =		−54.47		
$\ln K_f$ =		21.97		
Liquid phase				
$\Delta_fH°$ =	−235.70	−234.12	−1.58	53SMI/BJE

1,2-Dichloroethane $C_2H_4Cl_2$

(2×C–(H)$_2$(C)(Cl)), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−129.10	−138.90	9.80	58SIN/STU
$C_p°$ =	78.66	75.06	3.60	69STU/WES
$S°$ =	308.19	312.72	−4.53	69STU/WES
$\Delta_fS°$ =		−182.88		
$\Delta_fG°$ =		−84.38		
$\ln K_f$ =		34.04		
Liquid phase				
$\Delta_fH°$ =	−164.50	−173.80	9.30	58SIN/STU
$C_p°$ =	128.87	127.52	1.35	40PIT
$S°$ =	208.53	208.54	−0.01	40PIT
$\Delta_fS°$ =		−287.05		
$\Delta_fG°$ =		−88.21		
$\ln K_f$ =		35.59		

1,2-Dichloropropane $C_3H_6Cl_2$

(1×C–(H)$_2$(C)(Cl)) + (1×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(Cl)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−162.80	−167.32	4.52	49DRE/MAR
$C_p°$ =	98.20	98.26	−0.06	69STU/WES
$S°$ =	351.46	348.77	2.69	69STU/WES
$\Delta_fS°$ =		−283.14		
$\Delta_fG°$ =		−82.90		
$\ln K_f$ =		33.44		
Liquid phase				
$\Delta_fH°$ =	−198.80	−205.68	6.88	49DRE/MAR
$C_p°$ =		166.26		

TABLE 51. Chlorides (116) — Continued

1,3-Dichloropropane $C_3H_6Cl_2$

$(1\times C\text{-}(H)_2(C)_2)+(2\times C\text{-}(H)_2(C)(Cl))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−159.20	−159.53	0.33	68WAD
$C_p°$ =	99.62	97.95	1.67	69STU/WES
$S°$ =	351.08	351.88	−0.80	69STU/WES
$\Delta_fS°$ =		−280.03		
$\Delta_fG°$ =		−76.04		
$\ln K_f$ =		30.67		
Liquid phase				
$\Delta_fH°$ =	−200.00	−199.53	−0.47	53SMI/BJE
$C_p°$ =		157.94		
$S°$ =		240.92		
$\Delta_fS°$ =		−390.98		
$\Delta_fG°$ =		−82.96		
$\ln K_f$ =		33.46		

1,1-Dichloroethane $C_2H_4Cl_2$

$(1\times C\text{-}(H)_3(C))+(1\times C\text{-}(H)(C)(Cl)_2)$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−127.60	−121.36	−6.24	67LAC/AMA
$C_p°$ =	76.23	76.42	−0.19	69STU/WES
$S°$ =	304.97	301.47	3.50	69STU/WES
$\Delta_fS°$ =		−194.13		
$\Delta_fG°$ =		−63.48		
$\ln K_f$ =		25.61		
Liquid phase				
$\Delta_fH°$ =	−158.40	−150.21	−8.19	56LI/PIT
$C_p°$ =	126.27	121.50	4.77	56LI/PIT
$S°$ =	211.75	211.75	0.00	56LI/PIT
$\Delta_fS°$ =		−283.84		
$\Delta_fG°$ =		−65.58		
$\ln K_f$ =		26.46		

2,2-Dichloropropane $C_3H_6Cl_2$

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(C)_2(Cl)_2)+$
$(2\times \text{-}CH_3$ corr (quaternary)), $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−173.20		
$C_p°$ =	105.86	105.86	0.00	69STU/WES
$S°$ =	326.02	326.02	0.00	69STU/WES
$\Delta_fS°$ =		−305.89		
$\Delta_fG°$ =		−82.00		
$\ln K_f$ =		33.08		

TABLE 51. Chlorides (116) — Continued

2,2-Dichloropropane (Continued) $C_3H_6Cl_2$

$(2\times C\text{-}(H)_3(C))+(1\times C\text{-}(C)_2(Cl)_2)+$
$(2\times \text{-}CH_3$ corr (quaternary)), $\sigma = 18$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−205.80	−205.80	0.00	53SMI/BJE
$C_p°$ =		147.20		

1,1,1-Trichloroethane $C_2H_3Cl_3$

$(1\times C\text{-}(H)_3(C))+(1\times C\text{-}(C)(Cl)_3)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−145.00	−124.24	−20.76	71MAN/RIN
$C_p°$ =		93.91		
Liquid phase				
$\Delta_fH°$ =	−174.50	−160.54	−13.96	71MAN/RIN
$C_p°$ =	144.39	138.68	5.71	73AND/COU
$S°$ =	226.69	229.21	−2.52	73AND/COU
$\Delta_fS°$ =		−312.58		
$\Delta_fG°$ =		−67.34		
$\ln K_f$ =		27.17		

1,1,2-Trichloroethane $C_2H_3Cl_3$

$(1\times C\text{-}(H)(C)(Cl)_2)+(1\times C\text{-}(H)_2(C)(Cl))$, $\sigma = 1$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−151.20	−148.55	−2.65	72LAY/WAD
$C_p°$ =	88.99	88.22	0.77	69STU/WES
$S°$ =	337.10	342.52	−5.42	69STU/WES
$\Delta_fS°$ =		−199.27		
$\Delta_fG°$ =		−89.14		
$\ln K_f$ =		35.96		
Liquid phase				
$\Delta_fH°$ =	−191.50	−189.50	−2.00	56KIR
$C_p°$ =		148.78		
$S°$ =		232.72		
$\Delta_fS°$ =		−309.07		
$\Delta_fG°$ =		−97.35		
$\ln K_f$ =		39.27		

TABLE 51. Chlorides (116) — Continued

1,2,3-Trichloropropane $C_3H_5Cl_3$
(2×C–(H)$_2$(C)(Cl))+(1×C–(H)(C)$_2$(Cl)), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−194.51		
$C_p°$ =	112.21	110.06	2.15	69STU/WES
$S°$ =	382.92	384.06	−1.14	69STU/WES
$\Delta_fS°$ =		−294.05		
$\Delta_fG°$ =		−106.84		
$\ln K_f$ =		43.10		
Liquid phase				
$\Delta_fH°$ =	−230.60	−244.97	14.37	54BJE/SMI
$C_p°$ =	183.68	193.54	−9.86	41NEL/NEW

1,1,2,2-Tetrachloroethane $C_2H_2Cl_4$
(2×C–(H)(C)(Cl)$_2$), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−148.80	−158.20	9.40	72LAY/WAD
$C_p°$ =	100.79	101.38	−0.59	69STU/WES
$S°$ =	362.71	360.80	1.91	69STU/WES
$\Delta_fS°$ =		−227.20		
$\Delta_fG°$ =		−90.46		
$\ln K_f$ =		36.49		
Liquid phase				
$\Delta_fH°$ =	−194.60	−205.20	10.60	53SMI/BJE
$C_p°$ =	165.27	170.04	−4.77	48KUR
$S°$ =		256.90		
$\Delta_fS°$ =		−331.10		
$\Delta_fG°$ =		−106.48		
$\ln K_f$ =		42.95		

1,2,2,3-Tetrachloropropane $C_3H_4Cl_4$
(2×C–(H)$_2$(C)(Cl))+(1×C–(C)$_2$(Cl)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−218.46		
$C_p°$ =		129.46		
Liquid phase				
$\Delta_fH°$ =	−251.80	−275.60	23.80	69HU/SIN
$C_p°$ =		201.76		

TABLE 51. Chlorides (116) — Continued

1,1,1,3-Tetrachloropropane $C_3H_4Cl_4$
(1×C–(H)$_2$(C)$_2$)+(1×C–(C)(Cl)$_3$)+(1×C–(H)$_2$(C)(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−172.06		
$C_p°$ =		128.60		
Liquid phase				
$\Delta_fH°$ =	−208.70	−225.56	16.86	70KOL/TOM
$C_p°$ =	196.40	196.38	0.02	74KOL/VOR
$S°$ =	284.30	282.56	1.74	74KOL/VOR
$\Delta_fS°$ =		−441.75		
$\Delta_fG°$ =		−93.85		
$\ln K_f$ =		37.86		

Pentachloroethane C_2HCl_5
(1×C–(C)(Cl)$_3$)+(1×C–(H)(C)(Cl)$_2$), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−142.00	−161.08	19.08	56KIR
$C_p°$ =	117.74	118.87	−1.13	69STU/WES
$S°$ =	380.53	376.29	4.24	69STU/WES
$\Delta_fS°$ =		−257.91		
$\Delta_fG°$ =		−84.18		
$\ln K_f$ =		33.96		
Liquid phase				
$\Delta_fH°$ =	−189.90	−215.53	25.63	56KIR
$C_p°$ =	196.23	187.22	9.01	48KUR
$S°$ =		274.36		
$\Delta_fS°$ =		−359.84		
$\Delta_fG°$ =		−108.25		
$\ln K_f$ =		43.67		

Hexachloroethane C_2Cl_6
(2×C–(C)(Cl)$_3$), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−143.50	−163.96	20.46	63PUY/BAL
$C_p°$ =	136.36	136.36	0.00	69STU/WES
$S°$ =	396.52	398.52	−2.00	69STU/WES
$\Delta_fS°$ =		−281.88		
$\Delta_fG°$ =		−79.92		
$\ln K_f$ =		32.24		
Liquid phase				
$\Delta_fH°$ =		−225.86		
$C_p°$ =	198.24	204.40	−6.16	75RAK/GUT
$S°$ =	237.32	291.82	−54.50	75RAK/GUT
$\Delta_fS°$ =		−388.58		
$\Delta_fG°$ =		−110.01		
$\ln K_f$ =		44.38		

TABLE 51. Chlorides (116) – Continued

Tetrachloroethylene C_2Cl_4
$(2\times C_d-(Cl)_2)$, $\sigma = 4$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−10.80	−23.02	12.22	26MAT
C_p° =	94.93	93.72	1.21	69STU/WES
S° =	340.83	339.29	1.54	69STU/WES
Δ_fS° =		−118.13		
Δ_fG° =		12.20		
$\ln K_f$ =		−4.92		
Liquid phase				
Δ_fH° =	−50.60	−64.16	13.56	53SMI/BJE
C_p° =	146.48	152.94	−6.46	82GRO/ING
S° =		230.70		
Δ_fS° =		−226.72		
Δ_fG° =		3.44		
$\ln K_f$ =		−1.39		

Chloroethylene C_2H_3Cl
$(1\times C_d-(H)_2)+(1\times C_d-(H)(Cl))$, $\sigma = 1$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	35.30	30.69	4.61	62LAC/GOT
C_p° =	53.72	54.13	−0.41	69STU/WES
S° =	263.93	263.37	0.56	69STU/WES
Δ_fS° =		−55.45		
Δ_fG° =		47.22		
$\ln K_f$ =		−19.05		

2-Chloro-1-propene C_3H_5Cl
$(1\times C_d-(C)(Cl))+(1\times C-(H)_3(C))+(1\times C_d-(H)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−21.00	−21.00	0.00	70SHE/ROZ

3-Chloro-1-propene C_3H_5Cl
$(1\times C_d-(H)_2)+(1\times C_d-(H)(C))+(1\times C-(H)_2(C)(Cl))$, $\sigma = 1$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−6.81		
C_p° =	75.35	77.65	−2.30	69STU/WES
S° =	306.64	307.81	−1.17	69STU/WES
Δ_fS° =		−147.32		
Δ_fG° =		37.11		
$\ln K_f$ =		−14.97		

TABLE 51. Chlorides (116) – Continued

1,1-Dichloroethylene $C_2H_2Cl_2$
$(1\times C_d-(H)_2)+(1\times C_d-(Cl)_2)$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	2.60	14.81	−12.21	59HIL/MCD
C_p° =	67.03	68.24	−1.21	69STU/WES
S° =	288.07	285.17	2.90	69STU/WES
Δ_fS° =		−79.86		
Δ_fG° =		38.62		
$\ln K_f$ =		−15.58		
Liquid phase				
Δ_fH° =	−24.10	−10.33	−13.77	71MAN/RIN
C_p° =	111.29	104.84	6.45	59HIL/MCD
S° =	201.54	201.54	0.00	59HIL/MCD
Δ_fS° =		−163.48		
Δ_fG° =		38.41		
$\ln K_f$ =		−15.50		

1,2-Dichloroethylene (Z) $C_2H_2Cl_2$
$(2\times C_d-(H)(Cl))+(1\times cis\ corr-(X)(X))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	4.60	4.74	−0.14	47KET/VAN
C_p° =	65.05	65.50	−0.45	69STU/WES
S° =	289.53	289.94	−0.41	69STU/WES
Δ_fS° =		−75.09		
Δ_fG° =		27.13		
$\ln K_f$ =		−10.94		
Liquid phase				
Δ_fH° =	−26.40	−25.34	−1.06	53SMI/BJE
C_p° =	113.80	113.24	0.56	34MEH2

1,2-Dichloroethylene (E) $C_2H_2Cl_2$
$(2\times C_d-(H)(Cl))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	5.00	8.74	−3.74	47KET/VAN
C_p° =	66.65	65.50	1.15	69STU/WES
S° =	289.90	289.94	−0.04	69STU/WES
Δ_fS° =		−75.09		
Δ_fG° =		31.13		
$\ln K_f$ =		−12.56		
Liquid phase				
Δ_fH° =	−24.30	−25.34	1.04	53SMI/BJE
C_p° =	112.97	113.24	−0.27	34MEH2

TABLE 51. Chlorides (116) – Continued

Trichloroethylene C_2HCl_3

$(1\times C_d-(H)(Cl))+(1\times C_d-(Cl)_2)$, $\sigma = 1$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−8.00	−7.14	−0.86	44MCD
$C_p°$ =	80.21	79.61	0.60	69STU/WES
$S°$ =	324.80	323.26	1.54	69STU/WES
$\Delta_fS°$ =		−87.96		
$\Delta_fG°$ =		19.09		
$\ln K_f$ =		−7.70		
Liquid phase				
$\Delta_fH°$ =	−44.40	−44.75	0.35	53SMI/BJE
$C_p°$ =	124.68	133.09	−8.41	33TRE/WAT

1,2,3-Trichloropropene $C_3H_3Cl_3$

$(1\times C-(H)_2(C)(Cl))+(1\times C_d-(C)(Cl))+(1\times C_d-(H)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−70.14		
Liquid phase				
$\Delta_fH°$ =	−101.80	−101.80	0.00	69HU/SIN

1-Chloropropyne C_3H_3Cl

$(1\times C-(H)_3(C))+(1\times C_t-(C))+(1\times C_t-(Cl))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$C_p°$ =	71.96	71.96	0.00	69STU/WES
$S°$ =	284.51	284.51	0.00	69STU/WES
$\Delta_fS°$ =		−40.06		

Hexachlorobenzene C_6Cl_6

$(6\times C_B-(Cl)(C_B)_2)+(6\times$ *ortho* corr$-(Cl)(Cl))$, $\sigma = 12$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−44.70	−45.18	0.48	83PLA/SIM
$C_p°$ =	175.31	175.98	−0.67	69STU/WES
$S°$ =	441.20	441.82	−0.62	69STU/WES
$\Delta_fS°$ =		−261.54		
$\Delta_fG°$ =		32.80		
$\ln K_f$ =		−13.23		

Hexachlorobenzene (Continued) C_6Cl_6

$(6\times C_B-(Cl)(C_B)_2)+(6\times$ *ortho* corr$-(Cl)(Cl))$, $\sigma = 12$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−111.45	−109.20	−2.25	69PLA/GLA
$C_p°$ =		211.62		
$S°$ =		332.82		
$\Delta_fS°$ =		−370.54		
$\Delta_fG°$ =		1.28		
$\ln K_f$ =		−0.51		
Solid phase				
$\Delta_fH°$ =	−141.77	−141.00	−0.77	83PLA/SIM
$C_p°$ =	201.29	201.30	−0.01	58HIL/KRA
$S°$ =	260.24	260.22	0.02	58HIL/KRA
$\Delta_fS°$ =		−443.14		
$\Delta_fG°$ =		−8.88		
$\ln K_f$ =		3.58		

Chlorobenzene C_6H_5Cl

$(1\times C_B-(Cl)(C_B)_2)+(5\times C_B-(H)(C_B)_2)$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	50.90	52.02	−1.12	68WAD
$C_p°$ =	98.03	97.38	0.65	69STU/WES
$S°$ =	313.46	312.87	0.59	69STU/WES
$\Delta_fS°$ =		−159.49		
$\Delta_fG°$ =		99.57		
$\ln K_f$ =		−40.17		
Liquid phase				
$\Delta_fH°$ =	10.50	8.60	1.90	54HUB/KNO
$C_p°$ =	150.08	148.67	1.41	37STU
$S°$ =	197.48	199.82	−2.34	37STU
$\Delta_fS°$ =		−272.53		
$\Delta_fG°$ =		89.86		
$\ln K_f$ =		−36.25		

1-Chloro-4-methylbenzene; p-Chlorotoluene C_7H_7Cl

$(1\times C_B-(Cl)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		19.59		
$C_p°$ =		119.25		

TABLE 51. Chlorides (116) – Continued

1-Chloro-4-methylbenzene; *p*-Chlorotoluene (Continued) C_7H_7Cl

$(1\times C_B-(Cl)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Liquid phase				
Δ_fH° =	−19.90	−28.01	8.11	53SMI/BJE
C_p° =		172.57		
S° =		234.75		
Δ_fS° =		−373.91		
Δ_fG° =		83.47		
$\ln K_f$ =		−33.67		

Benzyl chloride C_7H_7Cl

$(5\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_2(C_B)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	18.90	18.90	0.00	70COX/PIL
Liquid phase				
Δ_fH° =	−32.60	−32.60	0.00	56KIR

1-Chloro-2-ethylbenzene C_8H_9Cl

$(1\times C_B-(Cl)(C_B)_2)+(1\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))+(1\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times$ *ortho* corr–(alk)(X))

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−6.70	0.76	−7.46	49DRE/MAR
C_p° =		144.86		
Liquid phase				
Δ_fH° =	−54.10	−46.52	−7.58	54HUB/KNO
C_p° =		195.47		
S° =		282.15		
Δ_fS° =		−462.83		
Δ_fG° =		91.47		
$\ln K_f$ =		−36.90		

1-Chloro-4-ethylbenzene C_8H_9Cl

$(1\times C_B-(Cl)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−3.64	−1.75	−1.89	49DRE/MAR
C_p° =		144.86		

TABLE 51. Chlorides (116) – Continued

1-Chloro-4-ethylbenzene (Continued) C_8H_9Cl

$(1\times C_B-(Cl)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_3(C))+(1\times C-(H)_2(C)(C_B))$

	Literature	Calculated	Residual	Reference
Liquid phase				
Δ_fH° =	−51.76	−52.82	1.06	54HUB/KNO
C_p° =		195.47		
S° =		282.15		
Δ_fS° =		−462.83		
Δ_fG° =		85.17		
$\ln K_f$ =		−34.36		

(1-Chloroethyl)benzene C_8H_9Cl

$(5\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_2(C)(C_B))+(1\times C-(H)_2(C)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		1.90		
C_p° =		140.94		
Liquid phase				
Δ_fH° =	−58.20	−51.75	−6.45	69HU/SIN
C_p° =		210.16		
S° =		276.52		
Δ_fS° =		−468.46		
Δ_fG° =		87.92		
$\ln K_f$ =		−35.47		

1-Chloronaphthalene $C_{10}H_7Cl$

$(1\times C_B-(Cl)(C_B)_2)+(7\times C_B-(H)(C_B)_2)+(2\times C_{BF}-(C_{BF})(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	119.60	119.84	−0.24	70COX/PIL
C_p° =		124.60		
Liquid phase				
Δ_fH° =	54.40	56.58	−2.18	56SMI
C_p° =		213.07		
S° =		246.48		
Δ_fS° =		−379.40		
Δ_fG° =		169.70		
$\ln K_f$ =		−68.46		

TABLE 51. Chlorides (116) – Continued

2-Chloronaphthalene $C_{10}H_7Cl$

$(1 \times C_B-(Cl)(C_B)_2) + (7 \times C_B-(H)(C_B)_2) + (2 \times C_{BF}-(C_{BF})(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	137.20	119.84	17.36	70COX/PIL
$C_p°$ =		124.60		
Liquid phase				
$\Delta_f H°$ =		56.58		
$C_p°$ =		213.07		
$S°$ =		246.48		
$\Delta_f S°$ =		−379.40		
$\Delta_f G°$ =		169.70		
$\ln K_f$ =		−68.46		
Solid phase				
$\Delta_f H°$ =	55.20	41.91	13.29	56SMI
$C_p°$ =		179.06		
$S°$ =		190.62		
$\Delta_f S°$ =		−435.26		
$\Delta_f G°$ =		171.68		
$\ln K_f$ =		−69.26		

1,2-Dichlorobenzene $C_6H_4Cl_2$

$(4 \times C_B-(H)(C_B)_2) + (2 \times C_B-(Cl)(C_B)_2) + (1 \times$ *ortho* corr$-(Cl)(Cl))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	29.63	30.68	−1.05	49DRE/MAR
$C_p°$ =	113.47	113.10	0.37	69STU/WES
$S°$ =	341.46	341.64	−0.18	69STU/WES
$\Delta_f S°$ =		−176.92		
$\Delta_f G°$ =		83.43		
$\ln K_f$ =		−33.65		
Liquid phase				
$\Delta_f H°$ =	−18.07	−17.76	−0.31	54HUB/KNO
$C_p°$ =		161.26		
$S°$ =		226.42		
$\Delta_f S°$ =		−292.13		
$\Delta_f G°$ =		69.34		
$\ln K_f$ =		−27.97		

TABLE 51. Chlorides (116) – Continued

1,3-Dichlorobenzene $C_6H_4Cl_2$

$(4 \times C_B-(H)(C_B)_2) + (2 \times C_B-(Cl)(C_B)_2) + (1 \times$ *meta* corr$-(Cl)(Cl))$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	25.50	16.18	9.32	49DRE/MAR
$C_p°$ =	113.80	113.10	0.70	69STU/WES
$S°$ =	343.46	341.64	1.82	69STU/WES
$\Delta_f S°$ =		−176.92		
$\Delta_f G°$ =		68.93		
$\ln K_f$ =		−27.81		
Liquid phase				
$\Delta_f H°$ =	−20.90	−21.76	0.86	54HUB/KNO
$C_p°$ =		161.26		
$S°$ =		226.42		
$\Delta_f S°$ =		−292.13		
$\Delta_f G°$ =		65.34		
$\ln K_f$ =		−26.36		

1,4-Dichlorobenzene $C_6H_4Cl_2$

$(4 \times C_B-(H)(C_B)_2) + (2 \times C_B-(Cl)(C_B)_2)$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	22.18	21.18	1.00	61WAL/SMI
$C_p°$ =	113.89	113.10	0.79	69STU/WES
$S°$ =	336.69	341.64	−4.95	69STU/WES
$\Delta_f S°$ =		−176.92		
$\Delta_f G°$ =		73.93		
$\ln K_f$ =		−29.82		
Liquid phase				
$\Delta_f H°$ =		−31.76		
$C_p°$ =		161.26		
$S°$ =		226.42		
$\Delta_f S°$ =		−292.13		
$\Delta_f G°$ =		55.34		
$\ln K_f$ =		−22.32		
Solid phase				
$\Delta_f H°$ =	−42.84	−37.88	−4.96	54HUB/KNO
$C_p°$ =	147.76	147.62	0.14	76DWO/FIG
$S°$ =	175.41	177.74	−2.33	76DWO/FIG
$\Delta_f S°$ =		−340.81		
$\Delta_f G°$ =		63.73		
$\ln K_f$ =		−25.71		

TABLE 51. Chlorides (116) – Continued

2,5-Dichlorostyrene $C_8H_6Cl_2$

$(1\times C_d\text{-}(H)_2)+(1\times C_d\text{-}(H)(C_B))+(1\times C_B\text{-}(C_d)(C_B)_2)+(3\times C_B\text{-}(H)(C_B)_2)+(2\times C_B\text{-}(Cl)(C_B)_2)+(2\times \textit{ortho}\text{ corr-}(alk)(X))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		91.16		
$C_p°$ =		153.53		
Liquid phase				
$\Delta_fH°$ =	35.90	35.73	0.17	58SIN/STU
$C_p°$ =		208.06		
$S°$ =		288.00		
$\Delta_fS°$ =		−372.60		
$\Delta_fG°$ =		146.82		
$\ln K_f$ =		−59.23		

2,2′-Dichlorobiphenyl $C_{12}H_8Cl_2$

$(8\times C_B\text{-}(H)(C_B)_2)+(2\times C_B\text{-}(Cl)(C_B)_2)+(2\times C_B\text{-}(C_B)_3)+(1\times \textit{ortho}\text{ corr-}(Cl)(Cl'))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	127.90	127.74	0.16	64SMI/GOR
$C_p°$ =		193.78		
Liquid phase				
$\Delta_fH°$ =		43.30		
$C_p°$ =		286.12		
Solid phase				
$\Delta_fH°$ =	31.70	30.30	1.40	64SMI/GOR
$C_p°$ =		224.70		
$S°$ =		256.74		
$\Delta_fS°$ =		557.40		
$\Delta_fG°$ =		196.49		
$\ln K_f$ =		−79.26		

4,4′-Dichlorobiphenyl $C_{12}H_8Cl_2$

$(8\times C_B\text{-}(H)(C_B)_2)+(2\times C_B\text{-}(Cl)(C_B)_2)+(2\times C_B\text{-}(C_B)_3)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	121.10	119.74	1.36	64SMI/GOR
$C_p°$ =		193.78		
Liquid phase				
$\Delta_fH°$ =		35.30		
$C_p°$ =		286.12		

4,4′-Dichlorobiphenyl (Continued) $C_{12}H_8Cl_2$

$(8\times C_B\text{-}(H)(C_B)_2)+(2\times C_B\text{-}(Cl)(C_B)_2)+(2\times C_B\text{-}(C_B)_3)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	17.30	22.30	−5.00	64SMI/GOR
$C_p°$ =		224.70		
$S°$ =		256.74		
$\Delta_fS°$ =		−557.40		
$\Delta_fG°$ =		188.49		
$\ln K_f$ =		−76.03		

1,2,4,5-Tetrachloro-3,6-dimethylbenzene $C_8H_6Cl_4$

$(2\times C\text{-}(H)_3(C))+(2\times C_B\text{-}(C)(C_B)_2)+(4\times C_B\text{-}(Cl)(C_B)_2)+(2\times \textit{ortho}\text{ corr-}(Cl)(Cl))+(4\times \textit{ortho}\text{ corr-}(alk)(X))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−76.32		
$C_p°$ =		188.28		
Liquid phase				
$\Delta_fH°$ =		−132.50		
$C_p°$ =		234.24		
$S°$ =		349.48		
$\Delta_fS°$ =		−534.10		
$\Delta_fG°$ =		26.74		
$\ln K_f$ =		−10.79		
Solid phase				
$\Delta_fH°$ =	−173.90	−176.68	2.78	69HU/SIN
$C_p°$ =		222.58		
$S°$ =		275.86		
$\Delta_fS°$ =		−607.72		
$\Delta_fG°$ =		4.51		
$\ln K_f$ =		−1.82		

Pentachlorobenzene C_6HCl_5

$(1\times C_B\text{-}(H)(C_B)_2)+(5\times C_B\text{-}(Cl)(C_B)_2)+(4\times \textit{ortho}\text{ corr-}(Cl)(Cl))+(1\times \textit{meta}\text{ corr-}(Cl)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−40.00	−38.34	−1.66	85PLA/SIM
$C_p°$ =		160.26		
Liquid phase				
$\Delta_fH°$ =		−86.84		
$C_p°$ =		199.03		
$S°$ =		306.22		
$\Delta_fS°$ =		−350.94		
$\Delta_fG°$ =		17.79		
$\ln K_f$ =		−7.18		

TABLE 51. Chlorides (116) — Continued

Pentachlorobenzene (Continued) C_6HCl_5
$(1 \times C_B-(H)(C_B)_2) + (5 \times C_B-(Cl)(C_B)_2) +$
$(4 \times$ *ortho* corr$-(Cl)(Cl)) + (1 \times$ *meta* corr$-(Cl)(Cl))$

	Literature	Calculated	Residual	Reference
Solid phase				
Δ_fH° =	−120.40	−115.47	−4.93	85PLA/SIM
C_p° =		187.88		
S° =		239.60		
Δ_fS° =		−417.56		
Δ_fG° =		9.02		
$\ln K_f$ =		−3.64		

Chlorocyclohexane $C_6H_{11}Cl$
$(5 \times C-(H)_2(C)_2) + (1 \times C-(H)(C)_2(Cl)) +$
$(1 \times$ Cyclohexane (sub) rsc$)$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−163.70	−159.15	−4.55	70COX/PIL
C_p° =		126.63		
Liquid phase				
Δ_fH° =	−207.20	−201.88	−5.32	56KIR
C_p° =		191.91		

3-Chlorophenol C_6H_5ClO
$(4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(Cl)(C_B)_2) + (1 \times C_B-(O)(C_B)_2) +$
$(1 \times O-(H)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−153.30	−126.84	−26.46	38WOL/WEG
C_p° =		117.79		
Liquid phase				
Δ_fH° =	−189.30	−196.92	7.62	53SMI/BJE
C_p° =		210.34		
S° =		204.25		
Δ_fS° =		−370.62		
Δ_fG° =		−86.42		
$\ln K_f$ =		34.86		
Solid phase				
Δ_fH° =	−206.40	−204.13	−2.27	53SMI/BJE
C_p° =		143.03		
S° =		164.58		
Δ_fS° =		−410.30		
Δ_fG° =		−81.80		
$\ln K_f$ =		33.00		

4-Chlorophenol C_6H_5ClO
$(4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(Cl)(C_B)_2) + (1 \times C_B-(O)(C_B)_2) +$
$(1 \times O-(H)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =	−145.80	−126.84	−18.96	38WOL/WEG
C_p° =		117.79		
Liquid phase				
Δ_fH° =	−181.30	−196.92	15.62	53SMI/BJE
C_p° =		210.34		
S° =		204.25		
Δ_fS° =		−370.62		
Δ_fG° =		−86.42		
$\ln K_f$ =		34.86		
Solid phase				
Δ_fH° =	−197.70	−204.13	6.43	53SMI/BJE
C_p° =		143.03		
S° =		164.58		
Δ_fS° =		−410.30		
Δ_fG° =		−81.80		
$\ln K_f$ =		33.00		

2-Chloro-1,3-propanediol $C_3H_7ClO_2$
$(2 \times O-(H)(C)) + (2 \times C-(H)_2(O)(C)) + (1 \times C-(H)(C)_2(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−440.07		
C_p° =		111.98		
Liquid phase				
Δ_fH° =	−517.50	−525.77	8.27	54BJE/SMI
C_p° =		222.58		

3-Chloro-1,2-propanediol $C_3H_7ClO_2$
$(1 \times C-(H)_2(C)(Cl)) + (1 \times C-(H)(O)(C)_2$ (alcohols,peroxides)$) +$
$(1 \times C-(H)_2(O)(C)) + (2 \times O-(H)(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
Δ_fH° =		−447.11		
C_p° =		114.14		
Liquid phase				
Δ_fH° =	−525.30	−533.30	8.00	54BJE/SMI
C_p° =		236.51		
S° =		194.81		
Δ_fS° =		−595.94		
Δ_fG° =		−355.62		
$\ln K_f$ =		143.46		

TABLE 51. Chlorides (116) – Continued

1,3-Dichloro-2-propanol $C_3H_6Cl_2O$
(2×C–(H)$_2$(C)(Cl)) + (1×C–(H)(O)(C)$_2$ (alcohols,peroxides)) + (1×O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−318.40	−324.33	5.93	70COX/PIL
$C_p°$ =		113.18		
Liquid phase				
$\Delta_fH°$ =	−385.30	−392.90	7.60	54BJE/SMI
$C_p°$ =		221.99		
$S°$ =		222.60		
$\Delta_fS°$ =		−511.83		
$\Delta_fG°$ =		−240.30		
$\ln K_f$ =		96.93		

2,3-Dichloro-1-propanol $C_3H_6Cl_2O$
(1×C–(H)$_2$(C)(Cl)) + (1×C–(H)(C)$_2$(Cl)) + (1×C–(H)$_2$(O)(C)) + (1×O–(H)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−316.30	−317.29	0.99	70COX/PIL
$C_p°$ =		111.02		
Liquid phase				
$\Delta_fH°$ =	−381.50	−385.37	3.87	54BJE/SMI
$C_p°$ =		208.06		

2,3-Dichloro-1,4-benzenediol $C_6H_4Cl_2O_2$
(2×C_B–(H)(C_B)$_2$) + (2×C_B–(Cl)(C_B)$_2$) + (2×C_B–(O)(C_B)$_2$) + (2×O–(H)(C_B)) + (1×*ortho* corr–(Cl)(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−327.04		
$C_p°$ =		153.92		
Liquid phase				
$\Delta_fH°$ =		−428.80		
$C_p°$ =		284.60		
$S°$ =		235.28		
$\Delta_fS°$ =		−488.32		
$\Delta_fG°$ =		−283.21		
$\ln K_f$ =		114.24		
Solid phase				
$\Delta_fH°$ =	−416.00	−438.94	22.94	53SMI/BJE
$C_p°$ =		165.28		
$S°$ =		192.66		
$\Delta_fS°$ =		−530.94		
$\Delta_fG°$ =		−280.64		
$\ln K_f$ =		113.21		

2,5-Dichloro-1,4-benzenediol $C_6H_4Cl_2O_2$
(2×C_B–(H)(C_B)$_2$) + (2×C_B–(Cl)(C_B)$_2$) + (2×C_B–(O)(C_B)$_2$) + (2×O–(H)(C_B))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−336.54		
$C_p°$ =		153.92		
Liquid phase				
$\Delta_fH°$ =		−442.80		
$C_p°$ =		284.60		
$S°$ =		235.28		
$\Delta_fS°$ =		−488.32		
$\Delta_fG°$ =		−297.21		
$\ln K_f$ =		119.89		
Solid phase				
$\Delta_fH°$ =	−427.30	−447.44	20.14	53SMI/BJE
$C_p°$ =		165.28		
$S°$ =		192.66		
$\Delta_fS°$ =		−530.94		
$\Delta_fG°$ =		−289.14		
$\ln K_f$ =		116.64		

2,6-Dichloro-1,4-benzenediol $C_6H_4Cl_2O_2$
(2×C_B–(H)(C_B)$_2$) + (2×C_B–(Cl)(C_B)$_2$) + (2×C_B–(O)(C_B)$_2$) + (2×O–(H)(C_B)) + (1×*meta* corr–(Cl)(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−331.50	−341.54	10.04	27COO/COO
$C_p°$ =		153.92		
Liquid phase				
$\Delta_fH°$ =		−432.80		
$C_p°$ =		284.60		
$S°$ =		235.28		
$\Delta_fS°$ =		−488.32		
$\Delta_fG°$ =		−287.21		
$\ln K_f$ =		115.86		
Solid phase				
$\Delta_fH°$ =	−423.50	−443.44	19.94	53SMI/BJE
$C_p°$ =		165.28		
$S°$ =		192.66		
$\Delta_fS°$ =		−530.94		
$\Delta_fG°$ =		−285.14		
$\ln K_f$ =		115.02		

TABLE 51. Chlorides (116) — Continued

2,3,5-Trichloro-1,4-benzenediol $C_6H_3Cl_3O_2$
$(1\times C_B-(H)(C_B)_2)+(3\times C_B-(Cl)(C_B)_2)+(2\times O-(H)(C_B))+(2\times C_B-(O)(C_B)_2)+(1\times ortho\ corr-(Cl)(Cl))+(1\times meta\ corr-(Cl)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−339.40	−362.88	23.48	27COO/COO
$C_p°$ =		169.64		
Liquid phase				
$\Delta_fH°$ =		−459.16		
$C_p°$ =		297.19		
$S°$ =		261.88		
$\Delta_fS°$ =		−507.92		
$\Delta_fG°$ =		−307.72		
$\ln K_f$ =		124.13		
Solid phase				
$\Delta_fH°$ =	−440.70	−473.47	32.77	53SMI/BJE
$C_p°$ =		178.70		
$S°$ =		213.28		
$\Delta_fS°$ =		−556.52		
$\Delta_fG°$ =		−307.54		
$\ln K_f$ =		124.06		

2,3,5,6-Tetrachloro-1,4-benzenediol $C_6H_2Cl_4O_2$
$(4\times C_B-(Cl)(C_B)_2)+(2\times O-(H)(C_B))+(2\times C_B-(O)(C_B)_2)+(2\times ortho\ corr-(Cl)(Cl))+(2\times meta\ corr-(Cl)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−389.22		
$C_p°$ =		185.36		
Liquid phase				
$\Delta_fH°$ =		−475.52		
$C_p°$ =		309.78		
$S°$ =		288.48		
$\Delta_fS°$ =		−527.52		
$\Delta_fG°$ =		−318.24		
$\ln K_f$ =		128.38		
Solid phase				
$\Delta_fH°$ =	−453.60	−499.50	45.90	53SMI/BJE
$C_p°$ =		192.12		
$S°$ =		233.90		
$\Delta_fS°$ =		−582.10		
$\Delta_fG°$ =		−325.95		
$\ln K_f$ =		131.48		

TABLE 51. Chlorides (116) — Continued

Pentachlorophenol C_6HCl_5O
$(1\times O-(H)(C_B))+(1\times C_B-(O)(C_B)_2)+(5\times C_B-(Cl)(C_B)_2)+(4\times ortho\ corr-(Cl)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−225.10	−212.20	−12.90	70COX/PIL
$C_p°$ =		180.67		
Liquid phase				
$\Delta_fH°$ =		−302.36		
$C_p°$ =		260.70		
$S°$ =		310.65		
$\Delta_fS°$ =		−449.03		
$\Delta_fG°$ =		−168.48		
$\ln K_f$ =		67.96		
Solid phase				
$\Delta_fH°$ =	−292.50	−324.25	31.75	58SIN/STU
$C_p°$ =		196.71		
$S°$ =		247.06		
$\Delta_fS°$ =		−512.62		
$\Delta_fG°$ =		−171.41		
$\ln K_f$ =		69.15		

2-Chloro-1,4-benzenediol $C_6H_5ClO_2$
$(3\times C_B-(H)(C_B)_2)+(1\times C_B-(Cl)(C_B)_2)+(2\times O-(H)(C_B))+(2\times C_B-(O)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−314.00	−305.70	−8.30	27COO/COO
$C_p°$ =		138.20		
Liquid phase				
$\Delta_fH°$ =		−402.44		
$C_p°$ =		272.01		
$S°$ =		208.68		
$\Delta_fS°$ =		−468.72		
$\Delta_fG°$ =		−262.69		
$\ln K_f$ =		105.97		
Solid phase				
$\Delta_fH°$ =	−383.00	−408.91	25.91	53SMI/BJE
$C_p°$ =		151.86		
$S°$ =		172.04		
$\Delta_fS°$ =		−505.36		
$\Delta_fG°$ =		−258.24		
$\ln K_f$ =		104.17		

TABLE 51. Chlorides (116) – Continued

Chloroacetic acid $C_2H_3ClO_2$
(1×C–(H)$_2$(CO)(Cl)) + (1×CO–(C)(O)) + (1×O–(H)(CO))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	−435.20	−435.80	0.60	49SRE/MAR
Liquid phase				
$\Delta_f H°$ =		−493.42		
Solid phase				
$\Delta_f H°$ =	−510.50	−510.50	0.00	53SMI/BJE

2-Chloropropanoic acid $C_3H_5ClO_2$
(1×O–(H)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_3$(C)) + (1×C–(H)(C)(CO)(Cl))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−473.68		
Liquid phase				
$\Delta_f H°$ =	−522.50	−518.08	−4.42	53SMI/BJE
$C_p°$ =		168.73		

3-Chloropropanoic acid $C_3H_5ClO_2$
(1×O–(H)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_2$(CO)(C)) + (1×C–(H)$_2$(C)(Cl))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−482.83		
$C_p°$ =		103.01		
Liquid phase				
$\Delta_f H°$ =		−546.05		
$C_p°$ =		175.85		
$S°$ =		215.14		
$\Delta_f S°$ =		−445.04		
$\Delta_f G°$ =		−413.36		
$\ln K_f$ =		166.75		
Solid phase				
$\Delta_f H°$ =	−549.30	−549.30	0.00	53SMI/BJE

2-Chlorobutanoic acid $C_4H_7ClO_2$
(1×O–(H)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_2$(CO)(Cl)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)$_3$(C))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−498.69		
Liquid phase				
$\Delta_f H°$ =	−575.50	−566.76	−8.74	53SMI/BJE
Solid phase				
$\Delta_f H°$ =		−586.65		

3-Chlorobutanoic acid $C_4H_7ClO_2$
(1×O–(H)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_2$(CO)(C)) + (1×C–(H)(C)$_2$(Cl)) + (1×C–(H)$_3$(C))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−511.25		
$C_p°$ =		126.21		
Liquid phase				
$\Delta_f H°$ =	−556.30	−577.93	21.63	53SMI/BJE
$C_p°$ =		214.59		

4-Chlorobutanoic acid $C_4H_7ClO_2$
(1×O–(H)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_2$(CO)(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(C)(Cl))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		−503.46		
$C_p°$ =		125.90		
Liquid phase				
$\Delta_f H°$ =	−566.30	−571.78	5.48	53SMI/BJE
$C_p°$ =		206.27		
$S°$ =		247.52		
$\Delta_f S°$ =		−548.97		
$\Delta_f G°$ =		−408.11		
$\ln K_f$ =		164.63		

TABLE 51. Chlorides (116) — Continued

Dichloroacetic acid $C_2H_2Cl_2O_2$

$(1\times O\text{–}(H)(CO))+(1\times CO\text{–}(C)(O))+(1\times C\text{–}(H)(CO)(Cl)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−431.94		
Liquid phase				
$\Delta_fH°$ =	−496.30	−490.12	−6.18	53SMI/BJE

2-Chlorobenzoic acid $C_7H_5ClO_2$

$(4\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(Cl)(C_B)_2)+(1\times O\text{–}(H)(CO))+(1\times CO\text{–}(O)(C_B))+(1\times C_B\text{–}(CO)(C_B)_2)+(1\times \textit{ortho}\ \text{corr–}(Cl)(COOH))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−325.00	−325.59	0.59	38WOL/WEG
Liquid phase				
$\Delta_fH°$ =		−414.70		
$C_p°$ =		216.36		
Solid phase				
$\Delta_fH°$ =	−404.83	−404.88	0.05	74JOH/PRO
$C_p°$ =		159.53		
$S°$ =		188.36		
$\Delta_fS°$ =		−494.78		
$\Delta_fG°$ =		−257.36		
$\ln K_f$ =		103.82		

3-Chlorobenzoic acid $C_7H_5ClO_2$

$(4\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(Cl)(C_B)_2)+(1\times O\text{–}(H)(CO))+(1\times CO\text{–}(O)(C_B))+(1\times C_B\text{–}(CO)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−342.30	−325.59	−16.71	38WOL/WEG
Liquid phase				
$\Delta_fH°$ =		−414.70		
$C_p°$ =		216.36		
Solid phase				
$\Delta_fH°$ =	−424.59	−424.88	0.29	74JOH/PRO
$C_p°$ =		159.53		
$S°$ =		188.36		
$\Delta_fS°$ =		494.78		
$\Delta_fG°$ =		−277.36		
$\ln K_f$ =		111.89		

4-Chlorobenzoic acid $C_7H_5ClO_2$

$(4\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(Cl)(C_B)_2)+(1\times O\text{–}(H)(CO))+(1\times CO\text{–}(O)(C_B))+(1\times C_B\text{–}(CO)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−341.00	−325.59	−15.41	38WOL/WEG
Liquid phase				
$\Delta_fH°$ =		−414.70		
$C_p°$ =		216.36		
Solid phase				
$\Delta_fH°$ =	−428.16	−424.88	−3.28	74JOH/PRO
$C_p°$ =		159.53		
$S°$ =		188.36		
$\Delta_fS°$ =		−494.78		
$\Delta_fG°$ =		−277.36		
$\ln K_f$ =		111.89		

2-Chlorobenzaldehyde C_7H_5ClO

$(4\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(CO)(C_B)_2)+(1\times C_B\text{–}(Cl)(C_B)_2)+(1\times CO\text{–}(H)(C_B))+(1\times \textit{ortho}\ \text{corr–}(Cl)(CHO))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−62.70	−74.39	11.69	49DRE/MAR
Liquid phase				
$\Delta_fH°$ =	−118.40	−118.68	0.28	53SMI/BJE
$C_p°$ =		184.60		

3-Chlorobenzaldehyde C_7H_5ClO

$(4\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(Cl)(C_B)_2)+(1\times C_B\text{–}(CO)(C_B)_2)+(1\times CO\text{–}(H)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−67.64		
Liquid phase				
$\Delta_fH°$ =	−125.90	−127.18	1.28	53SMI/BJE
$C_p°$ =		184.60		

TABLE 51. Chlorides (116) — Continued

4-Chlorobenzaldehyde C_7H_5ClO
$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(Cl)(C_B)_2)+(1\times C_B-(CO)(C_B)_2)+(1\times CO-(H)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−67.64		
Liquid phase				
$\Delta_fH°$ =		−127.18		
$C_p°$ =		184.60		
Solid phase				
$\Delta_fH°$ =	−146.40	−157.91	11.51	53SMI/BJE

2,2,3-Trichlorobutanal $C_4H_5Cl_3O$
$(1\times C-(H)_3(C))+(1\times C-(H)(C)_2(Cl))+(1\times C-(C)_2(Cl)_2)+(1\times CO-(H)(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−301.82		
$C_p°$ =		144.13		
Liquid phase				
$\Delta_fH°$ =		−363.00		
$C_p°$ =	241.84	241.84	0.00	1881REI

2-Chloroethyl vinyl ether C_4H_7ClO
$(1\times C-(H)_2(C)(Cl))+(1\times C-(H)_2(O)(C))+(1\times O-(C)(C_d))+(1\times C_d-(O)(H))+(1\times C_d-(H)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−170.10	−169.04	−1.06	81TRO/NED
Liquid phase				
$\Delta_fH°$ =	−208.20	−203.62	−4.58	81TRO/NED
$C_p°$ =		201.58		

1-Chloro-2-ethoxyethane C_4H_9ClO
$(1\times C-(H)_2(C)(Cl))+(2\times C-(H)_2(O)(C))+(1\times O-(C)_2)+(1\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−301.30	−278.93	−22.37	67FAI/STI
$C_p°$ =		122.46		

1-Chloro-2-ethoxyethane (Continued) C_4H_9ClO
$(1\times C-(H)_2(C)(Cl))+(2\times C-(H)_2(O)(C))+(1\times O-(C)_2)+(1\times C-(H)_3(C))$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−335.60	−316.94	−18.66	67FAI/STI
$C_p°$ =		191.79		
$S°$ =		279.53		
$\Delta_fS°$ =		−545.01		
$\Delta_fG°$ =		−154.45		
$\ln K_f$ =		62.30		

Propyl chloroacetate $C_5H_9ClO_2$
$(1\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(1\times C-(H)_2(O)(C))+(1\times O-(C)(CO))+(1\times CO-(C)(O))+(1\times C-(H)_2(CO)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−467.00	−466.16	−0.84	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−515.60	−512.94	−2.66	54BJE/SMI

Butyl chloroacetate $C_6H_{11}ClO_2$
$(1\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(O)(C))+(1\times O-(C)(CO))+(1\times CO-(C)(O))+(1\times C-(H)_2(CO)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−487.40	−486.79	−0.61	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−538.40	−538.67	0.27	54BJE/SMI

Ethyl 2-chloropropanoate $C_5H_9ClO_2$
$(2\times C-(H)_3(C))+(1\times C-(H)(C)(CO)(Cl))+(1\times CO-(C)(O))+(1\times O-(C)(CO))+(1\times C-(H)_2(O)(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−483.41		
Liquid phase				
$\Delta_fH°$ =		−511.87		
$C_p°$ =	220.50	220.61	−0.11	54BJE/SMI

TABLE 51. Chlorides (116) — Continued

Propyl 3-chloropropanoate $C_6H_{11}ClO_2$

(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(O)(C)) + (1×O–(C)(CO)) + (1×CO–(C)(O)) + (1×C–(H)$_2$(C)(Cl)) + (1×C–(H)$_2$(CO)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−485.70	−513.19	27.49	70COX/PIL
C_p° =		167.53		
Liquid phase				
$\Delta_f H°$ =	−537.60	−565.57	27.97	53SMI/BJE
C_p° =		258.15		
$S°$ =		363.41		
$\Delta_f S°$ =		−705.70		
$\Delta_f G°$ =		−355.17		
$\ln K_f$ =		143.27		

Ethyl 4-chlorobutanoate $C_6H_{11}ClO_2$

(1×C–(H)$_2$(C)(Cl)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO)) + (1×C–(H)$_2$(O)(C)) + (1×C–(H)$_3$(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−513.80	−513.19	−0.61	70COX/PIL
C_p° =		167.53		
Liquid phase				
$\Delta_f H°$ =	−566.50	−565.57	−0.93	53SMI/BJE
C_p° =		258.15		
$S°$ =		363.41		
$\Delta_f S°$ =		−705.70		
$\Delta_f G°$ =		−355.17		
$\ln K_f$ =		143.27		

Butyl 2-chloropropanoate $C_7H_{13}ClO_2$

(1×C–(H)(C)(CO)(Cl)) + (2×C–(H)$_2$(C)$_2$) + (1×CO–(C)(O)) + (1×O–(C)(CO)) + (1×C–(H)$_2$(O)(C)) + (2×C–(H)$_3$(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−517.40	−524.67	7.27	70COX/PIL
Liquid phase				
$\Delta_f H°$ =	−571.70	−563.33	−8.37	53SMI/BJE
C_p° =		281.45		

TABLE 51. Chlorides (116) — Continued

Butyl 3-chloropropanoate $C_7H_{13}ClO_2$

(1×C–(H)$_2$(C)(Cl)) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO)) + (1×C–(H)$_2$(O)(C)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)$_3$(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−502.30	−533.82	31.52	70COX/PIL
C_p° =		190.42		
Liquid phase				
$\Delta_f H°$ =	−557.90	−591.30	33.40	53SMI/BJE
C_p° =		288.57		
$S°$ =		395.79		
$\Delta_f S°$ =		−809.63		
$\Delta_f G°$ =		−349.91		
$\ln K_f$ =		141.15		

Propyl 2-chlorobutanoate $C_7H_{13}ClO_2$

(2×C–(H)$_3$(C)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)(CO)(Cl)) + (1×CO–(C)(O)) + (1×O–(C)(CO)) + (1×C–(H)$_2$(O)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−578.40	−524.67	−53.73	70COX/PIL
Liquid phase				
$\Delta_f H°$ =	−630.70	−563.33	−67.37	53SMI/BJE
C_p° =		281.45		

Propyl 4-chlorobutanoate $C_7H_{13}ClO_2$

(1×C–(H)$_2$(C)(Cl)) + (2×C–(H)$_2$(C)$_2$) + (1×C–(H)$_2$(CO)(C)) + (1×CO–(C)(O)) + (1×O–(C)(CO)) + (1×C–(H)$_2$(O)(C)) + (1×C–(H)$_3$(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−537.90	−533.82	−4.08	70COX/PIL
C_p° =		190.42		
Liquid phase				
$\Delta_f H°$ =	−591.40	−591.30	−0.10	53SMI/BJE
C_p° =		288.57		
$S°$ =		395.79		
$\Delta_f S°$ =		−809.63		
$\Delta_f G°$ =		−349.91		
$\ln K_f$ =		141.15		

TABLE 51. Chlorides (116) – Continued

Ethyl 2,3-dichloropropanoate $C_5H_8Cl_2O_2$
(1×C–(H)$_2$(C)(Cl))+(1×C–(H)(C)(CO)(Cl))+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))+(1×C–(H)$_3$(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−510.60		
Liquid phase				
$\Delta_fH°$ =		−551.16		
$C_p°$ =	248.95	247.89	1.06	53SMI/BJE

3-Methylbutyl 2-chloropropanoate $C_8H_{15}ClO_2$
(3×C–(H)$_3$(C))+(1×C–(H)(C)(CO)(Cl))+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+(2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−575.00	−551.99	−23.01	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−627.30	−594.34	−32.96	53SMI/BJE
$C_p°$ =		308.89		

3-Methylbutyl 3-chloropropanoate $C_8H_{15}ClO_2$
(1×C–(H)$_2$(C)(Cl))+(1×C–(H)$_2$(CO)(C))+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+(2×C–(H)$_3$(C))+(2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−539.40	−561.14	21.74	70COX/PIL
$C_p°$ =		213.34		
Liquid phase				
$\Delta_fH°$ =	−593.40	−622.31	28.91	53SMI/BJE
$C_p°$ =		316.01		
$S°$ =		422.82		
$\Delta_fS°$ =		−918.91		
$\Delta_fG°$ =		−348.34		
$\ln K_f$ =		140.52		

Butyl 2-chlorobutanoate $C_8H_{15}ClO_2$
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)(CO)(Cl))+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−602.60	−545.30	−57.30	70COX/PIL

Butyl 2-chlorobutanoate (Continued) $C_8H_{15}ClO_2$
(2×C–(H)$_3$(C))+(3×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)(CO)(Cl))+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−655.30	−589.06	−66.24	53SMI/BJE
$C_p°$ =		311.87		

Butyl dichloroacetate $C_6H_{10}Cl_2O_2$
(1×C–(H)(CO)(Cl)$_2$)+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))+(2×C–(H)$_2$(C)$_2$)+(1×C–(H)$_3$(C))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−497.80	−482.93	−14.87	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−550.10	−535.37	−14.73	53SMI/BJE

2-Methylpropyl dichloroacetate $C_6H_{10}Cl_2O_2$
(1×C–(H)(CO)(Cl)$_2$)+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))+(1×C–(H)(C)$_3$)+(2×C–(H)$_3$(C))+(2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−501.50	−489.62	−11.88	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−553.80	−540.65	−13.15	53SMI/BJE

3-Methylbutyl dichloroacetate $C_7H_{12}Cl_2O_2$
(1×C–(H)(CO)(Cl)$_2$)+(1×CO–(C)(O))+(1×O–(C)(CO))+(1×C–(H)$_2$(O)(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_3$)+(2×C–(H)$_3$(C))+(2×–CH$_3$ corr (tertiary))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−519.40	−510.25	−9.15	70COX/PIL
Liquid phase				
$\Delta_fH°$ =	−575.00	−566.38	−8.62	53SMI/BJE

TABLE 51. Chlorides (116) – Continued

Acetyl chloride C_2H_3ClO

$(1\times C\text{-}(H)_3(CO)) + (1\times CO\text{-}(C)(Cl))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−242.70	−242.80	0.10	31MAT/FEH
C_p° =	67.82	67.82	0.00	69STU/WES
S° =	294.85	294.85	0.00	69STU/WES
$\Delta_f S^\circ$ =		−126.50		
$\Delta_f G^\circ$ =		−205.08		
$\ln K_f$ =		82.73		
Liquid phase				
$\Delta_f H^\circ$ =	−272.80	−272.90	0.10	49CAR/SKI
C_p° =	117.15	117.15	0.00	1881REI

Dichloroacetyl chloride C_2HCl_3O

$(1\times C\text{-}(H)(CO)(Cl)_2) + (1\times CO\text{-}(C)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−241.00	−240.94	−0.06	70COX/PIL
Liquid phase				
$\Delta_f H^\circ$ =	−280.40	−280.40	0.00	50PRI/SKI

Propanoyl chloride C_3H_5ClO

$(1\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)_2(CO)(C)) + (1\times CO\text{-}(C)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−264.64		
C_p° =		92.51		
Liquid phase				
$\Delta_f H^\circ$ =		−297.04		
C_p° =	147.28	146.44	0.84	1881REI

Butanoyl chloride C_4H_7ClO

$(1\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(CO)(C)) + (1\times CO\text{-}(C)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−285.27		
C_p° =		115.40		
Liquid phase				
$\Delta_f H^\circ$ =		−322.77		
C_p° =	170.71	176.86	−6.15	1881REI

TABLE 51. Chlorides (116) – Continued

Pentanoyl chloride C_5H_9ClO

$(1\times C\text{-}(H)_3(C)) + (2\times C\text{-}(H)_2(C)_2) + (1\times C\text{-}(H)_2(CO)(C)) + (1\times CO\text{-}(C)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−305.90		
C_p° =		138.29		
Liquid phase				
$\Delta_f H^\circ$ =		−348.50		
C_p° =	187.86	207.28	−19.42	1881REI

2-Methylpropanoyl chloride C_4H_7ClO

$(2\times C\text{-}(H)_3(C)) + (1\times C\text{-}(H)(CO)(C)_2) + (1\times CO\text{-}(C)(Cl)) + (2\times\text{-}CH_3 \text{ corr (tertiary)})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−289.83		
Liquid phase				
$\Delta_f H^\circ$ =		−328.76		
C_p° =	131.80	171.04	−39.24	1881REI

Benzoyl chloride C_7H_5ClO

$(5\times C_B\text{-}(H)(C_B)_2) + (1\times C_B\text{-}(CO)(C_B)_2) + (1\times CO\text{-}(C_B)(Cl))$

	Literature	Calculated	Risidual	Reference
Liquid phase				
$\Delta_f H^\circ$ =		−165.37		
C_p° =	187.00	187.00	0.00	1881REI

Chloroacetyl chloride $C_2H_2Cl_2O$

$(1\times CO\text{-}(C)(Cl)) + (1\times C\text{-}(H)_2(CO)(Cl))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−244.80	−244.80	0.00	70COX/PIL
Liquid phase				
$\Delta_f H^\circ$ =	−283.70	−283.70	0.00	50PRI/SKI

TABLE 51. Chlorides (116) – Continued

2-Chlorobenzoyl chloride $C_7H_4Cl_2O$

$(4\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(Cl)(C_B)_2)+(1\times C_B\text{–}(CO)(C_B)_2)+(1\times CO\text{–}(C_B)(Cl))+(1\times \textit{ortho}\ \text{corr–}(Cl)(COCl))$

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−171.30	−171.30	0.00	75MOS/PRI
$C_p°$ =		199.59		

3-Chlorobenzoyl chloride $C_7H_4Cl_2O$

$(4\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(Cl)(C_B)_2)+(1\times C_B\text{–}(CO)(C_B)_2)+(1\times CO\text{–}(C_B)(Cl))$

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−189.70	−205.73	16.03	75MOS/PRI
$C_p°$ =		199.59		

4-Chlorobenzoyl chloride $C_7H_4Cl_2O$

$(4\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(Cl)(C_B)_2)+(1\times C_B\text{–}(CO)(C_B)_2)+(1\times CO\text{–}(C_B)(Cl))$

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−191.70	−205.73	14.03	75MOS/PRI
$C_p°$ =		199.59		

1,2-Phthaloyl chloride $C_8H_4Cl_2O_2$

$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(CO)(C_B)_2)+(2\times CO\text{–}(C_B)(Cl))+(1\times \textit{ortho}\ \text{corr–}(COCl)(COCl))$

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−379.70		
$C_p°$ =	248.50	248.50	0.00	1881REI

TABLE 51. Chlorides (116) – Continued

1,3-Phthaloyl chloride $C_8H_4Cl_2O_2$

$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(CO)(C_B)_2)+(2\times CO\text{–}(C_B)(Cl))+(1\times \textit{meta}\ \text{corr–}(COCl)(COCl))$

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−379.70		
$C_p°$ =		237.92		
Solid phase				
$\Delta_fH°$ =	−367.50	−367.50	0.00	73SAP/MOC

1,4-Phthaloyl chloride $C_8H_4Cl_2O_2$

$(4\times C_B\text{–}(H)(C_B)_2)+(2\times C_B\text{–}(CO)(C_B)_2)+(2\times CO\text{–}(C_B)(Cl))$

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−379.70		
$C_p°$ =		237.92		
Solid phase				
$\Delta_fH°$ =	−384.60	−383.56	−1.04	73SAP/MOC

TABLE 52. Bromides (39)

Bromomethane; Methyl bromide CH_3Br
(1×C-(H)3(Br), methyl bromide), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−37.66	−37.66	0.00	38EGA/KEM
$C_p°$ =	42.43	42.43	0.00	69STU/WES
$S°$ =	245.81	245.81	0.00	69STU/WES
$\Delta_fS°$ =		−31.90		
$\Delta_fG°$ =		−28.15		
$\ln K_f$ =		11.36		
Liquid phase				
$\Delta_fH°$ =	−61.10	−61.10	0.00	66ADA/CAR

Bromoethane C_2H_5Br
(1×C-(H)3(C))+(1×C-(H)2(C)(Br)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−64.02	−64.04	0.02	69STU/WES
$C_p°$ =	64.64	63.55	1.09	69STU/WES
$S°$ =	287.48	291.50	−4.02	69STU/WES
$\Delta_fS°$ =		−122.52		
$\Delta_fG°$ =		−27.51		
$\ln K_f$ =		11.10		
Liquid phase				
$\Delta_fH°$ =	−91.51	−90.26	−1.25	69STU/WES
$C_p°$ =	100.80	102.48	−1.68	48KUR
$S°$ =		196.30		
$\Delta_fS°$ =		−217.71		
$\Delta_fG°$ =		−25.35		
$\ln K_f$ =		10.23		

1-Bromopropane C_3H_7Br
(1×C-(H)3(C))+(1×C-(H)2(C)2)+(1×C-(H)2(C)(Br)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−87.86	−84.67	−3.19	69STU/WES
$C_p°$ =	86.44	86.44	0.00	69STU/WES
$S°$ =	330.87	330.66	0.21	69STU/WES
$\Delta_fS°$ =		−219.67		
$\Delta_fG°$ =		−19.18		
$\ln K_f$ =		7.74		
Liquid phase				
$\Delta_fH°$ =	−119.76	−115.99	−3.77	66WAD2
$C_p°$ =	130.50	132.90	−2.40	1881REI
$S°$ =		228.68		
$\Delta_fS°$ =		−321.64		
$\Delta_fG°$ =		−20.09		
$\ln K_f$ =		8.10		

TABLE 52. Bromides (39) — Continued

1-Bromobutane C_4H_9Br
(1×C-(H)3(C))+(2×C-(H)2(C)2)+(1×C-(H)2(C)(Br)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−107.10	−105.30	−1.80	66WAD2
$C_p°$ =	109.33	109.33	0.00	69STU/WES
$S°$ =	369.82	369.82	0.00	69STU/WES
$\Delta_fS°$ =		−316.82		
$\Delta_fG°$ =		−10.84		
$\ln K_f$ =		4.37		
Liquid phase				
$\Delta_fH°$ =	−143.80	−141.72	−2.08	61BJE2
$C_p°$ =	152.21	163.32	−11.11	31DEE
$S°$ =		261.06		
$\Delta_fS°$ =		−425.57		
$\Delta_fG°$ =		−14.83		
$\ln K_f$ =		5.98		

1-Bromopentane $C_5H_{11}Br$
(1×C-(H)3(C))+(3×C-(H)2(C)2)+(1×C-(H)2(C)(Br)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−129.10	−125.93	−3.17	66WAD2
$C_p°$ =	132.21	132.22	−0.01	69STU/WES
$S°$ =	408.78	408.98	−0.20	69STU/WES
$\Delta_fS°$ =		−413.97		
$\Delta_fG°$ =		−2.50		
$\ln K_f$ =		1.01		
Liquid phase				
$\Delta_fH°$ =	−170.20	−167.45	−2.75	61BJE2
$C_p°$ =	171.59	193.74	−22.15	31DEE
$S°$ =		293.44		
$\Delta_fS°$ =		−529.51		
$\Delta_fG°$ =		−9.58		
$\ln K_f$ =		3.86		

1-Bromohexane $C_6H_{13}Br$
(1×C-(H)3(C))+(4×C-(H)2(C)2)+(1×C-(H)2(C)(Br))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−148.10	−146.56	−1.54	68WAD
$C_p°$ =		155.11		
Liquid phase				
$\Delta_fH°$ =	−194.20	−193.18	−1.02	61BJE2
$C_p°$ =	203.55	224.16	−20.61	31DEE
$S°$ =	452.92	325.82	127.10	31DEE
$\Delta_fS°$ =		−633.44		
$\Delta_fG°$ =		−4.32		
$\ln K_f$ =		1.74		

TABLE 52. Bromides (39) – Continued

1-Bromoheptane $C_7H_{15}Br$
(1 × C–(H)3(C)) + (5 × C–(H)2(C)2) + (1 × C–(H)2(C)(Br))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−167.70	−167.19	−0.51	68WAD
$C_p°$ =		178.00		
Liquid phase				
$\Delta_fH°$ =	−218.40	−218.91	0.51	61BJE2
$C_p°$ =		254.58		
$S°$ =		358.20		
$\Delta_fS°$ =		−737.37		
$\Delta_fG°$ =		0.94		
$\ln K_f$ =		−0.38		

1-Bromooctane $C_8H_{17}Br$
(1 × C–(H)3(C)) + (6 × C–(H)2(C)2) + (1 × C–(H)2(C)(Br))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−189.30	−187.82	−1.48	77MAN/SEL
$C_p°$ =		200.89		
Liquid phase				
$\Delta_fH°$ =	−245.10	−244.64	−0.46	61BJE2
$C_p°$ =		285.00		
$S°$ =		390.58		
$\Delta_fS°$ =		−841.30		
$\Delta_fG°$ =		6.19		
$\ln K_f$ =		−2.50		

1-Bromododecane $C_{12}H_{25}Br$
(1 × C–(H)3(C)) + (10 × C–(H)2(C)2) + (1 × C–(H)2(C)(Br))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−269.90	−270.34	0.44	76STR3
$C_p°$ =		292.45		
Liquid phase				
$\Delta_fH°$ =	−344.70	−347.56	2.86	76STR3
$C_p°$ =		406.68		
$S°$ =		520.10		
$\Delta_fS°$ =		−1257.02		
$\Delta_fG°$ =		27.22		
$\ln K_f$ =		−10.98		

TABLE 52. Bromides (39) – Continued

1-Bromohexadecane $C_{16}H_{33}Br$
(1 × C–(H)3(C)) + (14 × C–(H)2(C)2) + (1 × C–(H)2(C)(Br))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−350.10	−352.86	2.76	76STR3
$C_p°$ =		384.01		
Liquid phase				
$\Delta_fH°$ =	−444.50	−450.48	5.98	76STR3
$C_p°$ =		528.36		
$S°$ =		649.62		
$\Delta_fS°$ =		−1672.75		
$\Delta_fG°$ =		48.25		
$\ln K_f$ =		−19.46		

1-Bromo-3-methylbutane $C_5H_{11}Br$
(2 × C–(H)3(C)) + (1 × C–(H)2(C)2) + (1 × C–(H)(C)3) + (2 × –CH3 corr (tertiary)) + (1 × C–(H)2(C)(Br))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−132.62		
$C_p°$ =		132.25		
Liquid phase				
$\Delta_fH°$ =		−172.73		
$C_p°$ =	187.00	190.76	−3.76	48KUR
$S°$ =		288.09		
$\Delta_fS°$ =		−534.86		
$\Delta_fG°$ =		−13.26		
$\ln K_f$ =		5.35		

1-Bromo-2-methylpropane C_4H_9Br
(2 × C–(H)3(C)) + (1 × C–(H)(C)3) + (2 × –CH3 corr (tertiary)) + (1 × C–(H)2(C)(Br))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−111.99		
$C_p°$ =		109.36		
Liquid phase				
$\Delta_fH°$ =		−147.00		
$C_p°$ =	154.39	160.34	−5.95	48KUR
$S°$ =		255.71		
$\Delta_fS°$ =		−430.92		
$\Delta_fG°$ =		−18.52		
$\ln K_f$ =		7.47		

TABLE 52. Bromides (39) — Continued

2-Bromopropane C_3H_7Br
(2×C–(H)$_3$(C))+(1×C–(H)(C)$_2$(Br))+
(2×–CH$_3$ corr (tertiary)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−97.10	−99.79	2.69	62ROZ/AND
$C_p°$ =	88.99	88.23	0.76	69STU/WES
$S°$ =	316.02	321.06	−5.04	69STU/WES
$\Delta_fS°$ =		−229.26		
$\Delta_fG°$ =		−31.44		
$\ln K_f$ =		12.68		
Liquid phase				
$\Delta_fH°$ =	−127.30	−126.89	−0.41	66WAD2
$C_p°$ =	132.20	132.20	0.00	1881REI

2-Bromobutane C_4H_9Br
(2×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)$_2$(Br)), σ = 9

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−120.60	−115.90	−4.70	68WAD
$C_p°$ =	110.79	111.12	−0.33	69STU/WES
$S°$ =	370.28	360.22	10.06	69STU/WES
$\Delta_fS°$ =		−326.41		
$\Delta_fG°$ =		−18.58		
$\ln K_f$ =		7.49		
Liquid phase				
$\Delta_fH°$ =	−155.10	−148.26	−6.84	61BJE
$C_p°$ =	154.40	162.62	−8.22	48KUR

2-Bromo-2-methylpropane C_4H_9Br
(3×C–(H)$_3$(C))+(3×–CH$_3$ corr (quaternary))+
(1×C–(C)$_3$(Br)), σ = 81

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−131.60	−133.20	1.60	68WAD
$C_p°$ =	116.52	116.52	0.00	69STU/WES
$S°$ =	331.96	331.96	0.00	69STU/WES
$\Delta_fS°$ =		−354.67		
$\Delta_fG°$ =		−27.45		
$\ln K_f$ =		11.07		
Liquid phase				
$\Delta_fH°$ =	−163.40	−163.40	0.00	51BRY/HOW

TABLE 52. Bromides (39) — Continued

1,2-Dibromoethane $C_2H_4Br_2$
(2×C–(H)$_2$(C)(Br)), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−37.50	−43.56	6.06	38CON/KIS
$C_p°$ =	85.35	75.64	9.71	69STU/WES
$S°$ =	329.74	340.86	−11.12	69STU/WES
$\Delta_fS°$ =		−83.98		
$\Delta_fG°$ =		−18.52		
$\ln K_f$ =		7.47		
Liquid phase				
$\Delta_fH°$ =	−79.20	−85.30	6.10	68WAD
$C_p°$ =	135.98	132.00	3.98	40PIT
$S°$ =	223.30	226.00	−2.70	40PIT
$\Delta_fS°$ =		−198.83		
$\Delta_fG°$ =		−26.02		
$\ln K_f$ =		10.50		

1,2-Dibromopropane $C_3H_6Br_2$
(1×C–(H)$_3$(C))+(1×C–(H)$_2$(C)(Br))+
(1×C–(H)(C)$_2$(Br)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−71.50	−74.79	3.29	38CON/KIS
$C_p°$ =	102.80	100.32	2.48	69STU/WES
$S°$ =	376.14	376.19	−0.05	69STU/WES
$\Delta_fS°$ =		−184.96		
$\Delta_fG°$ =		−19.64		
$\ln K_f$ =		7.92		
Liquid phase				
$\Delta_fH°$ =		−117.57		
$C_p°$ =	172.80	161.72	11.08	48KUR

1,2-Dibromobutane $C_4H_8Br_2$
(1×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(Br))+
(1×C–(H)(C)$_2$(Br)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−92.20	−95.42	3.22	38CON/KIS
$C_p°$ =	127.11	123.21	3.90	69STU/WES
$S°$ =	408.78	415.35	−6.57	69STU/WES
$\Delta_fS°$ =		−282.11		
$\Delta_fG°$ =		−11.31		
$\ln K_f$ =		4.56		
Liquid phase				
$\Delta_fH°$ =	−146.90	−143.30	−3.60	61BJE
$C_p°$ =		192.14		

TABLE 52. Bromides (39) — Continued

1,2-Dibromoheptane $C_7H_{14}Br_2$
$(1 \times C\text{-}(H)_3(C)) + (4 \times C\text{-}(H)_2(C)_2) + (1 \times C\text{-}(H)_2(C)(Br)) + (1 \times C\text{-}(H)(C)_2(Br))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−157.90	−157.31	−0.59	41LIS
C_p° =		191.88		
Liquid phase				
$\Delta_f H^\circ$ =	−212.30	−220.49	8.19	41LIS
C_p° =		283.40		

1,3-Dibromopropane $C_3H_6Br_2$
$(1 \times C\text{-}(H)_2(C)_2) + (2 \times C\text{-}(H)_2(C)(Br))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−64.19		
C_p° =		98.53		
Liquid phase				
$\Delta_f H^\circ$ =		−111.03		
C_p° =	158.99	162.42	−3.43	48KUR
S° =		258.38		
$\Delta_f S^\circ$ =		−302.76		
$\Delta_f G^\circ$ =		−20.76		
$\ln K_f$ =		8.37		

2,3-Dibromobutane $C_4H_8Br_2$
$(2 \times C\text{-}(H)_3(C)) + (2 \times C\text{-}(H)(C)_2(Br))$, $\sigma = 18$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−102.40	−106.02	3.62	38CON/KIS
C_p° =	124.56	125.00	−0.44	69STU/WES
S° =	394.97	399.99	−5.02	69STU/WES
$\Delta_f S^\circ$ =		−297.47		
$\Delta_f G^\circ$ =		−17.33		
$\ln K_f$ =		6.99		
Liquid phase				
$\Delta_f H^\circ$ =	−139.70	−149.84	10.14	36TRI
C_p° =		191.44		

TABLE 52. Bromides (39) — Continued

1,4-Dibromobutane $C_4H_8Br_2$
$(2 \times C\text{-}(H)_2(C)_2) + (2 \times C\text{-}(H)_2(C)(Br))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−87.00	−84.82	−2.18	68WAD
C_p° =		121.42		
Liquid phase				
$\Delta_f H^\circ$ =	−140.10	−136.76	−3.34	72ROZ/NES
C_p° =		192.84		
S° =		290.76		
$\Delta_f S^\circ$ =		−406.69		
$\Delta_f G^\circ$ =		−15.50		
$\ln K_f$ =		6.25		

1,3-Dibromobutane $C_4H_8Br_2$
$(1 \times C\text{-}(H)_3(C)) + (1 \times C\text{-}(H)_2(C)_2) + (1 \times C\text{-}(H)_2(C)(Br)) + (1 \times C\text{-}(H)(C)_2(Br))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =		−95.42		
C_p° =		123.21		
Liquid phase				
$\Delta_f H^\circ$ =	−147.80	−143.30	−4.50	72ROZ/NES
C_p° =		192.14		

1,2-Dibromo-2-methylpropane $C_4H_8Br_2$
$(2 \times C\text{-}(H)_3(C)) + (2 \times \text{-}CH_3 \text{ corr (quaternary)}) + (1 \times C\text{-}(C)_3(Br)) + (1 \times C\text{-}(H)_2(C)(Br))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−113.30	−108.16	−5.14	74SUN/WUL
C_p° =		128.61		
Liquid phase				
$\Delta_f H^\circ$ =	−156.60	−154.05	−2.55	74SUN/WUL

2,3-Dibromo-2-methylbutane $C_5H_{10}Br_2$
$(3 \times C\text{-}(H)_3(C)) + (1 \times C\text{-}(H)(C)_2(Br)) + (1 \times C\text{-}(C)_3(Br)) + (2 \times \text{-}CH_3 \text{ corr (quaternary)})$, $\sigma = 27$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	−138.00	−139.39	1.39	38CON/KIS
C_p° =	148.57	153.29	−4.72	69STU/WES
S° =	412.54	425.79	−13.25	69STU/WES
$\Delta_f S^\circ$ =		−407.98		
$\Delta_f G^\circ$ =		−17.75		
$\ln K_f$ =		7.16		

TABLE 52. Bromides (39) — Continued

2,3-Dibromo-2-methylbutane (Continued) $C_5H_{10}Br_2$
(3 × C–(H)$_3$(C)) + (1 × C–(H)(C)$_2$(Br)) + (1 × C–(C)$_3$(Br)) + (2 × –CH$_3$ corr (quaternary)), σ = 27

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−186.32		

1,2,3-Tribromopropane $C_3H_5Br_3$
(2 × C–(H)$_2$(C)(Br)) + (1 × C–(H)(C)$_2$(Br))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		−54.31		
$C_p°$ =		112.41		
Liquid phase				
$\Delta_fH°$ =		−112.61		
$C_p°$ =	166.52	191.24	−24.72	48KUR

Bromoethylene C_2H_3Br
(1 × C$_d$–(H)$_2$) + (1 × C$_d$–(H)(Br)), σ = 1

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	79.20	77.26	1.94	57LAC/KIA2
$C_p°$ =	55.48	55.48	0.00	69STU/WES
$S°$ =	275.43	275.43	0.00	69STU/WES
$\Delta_fS°$ =		−8.01		
$\Delta_fG°$ =		79.65		
$\ln K_f$ =		−32.13		
Liquid phase				
$C_p°$ =	107.50	107.50	0.00	34MEH2

3-Bromo-1-propene C_3H_5Br
(1 × C$_d$–(H)$_2$) + (1 × C$_d$–(H)(C)) + (1 × C–(H)$_2$(C)(Br)), σ = 1

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	49.37	40.86	8.51	69STU/WES
$C_p°$ =	77.66	77.94	−0.28	69STU/WES
$S°$ =	317.15	321.88	−4.73	69STU/WES
$\Delta_fS°$ =		−97.87		
$\Delta_fG°$ =		70.04		
$\ln K_f$ =		−28.25		

TABLE 52. Bromides (39) — Continued

3-Bromo-1-propene (Continued) C_3H_5Br
(1 × C$_d$–(H)$_2$) + (1 × C$_d$–(H)(C)) + (1 × C–(H)$_2$(C)(Br)), σ = 1

	Literature	– Calculated	= Residual	Reference
Liquid phase				
$\Delta_fH°$ =	12.20	10.15	2.05	49GEL/SKI
$C_p°$ =		118.97		
$S°$ =		227.77		
$\Delta_fS°$ =		−191.98		
$\Delta_fG°$ =		67.39		
$\ln K_f$ =		−27.18		

1-Bromo-1-propene (Z) C_3H_5Br
(1 × C–(H)$_3$(C)) + (1 × C$_d$–(H)(C)) + (1 × C$_d$–(H)(Br)) + (1 × *cis* corr–(alk)(X))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	40.80	41.00	−0.20	73ALF/GOL
$C_p°$ =		78.57		
Liquid phase				
$C_p°$ =		140.21		

1-Bromo-1-propene (E) C_3H_5Br
(1 × C–(H)$_3$(C)) + (1 × C$_d$–(H)(C)) + (1 × C$_d$–(H)(Br))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	43.90	45.00	−1.10	73ALF/GOL
$C_p°$ =		78.57		
Liquid phase				
$C_p°$ =		140.21		

1-Bromopropyne C_3H_3Br
(1 × C–(H)$_3$(C)) + (1 × C$_t$–(C)) + (1 × C$_t$–(Br)), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas phase				
$C_p°$ =	73.64	73.64	0.00	69STU/WES
$S°$ =	295.81	295.81	0.00	69STU/WES
$\Delta_fS°$ =		6.62		

TABLE 52. Bromides (39) – Continued

Bromobenzene C_6H_5Br

$(1 \times C_B\text{–}(Br)(C_B)_2) + (5 \times C_B\text{–}(H)(C_B)_2)$, $\sigma = 2$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	105.40	105.40	0.00	68WAD
$C_p°$ =	97.70	97.70	0.00	69STU/WES
$S°$ =	324.39	324.39	0.00	69STU/WES
$\Delta_f S°$ =		−112.59		
$\Delta_f G°$ =		138.97		
$\ln K_f$ =		−56.06		
Liquid phase				
$\Delta_f H°$ =	60.70	60.70	0.00	56CHE/SKI
$C_p°$ =	154.31	154.31	0.00	75MAS/SCO
$S°$ =	219.20	219.20	0.00	75MAS/SCO
$\Delta_f S°$ =		−217.77		
$\Delta_f G°$ =		125.63		
$\ln K_f$ =		−50.68		

Benzyl bromide C_7H_7Br

$(5 \times C_B\text{–}(H)(C_B)_2) + (1 \times C_B\text{–}(C)(C_B)_2) + (1 \times C\text{–}(H)_2(C_B)(Br))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	63.20	63.20	0.00	57BEN/BUS
Liquid phase				
$\Delta_f H°$ =	15.90	15.90	0.00	63ASH/CAR

1,2-Dibromocyclopentane $C_5H_8Br_2$

$(3 \times C\text{–}(H)_2(C)_2) + (2 \times C\text{–}(H)(C)_2(Br)) +$
$(1 \times \text{Cyclopentane (sub) rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−54.90	−63.84	8.94	41LIS
$C_p°$ =		114.34		
Liquid phase				
$\Delta_f H°$ =	−102.70	−108.22	5.52	41LIS
$C_p°$ =		186.42		

TABLE 52. Bromides (39) – Continued

1,2-Dibromocyclohexane $C_6H_{10}Br_2$

$(4 \times C\text{–}(H)_2(C)_2) + (2 \times C\text{–}(H)(C)_2(Br)) +$
$(1 \times \text{Cyclohexane (sub) rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−114.80	−104.41	−10.39	41LIS
$C_p°$ =		142.28		
Liquid phase				
$\Delta_f H°$ =	−162.80	−159.60	−3.20	41LIS
$C_p°$ =		213.95		

1,2-Dibromocycloheptane $C_7H_{12}Br_2$

$(5 \times C\text{–}(H)_2(C)_2) + (2 \times C\text{–}(H)(C)_2(Br)) + (1 \times \text{Cycloheptane rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−105.60	−98.31	−7.29	41LIS
$C_p°$ =		150.85		
Liquid phase				
$\Delta_f H°$ =	−157.70	−159.77	2.07	41LIS
$C_p°$ =		238.39		

1,2-Dibromocyclooctane $C_8H_{14}Br_2$

$(6 \times C\text{–}(H)_2(C)_2) + (2 \times C\text{–}(H)(C)_2(Br)) + (1 \times \text{Cyclooctane rsc})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−118.70	−104.63	−14.07	41LIS
$C_p°$ =		167.71		
Liquid phase				
$\Delta_f H°$ =	−173.30	−170.90	−2.40	41LIS
$C_p°$ =		273.12		

4-Bromobenzoic acid $C_7H_5BrO_2$

$(4 \times C_B\text{–}(H)(C_B)_2) + (1 \times C_B\text{–}(Br)(C_B)_2) + (1 \times O\text{–}(H)(CO)) +$
$(1 \times CO\text{–}(O)(C_B)) + (1 \times C_B\text{–}(CO)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−272.00	−272.21	0.21	87FER/PIL
Liquid phase				
$\Delta_f H°$ =		−362.60		
$C_p°$ =		222.00		

TABLE 52. Bromides (39) — Continued

4-Bromobenzoic acid (Continued) $C_7H_5BrO_2$

$(4\times C_B\text{–}(H)(C_B)_2)+(1\times C_B\text{–}(Br)(C_B)_2)+(1\times O\text{–}(H)(CO))+(1\times CO\text{–}(O)(C_B))+(1\times C_B\text{–}(CO)(C_B)_2)$

	Literature	Calculated	Residual	Reference
Solid phase				
$\Delta_fH°$ =	−379.60	−379.38	−0.22	87FER/PIL
$S°$ =		199.44		
$\Delta_fS°$ =		−448.32		
$\Delta_fG°$ =		−245.71		
$\ln K_f$ =		99.12		

Acetyl bromide C_2H_3BrO

$(1\times C\text{–}(H)_3(CO))+(1\times CO\text{–}(C)(Br))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−190.80	−190.80	0.00	26MAT
Liquid phase				
$\Delta_fH°$ =	−223.90	−223.10	−0.80	49CAR/SKI

TABLE 53. Iodides (39)

Iodomethane; Methyl iodide CH_3I

$(1\times C\text{–}(H)_3(I)$, methyl iodide), $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	14.30	14.30	0.00	65GOL/WAL
$C_p°$ =	44.14	44.14	0.00	69STU/WES
$S°$ =	254.01	254.01	0.00	69STU/WES
$\Delta_fS°$ =		−5.66		
$\Delta_fG°$ =		15.99		
$\ln K_f$ =		−6.45		
Liquid phase				
$\Delta_fH°$ =	−11.70	−11.70	0.00	61CAR/CAR
$C_p°$ =	82.76	82.76	0.00	62LOW/MOE

Iodoethane C_2H_5I

$(1\times C\text{–}(H)_3(C))+(1\times C\text{–}(H)_2(C)(I))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−7.50	−8.72	1.22	68WAD
$C_p°$ =	65.94	66.67	−0.73	69STU/WES
$S°$ =	296.31	295.97	0.34	69STU/WES
$\Delta_fS°$ =		−100.01		
$\Delta_fG°$ =		21.10		
$\ln K_f$ =		−8.51		
Liquid phase				
$\Delta_fH°$ =	−39.50	−43.47	3.97	65ASH/CAR
$C_p°$ =	115.10	101.84	13.26	48KUR

1-Iodopropane C_3H_7I

$(1\times C\text{–}(H)_3(C))+(1\times C\text{–}(H)_2(C)_2)+(1\times C\text{–}(H)_2(C)(I))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−30.84	−29.35	−1.49	69FUR/GOL
$C_p°$ =	89.87	89.56	0.31	69STU/WES
$S°$ =	336.06	335.13	0.93	69STU/WES
$\Delta_fS°$ =		−197.16		
$\Delta_fG°$ =		29.43		
$\ln K_f$ =		−11.87		
Liquid phase				
$\Delta_fH°$ =	−67.04	−69.20	2.16	68WAD
$C_p°$ =	126.80	132.26	−5.46	1881REI

TABLE 53. Iodides (39) – Continued

1-Iodo-3-methylbutane $C_5H_{11}I$

(2×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)$_2$) + (1×C–(H)(C)$_3$) + (2×–CH$_3$ corr (tertiary)) + (1×C–(H)$_2$(C)(I))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		–77.30		
$C_p°$ =		135.37		
Liquid phase				
$\Delta_f H°$ =		–125.94		
$C_p°$ =	178.70	190.12	–11.42	48KUR

1-Iodo-2-methylpropane C_4H_9I

(2×C–(H)$_3$(C)) + (1×C–(H)(C)$_3$) + (2×–CH$_3$ corr (tertiary)) + (1×C–(H)$_2$(C)(I))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =		–56.67		
$C_p°$ =		112.48		
Liquid phase				
$\Delta_f H°$ =		–100.21		
$C_p°$ =	163.32	159.70	3.62	48KUR

2-Iodopropane C_3H_9I

(2×C–(H)$_3$(C)) + (1×C–(H)(C)$_2$(I)) + (2×–CH$_3$ corr (tertiary)), σ = 9

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	–39.50	–40.30	0.80	69FUR/GOL
$C_p°$ =	90.08	90.08	0.00	69STU/WES
$S°$ =	324.47	324.47	0.00	69STU/WES
$\Delta_f S°$ =		–338.39		
$\Delta_f G°$ =		60.59		
$\ln K_f$ =		–24.44		
Liquid phase				
$\Delta_f H°$ =	–73.60	–74.80	1.20	68WAD

TABLE 53. Iodides (39)

2-Iodo-2-methylpropane C_4H_9I

(3×C–(H)$_3$(C)) + (3×–CH$_3$ corr (quaternary)) + (1×C–(C)$_3$(I)), σ = 81

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	–72.00	–72.00	0.00	62BEN/AMA2
$C_p°$ =	118.28	118.28	0.00	69STU/WES
$S°$ =	342.21	342.21	0.00	69STU/WES
$\Delta_f S°$ =		–326.39		
$\Delta_f G°$ =		25.31		
$\ln K_f$ =		–10.21		
Liquid phase				
$\Delta_f H°$ =	–107.40	–107.40	0.00	68WAD

1,2-Diiodoethane $C_2H_4I_2$

(2×C–(H)$_2$(C)(I)), σ = 2

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	66.80	67.08	–0.28	54ABR/DAV
$C_p°$ =	82.30	81.88	0.42	69STU/WES
$S°$ =	348.53	349.80	–1.27	69STU/WES
$\Delta_f S°$ =		–38.97		
$\Delta_f G°$ =		78.70		
$\ln K_f$ =		–31.75		
Liquid phase				
$\Delta_f H°$ =	1.10	8.28	–7.18	54ABR/DAV
$C_p°$ =		130.72		

1,2-Diiodopropane $C_3H_6I_2$

(1×C–(H)$_3$(C)) + (1×C–(H)$_2$(C)(I)) + (1×C–(H)(C)$_2$(I)), σ = 3

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_f H°$ =	35.60	40.02	–4.42	62BEN/AMA
$C_p°$ =	103.64	105.29	–1.65	69STU/WES
$S°$ =	395.81	384.07	11.74	69STU/WES
$\Delta_f S°$ =		–141.01		
$\Delta_f G°$ =		82.06		
$\ln K_f$ =		–33.10		
Liquid phase				
$\Delta_f H°$ =		–18.69		

TABLE 53. Iodides (39) — Continued

1,2-Diiodobutane $C_4H_8I_2$
(1×C–(H)$_3$(C))+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)$_2$(C)(I))+(1×C–(H)(C)$_2$(I)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	12.30	19.39	−7.09	37CLI/KIS
C_p° =	127.95	128.18	−0.23	69STU/WES
$S°$ =	425.93	423.23	2.70	69STU/WES
$\Delta_fS°$ =		−238.16		
$\Delta_fG°$ =		90.40		
$\ln K_f$ =		−36.47		
Liquid phase				
$\Delta_fH°$ =		−44.42		

3-Iodo-1-propene C_3H_5I
(1×C$_d$–(H)$_2$)+(1×C$_d$–(H)(C))+(1×C–(H)$_2$(C)(I)), σ = 1

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	93.10	96.18	−3.08	66ROD/GOL
C_p° =	82.63	81.06	1.57	69STU/WES
$S°$ =	319.91	326.35	−6.44	69STU/WES
$\Delta_fS°$ =		−75.37		
$\Delta_fG°$ =		118.65		
$\ln K_f$ =		−47.86		
Liquid phase				
$\Delta_fH°$ =	55.23	56.94	−1.71	49GEL/SKI
C_p° =		118.33		

1-Iodo-1-propene (Z) C_3H_5I
(1×C–(H)$_3$(C))+(1×C$_d$–(H)(C))+(1×C$_d$–(H)(I))+(1×*cis* corr-(alk)(X))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	86.40	92.42	−6.02	73ALF/GOL
C_p° =		81.29		

1-Iodo-1-propene (E) C_3H_5I
(1×C–(H)$_3$(C))+(1×C$_d$–(H)(C))+(1×C$_d$–(H)(I))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	93.10	96.42	−3.32	73ALF/GOL
C_p° =		81.29		

TABLE 53. Iodides (39) — Continued

1,2-Diiodoethylene (Z) $C_2H_2I_2$
(2×C$_d$–(H)(I))+(1×*cis* corr-(X)(X)), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	207.40	200.72	6.68	68FUR/GOL
C_p° =		73.64		
$S°$ =		333.14		
$\Delta_fS°$ =		74.95		
$\Delta_fG°$ =		178.37		
$\ln K_f$ =		−71.96		

1,2-Diiodoethylene (E) $C_2H_2I_2$
(2×C$_d$–(H)(I)), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	207.40	204.72	2.68	68FUR/GOL
C_p° =		73.64		
$S°$ =		333.14		
$\Delta_fS°$ =		74.95		
$\Delta_fG°$ =		182.37		
$\ln K_f$ =		−73.57		

1-Iodopropyne C_3H_3I
(1×C–(H)$_3$(C))+(1×C$_t$–(C))+(1×C$_t$–(I)), σ = 3

	Literature	Calculated	Residual	Reference
Gas phase				
C_p° =	74.48	74.48	0.00	69STU/WES
$S°$ =	302.92	302.92	0.00	69STU/WES
$\Delta_fS°$ =		31.77		

Iodobenzene C_6H_5I
(1×C$_B$–(I)(C$_B$)$_2$)+(5×C$_B$–(H)(C$_B$)$_2$), σ = 2

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	164.85	163.55	1.30	70COX/PIL
C_p° =	100.75	100.75	0.00	69STU/WES
$S°$ =	334.05	334.05	0.00	69STU/WES
$\Delta_fS°$ =		−84.89		
$\Delta_fG°$ =		188.86		
$\ln K_f$ =		−76.18		
Liquid phase				
$\Delta_fH°$ =	117.15	114.50	2.65	56SMI
C_p° =	158.57	158.57	0.00	37STU
$S°$ =	205.43	205.43	0.00	37STU
$\Delta_fS°$ =		−213.51		
$\Delta_fG°$ =		178.16		
$\ln K_f$ =		−71.87		

TABLE 53. Iodides (39) – Continued

Benzyl iodide C_7H_7I

$(5\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(C)(C_B)_2)+(1\times C\text{-}(H)_2(C_B)(I))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	100.00	100.00	0.00	57BEN/BUS
Liquid phase				
$\Delta_f H^\circ$ =	52.72	52.72	0.00	63ASH/CAR

1-Iodo-2-methylbenzene C_7H_7I

$(1\times C_B\text{-}(I)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(C)(C_B)_2)+(1\times C\text{-}(H)_3(C))+(1\times \textit{ortho}\text{ corr-(alk)(X)})$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	132.80	133.63	−0.83	70COX/PIL
C_p° =		122.62		
Liquid phase				
$\Delta_f H^\circ$ =	78.40	84.19	−5.79	56SMI
C_p° =		182.47		
S° =		240.36		
$\Delta_f S^\circ$ =		−314.89		
$\Delta_f G^\circ$ =		178.07		
$\ln K_f$ =		−71.83		

1-Iodo-3-methylbenzene C_7H_7

$(1\times C_B\text{-}(I)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(C)(C_B)_2)+(1\times C\text{-}(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	133.60	131.12	2.48	70COX/PIL
C_p° =		122.62		
Liquid phase				
$\Delta_f H^\circ$ =	79.20	77.89	1.31	56SMI
C_p° =		182.47		
S° =		240.36		
$\Delta_f S^\circ$ =		−314.89		
$\Delta_f G^\circ$ =		171.77		
$\ln K_f$ =		−69.29		

1-Iodo-4-methylbenzene C_7H_7I

$(1\times C_B\text{-}(I)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(C)(C_B)_2)+(1\times C\text{-}(H)_3(C))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	121.90	131.12	−9.22	70COX/PIL
C_p° =		122.62		

1-Iodo-4-methylbenzene (Continued) C_7H_7I

$(1\times C_B\text{-}(I)(C_B)_2)+(4\times C_B\text{-}(H)(C_B)_2)+(1\times C_B\text{-}(C)(C_B)_2)+(1\times C\text{-}(H)_3(C))$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_f H^\circ$ =	67.50	77.89	−10.39	56SMI
C_p° =		182.47		
S° =		240.36		
$\Delta_f S^\circ$ =		−314.89		
$\Delta_f G^\circ$ =		171.77		
$\ln K_f$ =		−69.29		

1-Iodonaphthalene $C_{10}H_7I$

$(1\times C_B\text{-}(I)(C_B)_2)+(7\times C_B\text{-}(H)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	233.90	231.37	2.53	70COX/PIL
C_p° =		127.97		
Liquid phase				
$\Delta_f H^\circ$ =	161.50	162.48	−0.98	56SMI
C_p° =		222.97		
S° =		252.09		
$\Delta_f S^\circ$ =		−320.38		
$\Delta_f G^\circ$ =		258.00		
$\ln K_f$ =		−104.08		
Solid phase				
$\Delta_f H^\circ$ =		144.31		
C_p° =		185.59		

2-Iodonaphthalene $C_{10}H_7I$

$(1\times C_B\text{-}(I)(C_B)_2)+(7\times C_B\text{-}(H)(C_B)_2)+(2\times C_{BF}\text{-}(C_{BF})(C_B)_2)$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H^\circ$ =	235.15	231.37	3.78	70COX/PIL
C_p° =		127.97		
Liquid phase				
$\Delta_f H^\circ$ =		162.48		
C_p° =		222.97		
S° =		252.09		
$\Delta_f S^\circ$ =		−320.38		
$\Delta_f G^\circ$ =		258.00		
$\ln K_f$ =		−104.08		
Solid phase				
$\Delta_f H^\circ$ =	144.35	144.31	0.04	56SMI
C_p° =		185.59		

TABLE 53. Iodides (39) – Continued

1,2-Diiodobenzene $C_6H_4I_2$
$(4 \times C_B-(H)(C_B)_2) + (2 \times C_B-(I)(C_B)_2) +$
$(1 \times$ *ortho* corr-(I)(I)), $\sigma = 2$

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	251.88	251.80	0.08	70COX/PIL
$C_p°$ =		119.84		
$S°$ =		384.00		
$\Delta_fS°$ =		–27.73		
$\Delta_fG°$ =		260.07		
$\ln K_f$ =		–104.91		
Liquid phase				
$\Delta_fH°$ =	187.00	187.00	0.00	56SMI2
$C_p°$ =		181.06		
$S°$ =		237.64		
$\Delta_fS°$ =		–174.08		
$\Delta_fG°$ =		238.90		
$\ln K_f$ =		–96.37		
Solid phase				
$\Delta_fH°$ =	172.40	172.42	–0.02	56SMI
$C_p°$ =		160.68		

1,3-Diiodobenzene $C_6H_4I_2$
$(4 \times C_B-(H)(C_B)_2) + (2 \times C_B-(I)(C_B)_2) + (1 \times$ *meta* corr-(I)(I))

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =		244.24		
$C_p°$ =		119.84		
Liquid phase				
$\Delta_fH°$ =		180.04		
$C_p°$ =		181.06		
$S°$ =		237.64		
$\Delta_fS°$ =		–174.08		
$\Delta_fG°$ =		231.94		
$\ln K_f$ =		–93.56		
Solid phase				
$\Delta_fH°$ =	187.00	187.00	0.00	56SMI
$C_p°$ =		160.68		

TABLE 53. Iodides (39) – Continued

1,4-Diiodobenzene $C_6H_4I_2$
$(4 \times C_B-(H)(C_B)_2) + (2 \times C_B-(I)(C_B)_2)$

	Literature	Calculated	– Residual	Reference
Gas phase				
$\Delta_fH°$ =		244.24		
$C_p°$ =		119.84		
Liquid phase				
$\Delta_fH°$ =		180.04		
$C_p°$ =		181.06		
$S°$ =		237.64		
$\Delta_fS°$ =		–174.08		
$\Delta_fG°$ =		231.94		
$\ln K_f$ =		–93.56		
Solid phase				
$\Delta_fH°$ =	160.70	166.92	–6.22	56SMI
$C_p°$ =		160.68		

Iodocyclohexane $C_6H_{11}I$
$(5 \times C-(H)_2(C)_2) + (1 \times C-(H)(C)_2(I)) +$
$(1 \times$ Cyclohexane (sub) rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	–50.00	–54.80	4.80	56BRE/UBB
$C_p°$ =		130.25		
Liquid phase				
$\Delta_fH°$ =	–97.20	–105.93	8.73	56SMI

1,3-Diiodocyclobutane(*cis/trans*) $C_4H_6I_2$
$(2 \times C-(H)_2(C)_2) + (2 \times C-(H)(C)_2(I)) + (1 \times$ Cyclobutane rsc)

	Literature	– Calculated	= Residual	Reference
Gas phase				
$\Delta_fH°$ =	193.30	167.11	26.19	73SUN/WUL
$C_p°$ =		103.68		
Liquid phase				
$\Delta_fH°$ =	134.70	104.74	29.96	73SUN/WUL

TABLE 53. Iodides (39) – Continued

2-Iodophenol C_6H_5IO

$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(I)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times O-(H)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−15.31		
$C_p°$ =		121.16		
Liquid phase				
$\Delta_fH°$ =		−91.02		
$C_p°$ =		220.24		
$S°$ =		209.86		
$\Delta_fS°$ =		−311.60		
$\Delta_fG°$ =		1.88		
$\ln K_f$ =		−0.76		
Solid phase				
$\Delta_fH°$ =	−95.80	−101.73	5.93	56SMI
$C_p°$ =		149.56		

3-Iodophenol C_6H_5IO

$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(I)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times O-(H)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−15.31		
$C_p°$ =		121.16		
Liquid phase				
$\Delta_fH°$ =		−91.02		
$C_p°$ =		220.24		
$S°$ =		209.86		
$\Delta_fS°$ =		−311.60		
$\Delta_fG°$ =		1.88		
$\ln K_f$ =		−0.76		
Solid phase				
$\Delta_fH°$ =	−94.50	−101.73	7.23	56SMI
$C_p°$ =		149.56		

4-Iodophenol C_6H_5IO

$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(I)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times O-(H)(C_B))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−15.31		
$C_p°$ =		121.16		

TABLE 53. Iodides (39) – Continued

4-Iodophenol (Continued) C_6H_5IO

$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(I)(C_B)_2)+(1\times C_B-(O)(C_B)_2)+(1\times O-(H)(C_B))$

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−91.02		
$C_p°$ =		220.24		
$S°$ =		209.86		
$\Delta_fS°$ =		−311.60		
$\Delta_fG°$ =		1.88		
$\ln K_f$ =		−0.76		
Solid phase				
$\Delta_fH°$ =	−95.40	−101.73	6.33	56SMI
$C_p°$ =		149.56		

3-Iodopropanoic acid $C_3H_5IO_2$

$(1\times O-(H)(CO))+(1\times CO-(C)(O))+(1\times C-(H)_2(CO)(C))+(1\times C-(H)_2(C)(I))$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−379.84		
$C_p°$ =		106.42		
Liquid phase				
$\Delta_fH°$ =		−455.01		
$C_p°$ =		177.45		
Solid phase				
$\Delta_fH°$ =	−460.00	−460.00	0.00	44ROT

2-Iodobenzoic acid $C_7H_5IO_2$

$(4\times C_B-(H)(C_B)_2)+(1\times C_B-(I)(C_B)_2)+(1\times O-(H)(CO))+(1\times CO-(O)(C_B))+(1\times C_B-(CO)(C_B)_2)+(1\times$ *ortho* corr-(I)(COOH))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−214.06		
Liquid phase				
$\Delta_fH°$ =		−308.80		
$C_p°$ =		226.26		
Solid phase				
$\Delta_fH°$ =	−302.30	−302.48	0.18	56SMI
$C_p°$ =		166.06		

TABLE 53. Iodides (39) – Continued

3-Iodobenzoic acid $C_7H_5IO_2$

(4×C_B–(H)(C_B)$_2$)+(1×C_B–(I)(C_B)$_2$)+(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO)(C_B)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−214.06		
Liquid phase				
$\Delta_f H°$ =		−308.80		
$C_p°$ =		226.26		
Solid phase				
$\Delta_f H°$ =	−316.90	−322.48	5.58	56SMI
$C_p°$ =		166.06		

4-Iodobenzoic acid $C_7H_5IO_2$

(4×C_B–(H)(C_B)$_2$)+(1×C_B–(I)(C_B)$_2$)+(1×O–(H)(CO))+(1×CO–(O)(C_B))+(1×C_B–(CO)(C_B)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−228.20	−214.06	−14.14	70COX/PIL
Liquid phase				
$\Delta_f H°$ =		−308.80		
$C_p°$ =		226.26		
Solid phase				
$\Delta_f H°$ =	−316.10	−322.48	6.38	56SMI
$C_p°$ =		166.06		

Methyl 2-iodobenzoate $C_8H_7IO_2$

(4×C_B–(H)(C_B)$_2$)+(1×C_B–(I)(C_B)$_2$)+(1×C_B–(CO)(C_B)$_2$)+(1×CO–(O)(C_B))+(1×O–(C)(CO))+(1×C–(H)$_3$(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−190.89		
Liquid phase				
$\Delta_f H°$ =	−243.10	−266.79	23.69	56SMI
$C_p°$ =		244.50		

TABLE 53. Iodides (39) – Continued

Methyl 3-iodobenzoate $C_8H_7IO_2$

(4×C_B–(H)(C_B)$_2$)+(1×C_B–(I)(C_B)$_2$)+(1×C_B–(CO)(C_B)$_2$)+(1×CO–(O)(C_B))+(1×O–(C)(CO))+(1×C–(H)$_3$(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−190.89		
Liquid phase				
$\Delta_f H°$ =		−266.79		
$C_p°$ =		244.50		
Solid phase				
$\Delta_f H°$ =	−278.30	−297.67	19.37	56SMI
$C_p°$ =		182.91		

Methyl 4-iodobenzoate $C_8H_7IO_2$

(4×C_B–(H)(C_B)$_2$)+(1×C_B–(I)(C_B)$_2$)+(1×C_B–(CO)(C_B)$_2$)+(1×CO–(O)(C_B))+(1×O–(C)(CO))+(1×C–(H)$_3$(O))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =		−190.89		
Liquid phase				
$\Delta_f H°$ =		−266.79		
$C_p°$ =		244.50		
Solid phase				
$\Delta_f H°$ =	−286.60	−297.67	11.07	56SMI
$C_p°$ =		182.91		

Acetyl iodide C_2H_3IO

(1×C–(H)$_3$(CO))+(1×CO–(C)(I))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_f H°$ =	−126.20	−126.20	0.00	70COX/PIL
Liquid phase				
$\Delta_f H°$ =	−164.70	−164.70	0.00	49CAR/SKI

TABLE 54. Mixed Halogen Compounds (18)

1-Chloro-1-fluoroethane C_2H_4ClF
(1×C–(H)$_3$(C))+(1×C–(H)(C)(Cl)(F))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−313.40	−313.40	0.00	73KOL/PAP

1,1,1-Trifluoro-2-iodoethane $C_2H_2F_3I$
(1×C–(C)(F)$_3$)+(1×C–(H)$_2$(C)(I))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−644.50	−640.27	−4.23	74WU/ROD
$C_p°$ =		93.93		

1,2-Dibromo-1,2-dichloroethane $C_2H_2Br_2Cl_2$
(2×C–(H)(C)(Br)(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−36.90	−36.90	0.00	39MUL/SCH
$C_p°$ =		103.76		

3,3-Dichloro-1,1,1-trifluoropropane $C_3H_3Cl_2F_3$
(1×C–(C)(F)$_3$)+(1×C–(H)$_2$(C)$_2$)+(1×C–(H)(C)(Cl)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−803.50	−773.54	−29.96	72KOL/SLA3
$C_p°$ =		126.57		
Liquid phase				
$\Delta_fH°$ =	−837.40	−837.40	0.00	72KOL/SLA3
$C_p°$ =	191.29	188.62	2.67	72KOL/VOR
$S°$ =	295.06	296.39	−1.33	72KOL/VOR
$\Delta_fS°$ =		−443.68		
$\Delta_fG°$ =		−705.12		
$\ln K_f$ =		284.44		

1-Chloro-1,1,3,3,3-pentafluoropropane $C_3H_2ClF_5$
(1×C–(C)(Cl)(F)$_2$)+(1×C–(H)$_2$(C)$_2$)+(1×C–(C)(F)$_3$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−1154.00	−1157.14	3.14	73SLA/KOL
$C_p°$ =		133.20		

TABLE 54. Mixed Halogen Compounds (18) – Continued

1-Chloro-1,1,3,3,3-pentafluoropropane $C_3H_2ClF_5$
(1×C–(C)(Cl)(F)$_2$)+(1×C–(H)$_2$(C)$_2$)+(1×C–(C)(F)$_3$)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−1180.90	−1200.80	19.90	73SLA/KOL
$C_p°$ =	196.48	187.24	9.24	74VOR/KOL
$S°$ =	311.62	306.25	5.37	74VOR/KOL
$\Delta_fS°$ =		−459.73		
$\Delta_fG°$ =		−1063.73		
$\ln K_f$ =		429.10		

1,2-Dibromotetrafluoroethane $C_2Br_2F_4$
(2×C–(C)(Br)(F)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−789.10	−789.10	0.00	56LAC/CAS
Liquid phase				
$C_p°$ =	170.79	170.80	−0.01	82KOS/ZHO
$S°$ =	299.41	299.40	0.01	82KOS/ZHO
$\Delta_fS°$ =		−269.65		

1,2-Dichlorotetrafluoroethane $C_2Cl_2F_4$
(2×C–(C)(Cl)(F)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−925.40	−925.40	0.00	82PAP/KOL
$C_p°$ =		114.64		
Liquid phase				
$\Delta_fH°$ =	−939.70	−932.00	−7.70	37PER
$C_p°$ =	164.01	167.28	−3.27	81KOL/KOS
$S°$ =	282.00	276.62	5.38	81KOL/KOS
$\Delta_fS°$ =		−363.20		
$\Delta_fG°$ =		−823.71		
$\ln K_f$ =		332.28		

1,1,2-Trichloro-1,2,2-trifluoroethane $C_2Cl_3F_3$
(1×C–(C)(Cl)$_2$(F))+(1×C–(C)(Cl)(F)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−777.30	−785.24	7.94	68KOL/TAL

TABLE 54. Mixed halogen compounds (18) — Continued

1,1,2-Trichloro-1,2,2-trifluoroethane (Continued) $C_2Cl_3F_3$
(1 × C–(C)(Cl)$_2$(F)) + (1 × C–(C)(Cl)(F)$_2$)

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =	−805.80	−809.87	4.07	63HIR/HIL
$C_p°$ =	172.80	172.93	−0.13	81KOL/KOS
$S°$ =	289.53	280.02	9.51	81KOL/KOS
$\Delta_fS°$ =		−369.94		
$\Delta_fG°$ =		−699.57		
$\ln K_f$ =		282.20		

1-Chloro-1,1-difluoroethane $C_2H_3ClF_2$
(1 × C–(H)$_3$(C)) + (1 × C–(C)(Cl)(F)$_2$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−504.96		
$C_p°$ =		83.05		
Liquid phase				
$\Delta_fH°$ =		−513.61		
$C_p°$ =	131.40	120.12	11.28	42REI
$S°$ =		221.61		
$\Delta_fS°$ =		−299.89		
$\Delta_fG°$ =		−424.20		
$\ln K_f$ =		171.12		

1,2-Difluorotetrachloroethane $C_2Cl_4F_2$
(2 × C–(C)(Cl)$_2$(F))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−645.08		
Liquid phase				
$\Delta_fH°$ =		−687.74		
$C_p°$ =	178.57	178.58	−0.01	78KIS/SUG
$S°$ =	283.42	283.42	0.00	78KIS/SUG
$\Delta_fS°$ =		−376.69		
$\Delta_fG°$ =		−575.43		
$\ln K_f$ =		232.12		

1-Bromo-2-chloroethane C_2H_4BrCl
(1 × C–(H)$_2$(C)(Cl)) + (1 × C–(H)$_2$(C)(Br))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−91.23		
$C_p°$ =		75.35		

TABLE 54. Mixed halogen compounds (18) — Continued

1-Bromo-2-chloroethane (Continued) C_2H_4BrCl
(1 × C–(H)$_2$(C)(Cl)) + (1 × C–(H)$_2$(C)(Br))

	Literature	Calculated	Residual	Reference
Liquid phase				
$\Delta_fH°$ =		−129.55		
$C_p°$ =	130.12	129.76	0.36	39RAI
$S°$ =		217.27		
$\Delta_fS°$ =		−242.94		
$\Delta_fG°$ =		−57.12		
$\ln K_f$ =		23.04		

1,1,1-Trichloro-3,3,3-trifluoropropane $C_3H_2Cl_3F_3$
(1 × C–(H)$_2$(C)$_2$) + (1 × C–(C)(Cl)$_3$) + (1 × C–(C)(F)$_3$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−776.42		
$C_p°$ =		144.06		
Liquid phase				
$\Delta_fH°$ =		−847.73		
$C_p°$ =	199.91	205.80	−5.89	71KOL/VOR
$S°$ =	311.42	313.85	−2.43	71KOL/VOR
$\Delta_fS°$ =		−472.42		
$\Delta_fG°$ =		−706.88		
$\ln K_f$ =		285.15		

1-Chloro-3,3,3-trifluoropropane $C_3H_4ClF_3$
(1 × C–(H)$_2$(C)(Cl)) + (1 × C–(H)$_2$(C)$_2$) + (1 × C–(C)(F)$_3$)

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−763.89		
$C_p°$ =		113.41		
Liquid phase				
$\Delta_fH°$ =		−821.70		
$C_p°$ =	171.08	167.36	3.72	74KOL/VOR
$S°$ =	271.67	272.21	−0.54	74KOL/VOR
$\Delta_fS°$ =		−421.66		
$\Delta_fG°$ =		−695.98		
$\ln K_f$ =		280.75		

TABLE 54. Mixed halogen compounds (18) – Continued

Chlorotrifluoroethylene C_2ClF_3

$(1\times C_d\text{–}(F)_2)+(1\times C_d\text{–}(Cl)(F))$, $\sigma = 3$

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−565.00	−565.00	0.00	63KOL/ZEN
$C_p°$ =	83.93	83.93	0.00	53MAN/ACQ
$S°$ =	322.11	322.11	0.00	53MAN/ACQ
$\Delta_fS°$ =		−104.88		
$\Delta_fG°$ =		−533.73		
$\ln K_f$ =		215.30		

Chloropentafluorobenzene C_6ClF_5

$(1\times C_B\text{–}(Cl)(C_B)_2)+(5\times C_B\text{–}(F)(C_B)_2)+(4\times$ *ortho* corr-(F)(F)) + (2 × *ortho* corr-(F)(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−810.00	−812.73	2.73	69COX/GUN
$C_p°$ =		159.83		
Liquid phase				
$\Delta_fH°$ =	−850.77	−851.20	0.43	69COX/GUN
$C_p°$ =	221.42	220.72	0.70	68AND/COU2
$S°$ =	300.70	326.42	−25.72	68AND/COU2
$\Delta_fS°$ =		−326.21		
$\Delta_fG°$ =		−753.94		
$\ln K_f$ =		304.13		

Bromopentafluorobenzene C_6BrF_5

$(1\times C_B\text{–}(Br)(C_B)_2)+(5\times C_B\text{–}(F)(C_B)_2)+(4\times$ *ortho* corr-(F)(F)) + (2 × *ortho* corr-(F)(Br))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−711.60	−711.85	0.25	77KRE/PRI
$C_p°$ =		160.15		
Liquid phase				
$\Delta_fH°$ =	−754.65	−754.90	0.25	77KRE/PRI
$C_p°$ =		226.36		
$S°$ =		345.80		
$\Delta_fS°$ =		−271.45		
$\Delta_fG°$ =		−673.97		
$\ln K_f$ =		271.87		

TABLE 54. Mixed halogen compounds (18) – Continued

Iodopentafluorobenzene C_6IF_5

$(1\times C_B\text{–}(I)(C_B)_2)+(5\times C_B\text{–}(F)(C_B)_2)+(4\times$ *ortho* corr-(F)(F)) + (2 × *ortho* corr-(F)(I))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =	−557.30	−557.40	0.10	74KRE/PRI
$C_p°$ =		163.20		
Liquid phase				
$\Delta_fH°$ =	−615.20	−615.20	0.00	74KRE/PRI
$C_p°$ =		230.62		
$S°$ =		332.03		
$\Delta_fS°$ =		−267.19		
$\Delta_fG°$ =		−535.54		
$\ln K_f$ =		216.03		

1,3,5-Trichloro-2,4,6-trifluorobenzene $C_6Cl_3F_3$

$(3\times C_B\text{–}(F)(C_B)_2)+(3\times C_B\text{–}(Cl)(C_B)_2)+(3\times$ *meta* corr-(F)(F)) + (3 × *meta* corr-(Cl)(Cl)) + (6 × *ortho* corr-(F)(Cl))

	Literature	Calculated	Residual	Reference
Gas phase				
$\Delta_fH°$ =		−528.87		
$C_p°$ =		166.29		
Liquid phase				
$\Delta_fH°$ =		−511.20		
$C_p°$ =		217.08		
$S°$ =		328.98		
$\Delta_fS°$ =		−343.94		
$\Delta_fG°$ =		−408.65		
$\ln K_f$ =		164.85		
Solid phase				
$\Delta_fH°$ =		−523.50		
$C_p°$ =	197.95	196.80	1.15	73AND/MAR2
$S°$ =	245.35	249.48	−4.13	73AND/MAR2
$\Delta_fS°$ =		−423.44		
$\Delta_fG°$ =		−397.25		
$\ln K_f$ =		160.25		

TABLE 55. Summary of residuals for C–H–N–O–S–Halogen families

This table provides information on how well agreement was achieved between literature and estimated values for values of $\Delta_f H°$(in kJ/mol), $C_p°$, and $S°$(in J/mol·K). Residuals having $< \pm 4$ indicate good agreement, those between $> \pm 4$ and $< \pm 8$ indicate agreement in the range from fair to just acceptable, and those $> \pm 8$ suggest problems such as poor experimental data, a poor choice of group value, an unaccounted for molecular interaction, or combinations of these problems. The distribution of residuals between gas to condensed phase is about half and half. Compounds which include a ring strain correction, rsc, (such as, "cyclohexane rsc") in their molecular description and compounds which are identified by a single group, such as, methane, formaldehyde, acetonitrile, methyl bromide, etc., are excluded from this tabulation because they have zero residuals. Also excluded are compounds containing a group value in their structural group representation which was derived from a single source of thermodynamic data because such compounds will produce zero residuals. The summary of residuals is divided among the various organic families, and then summed for CH, CHO, CHN, CHNO, CHS, and organic halogen compounds as well as for all families of compounds.

Family & residual range	Properties		
	$\Delta_f H°$	$C_p°$	$S°$
CH Compounds			
n-Alkanes			
< ±4	41	35	35
> ±4 to < ±8	1	0	0
> ±8	0	5	5
total	42	40	40
t-Alkanes			
< ±4	35	46	34
> ±4 to < ±8	5	2	9
> ±8	2	1	5
total	42	49	48
q-Alkanes			
< ±4	27	22	13
> ±4 to < ±8	3	4	9
> ±8	0	0	2
total	30	26	24
n-Alkenes			
< ±4	45	34	35
> ±4 to < ±8	3	2	1
> ±8	0	0	0
total	48	36	36
s-Alkenes			
< ±4	36	17	20
> ±4 to < ±8	16	7	5
> ±8	13	2	1
total	65	26	26
Alkynes			
< ±4	22	14	13
> ±4 to	3	0	0
> ±8	0	0	0
total	25	14	13

TABLE 55. Summary of residuals for C–H–N–O–S–Halogen families – Continued

Family & residual range	Properties		
	$\Delta_f H°$	$C_p°$	$S°$
CH Compounds (Continued)			
Alkynes			
< ±4	22	14	13
> ±4 to	3	0	0
> ±8	0	0	0
total	25	14	13
Aromat CH–01			
< ±4	54	41	30
> ±4 to < ±8	6	3	10
> ±8	5	2	6
total	65	46	46
Aromat CH 02			
< ±4	56	54	44
> ±4 to < ±8	15	7	11
> ±8	16	10	6
total	87	71	64
Cyclic CH–01			
< ±4	11	12	10
> ±4 to < ±8	6	2	4
> ±8	4	3	1
total	21	17	15
Cyclic CH–02			
< ±4	33	32	23
> ±4 to < ±8	14	3	4
> ±8	7	1	2
total	54	36	29
Cyclic CH–03			
< ±4	15	0	0
> ±4 to < ±8	18	0	0
> ±8	20	0	0
total	53	0	0
Total CH cpds	$\Delta_f H°$	$C_p°$	$S°$
< ±4	375	307	257
> ±4 to < ±8	90	30	53
> ±8	67	24	28
total	532	361	338
CHO Compounds			
Alcohols			
< ±4	94	56	45
> ±4 to < ±8	30	5	6
> ±8	19	13	5
total	143	74	55
Ethers			
< ±4	56	25	14
> ±4 to < ±8	10	8	11
> ±8	11	1	0
total	77	34	25

TABLE 55. Summary of Residuals for C–H–N–O–S–Halogen Families – Continued

Family & residual range	$\Delta_f H°$	$C_p°$	$S°$
CHO Compounds (Continued)			
Aldehydes			
< ±4	12	10	10
> ±4 to < ±8	5	0	2
> ±8	0	7	5
total	17	17	17
Ketones			
< ±4	43	14	9
> ± to < ±8	4	3	3
> ±8	1	0	2
total	48	17	14
Acids			
< ±4	68	16	11
> ±4 to < ±8	25	9	0
> ±8	43	3	0
total	136	28	11
Anhydrides			
< ±4	11	2	1
> ±4 to < ±8	3	0	0
> ±8	4	0	0
total	15	2	1
Esters			
< ±4	53	21	1
> ±4 to < ±8	21	6	0
> ±8	26	3	3
total	100	30	4
Peroxides			
< ±4	7	0	0
> ±4 to < ±8	0	0	0
> ±8	3	0	0
total	10	0	0
Hydroperoxides			
< ±4	4	0	0
> ±4 to < ±8	3	0	0
> ±8	4	0	0
total	11	0	0
Peroxyacids			
< ±4	2	0	0
> ±4 to < ±8	1	0	0
> ±8	5	0	0
total	8	0	0
Carbonates			
< ±4	2	1	1
> ±4 to < ±8	3	0	0
> ±8	0	0	0
total	5	1	1
Total CHO cpds	**$\Delta_f H°$**	**$C_p°$**	**$S°$**
< ±4	349	145	92
> ±4 to < ±8	105	31	21
> ±8	116	27	15
total	570	203	128

TABLE 55. Summary of Residuals for C–H–N–O–S–Halogen Families – Continued

Family & residual range	$\Delta_f H°$	$C_p°$	$S°$
CHN Compounds			
Amines			
< ±4	67	26	11
> ±4 to < ±8	6	3	5
> ±8	6	3	3
total	79	32	19
Imines			
< ±4	2	0	0
> ±4 to < ±8	1	0	0
> ±8	0	0	0
total	3	0	0
Nitriles			
< ±4	31	11	8
< ±8	4	0	1
> ±4 to > ±8	5	1	0
total	40	12	9
Hydrazines			
< ±4	12	4	4
> ±4 to < ±8	0	0	0
> ±8	0	0	0
total	12	4	4
Diazenes			
< ±4	14	0	0
> ±4 to < ±8	5	0	0
> ±8	1	0	0
total	20	0	0
Azides			
< ±4	9	0	0
> ±4 to < ±8	0	0	0
> ±8	0	0	0
total	9	0	0
Cyclic CHN			
< ±4	32	9	7
> ±4 to < ±8	3	1	0
> ±8	1	1	0
total	36	11	7
Total CHN cpds	**$\Delta_f H°$**	**$C_p°$**	**$S°$**
< ±4	167	50	30
> ±4 to < ±8	19	4	6
> ±8	13	5	3
total	199	59	39
CHNO Compounds			
Amides			
< ±4	22	12	1
> ±4 to < ±8	3	3	0
> ±8	11	0	1
total	36	15	2

TABLE 55. Summary of Residuals for C–H–N–O–S–Halogen Families – Continued

Family & residual range	$\Delta_f H°$	$C_p°$	$S°$
CHNO Compounds (Continued)			
Ureas			
< ±4	23	2	2
> ±4 to < ±8	6	0	0
> ±8	13	0	0
total	42	2	2
Amino Acids			
< ±4	28	16	5
> ±4 to < ±8	13	0	1
> ±8	5	6	5
total	46	22	11
Nitroso			
< ±4	8	0	0
> ±4 to < ±8	0	0	0
> ±8	0	0	0
total	8	0	0
Nitro			
< ±4	65	15	6
< ±8	5	1	0
> ±8	23	2	0
total	93	18	6
Nitrites and nitrates			
< ±4	15	7	6
> ±4 to < ±8	2	0	2
> ±8	0	1	0
total	17	8	8
Nitramines			
< ±4	13	0	0
> ±4 to < ±8	0	0	0
> ±8	1	0	0
total	14	0	0
Cyclic CHNO (Imides)			
< ±4	0	0	0
> ±4 to < ±8	0	0	0
> ±8	0	0	0
Total	0	0	0
Total CHNO cpds	$\Delta_f H°$	$C_p°$	$S°$
< ±4	174	52	20
> ±4 to < ±8	29	4	3
> ±8	53	9	6
total	256	65	29
CHS Compounds			
Thiols			
< ±4	50	29	30
> ±4 to < ±8	2	2	0
> ±8	0	0	2
total	52	31	32

TABLE 55. Summary of Residuals for C–H–N–O–S–Halogen Families – Continued

Family & residual range	$\Delta_f H°$	$C_p°$	$S°$
CHS Compounds (Continued)			
Sulfides			
< ±4	52	31	28
> ±4 to < ±8	3	2	1
> ±8	0	0	3
total	55	33	32
Disulfides			
< ±4	13	10	8
> ±4 to < ±8	1	0	3
> ±8	0	1	0
total	14	11	11
Sulfoxides			
< ±4	5	2	2
> ±4 to < ±8	2	0	0
> ±8	1	0	0
total	8	2	2
Sulfones			
< ±4	27	2	2
> ±4 to < ±8	15	0	0
> ±8	10	0	0
total	52	2	2
Sulfites and sulfates			
< ±4	5	0	0
> ±4 to < ±8	3	0	0
> ±8	1	0	0
total	9	0	0
Cyclic CHS			
< ±4	6	3	3
> ±4 to < ±8	2	2	1
> ±8	0	0	1
total	8	5	5
Total CHS	$\Delta_f H°$	$C_p°$	$S°$
< ±4	158	77	73
> ±4 to < ±8	28	6	6
> ±8	12	1	5
total	198	84	84
Halogens			
Fluorides			
< ±4	30	19	14
> ±4 to < ±8	15	5	2
> ±8	17	0	6
total	62	24	22
Chlorides			
< ±4	90	49	34
> ±4 to < ±8	23	7	4
> ±8	72	5	3
total	185	61	41

TABLE 55. Summary of Residuals for C–H–N–O–S–Halogen Families — Continued

Halogens (Continued)			
Bromides			
< ±4	44	22	9
> ±4 to < ±8	9	2	6
> ±8	6	9	1
total	59	33	16
Iodides			
< ±4	26	10	7
> ±4 to < ±8	13	1	1
> ±8	8	2	1
total	47	13	9
Mixed halogens			
< ±4	10	7	4
> ±4 to < ±8	4	1	3
> ±8	2	2	2
total	16	10	9
Total halogens	$\Delta_f H°$	$C_p°$	$S°$
< ±4	200	107	68
> ±4 to < ±8	64	16	16
> ±8	105	18	13
total	369	141	97

TABLE 55. Summary of Residuals for C–H–N–O–S–Halogen Families — Continued

All compounds	$\Delta_f H°$	(%)	$C_p°$	(%)	$S°$	(%)
< ±4	1423	(67)	738	(80)	540	(76)
> ±4 to < ±8	335	(16)	91	(10)	105	(14)
> ±8	366	(17)	84	(10)	70	(10)
Grand total	2124	(100)	913	(100)	715	(100)

TABLE 56. Name and Formula Index

TABLE 56. Name and Formula Index — Continued

Name	Formula	CAS Registry No.	Family	Page
L-Asparagine	$C_4H_8N_2O_3$	70–47–3	Amino acids	1018
L-Aspartic acid	$C_4H_7NO_4$	56–84–8	Amino acids	1017
1-Azabicyclo[3.3.0]octane	$C_7H_{13}N$	643–20–9	CyclCHN	1006
Azelaic acid	$C_9H_{16}O_4$	123–99–9	Acids	953
Azidobenzene	$C_6H_5N_3$	622–37–7	Azides	1000
Azidocyclohexane	$C_6H_{11}N_3$	19573–22–9	Azides	1000
Azidocyclopentane	$C_5H_9N_3$	33670–50–7	Azides	1000
2-Azidoethanol	$C_2H_5N_3O$	1517–05–1	Azides	1000
Aziridine	C_2H_5N	151–56–4	CyclCHN	1001
cis-Azobenzene	$C_{12}H_{10}N_2$	17082–12–1	Diazene	1000
trans-Azobenzene	$C_{12}H_{10}N_2$	1080–16–6	Diazene	999,1000
Azobutane	$C_8H_{18}N_2$	2159–75–3	Diazene	999
Azo-*tert*-butane	$C_8H_{18}N_2$	927–83–3	Diazene	999
Azoethane	$C_4H_{10}N_2$	821–14–7	Diazene	998
Azoisopropane	$C_6H_{14}N_2$	3880–49–7	Diazene	999
Azomethane	$C_2H_6N_2$	503–28–6	Diazene	998
Azopropane	$C_6H_{14}N_2$	821–67–0	Diazene	998
B				
Benzaldehyde	C_7H_6O	100–52–7	Aldehyde	938
Benzamide	C_7H_7NO	55–21–0	Amides	1010
1,2-Benzanthracene	$C_{18}H_{12}$	56–55–3	Aromat02	886
Benzenamine	C_6H_7N	62–53–3	Amines	989
Benzene	C_6H_6	71–43–2	Aromat01	863
1,2-Benzenediamine	$C_6H_8N_2$	95–54–5	Amines	991
1,3-Benzenediamine	$C_6H_8N_2$	108–45–2	Amines	991
1,4-Benzenediamine	$C_6H_8N_2$	106–50–3	Amines	991
1,2-Benzene dicarboxylic acid	$C_8H_6O_4$	88–99–3	Acids	961
1,3-Benzene dicarboxylic acid	$C_8H_6O_4$	121–91–5	Acids	962
1,4-Benzene dicarboxylic acid	$C_8H_6O_4$	100–21–0	Acids	962
1,2-Benzenediol	$C_6H_6O_2$	120–80–9	Alcohols	924
1,3-Benzenediol	$C_6H_6O_2$	108–46–3	Alcohols	924
1,4-Benzenediol	$C_6H_6O_2$	123–31–9	Alcohols	924
Benzenemethanol	C_7H_8O	100–51–6	Alcohols	914
Benzenethiol	C_6H_6S	108–98–5	Thiols	1041
1,2,3-Benzene tricarboxylic acid	$C_9H_6O_6$	528–44–9	Acids	962
1,3,5-Benzene tricarboxylic acid	$C_9H_6O_6$	554–95–0	Acids	962
Benzil	$C_{14}H_{10}O_2$	134–81–6	Ketones	945
1,4-Benzodinitrile	$C_8H_4N_2$	632–26–7	Nitriles	997
Benzoic acid	$C_7H_6O_2$	65–85–0	Acids	956, 957
Benzoic anhydride	$C_{14}H_{10}O_3$	93–97–0	Anhydrides	965
Benzonitrile	C_7H_5N	100–47–0	Nitriles	996
Benzophenone	$C_{13}H_{10}O$	119–61–9	Ketones	944
Benzoyl chloride	C_7H_5ClO	98–88–4	Chloride	1084
N-Benzoylglycine	$C_9H_9NO_3$	495–69–2	Amino acids	1019
Benzyl alcohol	C_7H_8O	100–51–6	Alcohols	914
Benzylamine	C_7H_9N	100–46–9	Amines	990
Benzylazide	$C_7H_7N_3$	622–79–7	Azides	1000,1001
Benzyl bromide	C_7H_7Br	100–39–0	Bromide	1091
Benzyl chloride	C_7H_7Cl	100–44–7	Chloride	1073
Benzylideneaniline	$C_{13}H_{11}N$	538–51–2	Imines	992
Benzyl iodide	C_7H_7I	620–05–3	Iodide	1095
Benzyl mercaptan	C_7H_8S	100–53–8	Thiols	1041
Benzyl methyl sulfone	$C_8H_{10}O_2S$	3112–90–1	Sulfones	1052
Biacetyl	$C_4H_6O_2$	431–03–8	Ketones	942
9,9′-Bianthracene	$C_{28}H_{18}$	1055–23–8	Cyclic03	908
Bibenzyl	$C_{14}H_{14}$	103–29–7	Aromat02	876
Bicyclo[1.1.0]butane	C_4H_6	157–33–5	Cyclic03	902
Bicyclobutane methyl carboxylate	$C_6H_8O_2$	4935–01–7	Esters	977
Bicyclo[2.2.1]hepta-2,5-diene	C_7H_8	121–46–0	Cyclic03	902
Bicyclo[2.2.1]heptane	C_7H_{12}	279–23–2	Cyclic03	903
Bicyclo[4.1.0]heptane	C_7H_{12}	286–08–8	Cyclic03	903
Bicyclo[2.2.1]hept-2-ene	C_7H_{10}	498–66–8	Cyclic03	903
Bicycloheptyl	$C_{14}H_{26}$	23183–11–1	Cyclic03	907
Bicyclo[3.1.0]hexane	C_6H_{10}	285–58–5	Cyclic03	902

TABLE 56. Name and Formula Index – Continued

Name	Formula	CAS Registry No.	Family	Page
Bicyclohexyl	$C_{12}H_{22}$	92–51–3	Cyclic03	907
Bicyclo[3.3.1]nonane	C_9H_{16}	280–65–9	Cyclic03	906
cis-Bicyclo[6.1.0]nonane	C_9H_{16}	13757–43–2	Cyclic03	906
trans-(+)-Bicyclo[6.1.0]nonane	C_9H_{16}	39124–79–3	Cyclic03	906
Bicyclo[2.2.2]octane	C_8H_{14}	280–33–1	Cyclic02	900
cis-Bicyclo[3.3.0]octane	C_8H_{14}	1755–05–1	Cyclic03	904
trans-Bicyclo[3.3.0]octane	C_8H_{14}	5597–89–7	Cyclic03	905
Bicyclo[4.2.0]octane	C_8H_{14}	278–30–8	Cyclic03	904
Bicyclo[5.1.0]octane	C_8H_{14}	286–43–1	Cyclic03	904
Bicyclo[2.2.2]oct-2-ene	C_8H_{12}	931–64–6	Cyclic03	904
Bicyclopentyl	$C_{10}H_{18}$	1636–39–1	Cyclic02	895
Bicyclopropyl	C_6H_{10}	5685–46–1	Cyclic03	902
Bicyclo[3.3.3]undecane	$C_{11}H_{20}$	29415–95–0	Cyclic02	901
9,9′-Biphenanthrene	$C_{28}H_{18}$	20532–03–0	Cyclic03	908
Biphenyl	$C_{12}H_{10}$	92–52–4	Aromat02	877,878
2,2′-Bis(hydroxymethyl)-1,3-propanediol	$C_5H_{12}O_4$	115–77–5	Alcohol	919
2,2-Bis(4-hydroxyphenyl)-propane	$C_{15}H_{16}O_2$	80–05–7	Alcohols	925
Bis-(3,3,3-trifluoropropyl)ether	$C_6H_8F_6O$	674–65–7	Fluoride	1065
N,N-Bisuccinimide	$C_8H_8N_2O_4$	500005–58–3	CyclCHNO	1035
Bromobenzene	C_6H_5Br	108–86–1	Bromide	1091
4-Bromobenzoic acid	$C_7H_5BrO_2$	586–76–5	Bromide	1091,1092
1-Bromobutane	C_4H_9Br	109–65–9	Bromide	1086
2-Bromobutane	C_4H_9Br	78–76–2	Bromide	1088
1-Bromo-2-chloroethane	C_2H_4BrCl	107–04–0	Mixed	1100
1-Bromododecane	$C_{12}H_{25}Br$	143–15–7	Bromide	1087
Bromoethane	C_2H_5Br	74–96–4	Bromide	1086
Bromoethylene	C_2H_3Br	593–60–2	Bromide	1090
1-Bromoheptane	$C_7H_{15}Br$	629–04–9	Bromide	1087
1-Bromohexadecane	$C_{16}H_{33}Br$	112–82–3	Bromide	1087
1-Bromohexane	$C_6H_{13}Br$	111–25–1	Bromide	1086
Bromomethane	CH_3Br	74–83–9	Bromide	1086
1-Bromo-3-methylbutane	$C_5H_{11}Br$	107–82–4	Bromide	1087
1-Bromo-2-methylpropane	C_4H_9Br	78–77–3	Bromide	1087
2-Bromo-2-methylpropane	C_4H_9Br	507–19–7	Bromide	1088
1-Bromooctane	$C_8H_{17}Br$	111–83–1	Bromide	1087
Bromopentafluorobenzene	C_6BrF_5	344–04–7	Mixed	1101
1-Bromopentane	$C_5H_{11}Br$	110–53–2	Bromide	1086
1-Bromopropane	C_3H_7Br	106–94–5	Bromide	1086
2-Bromopropane	C_3H_7Br	75–26–3	Bromide	1088
1-Bromo-1-propene (E)	C_3H_5Br	590–15–8	Bromide	1090
1-Bromo-1-propene (Z)	C_3H_5Br	590–13–6	Bromide	1090
3-Bromo-1-propene	C_3H_5Br	106–95–6	Bromide	1090
1-Bromopropyne	C_3H_3Br	2003–82–9	Bromide	1090
1,2-Butadiene	C_4H_6	590–19–2	*n*-Alkenes	850
1,3-Butadiene	C_4H_6	106–99–0	*n*-Alkenes	850
Butadiyne	C_4H_2	460–12–8	Alkynes	861
Butanal	C_4H_8O	123–72–8	Aldehyde	936
Butanamide	C_4H_9NO	541–35–5	Amides	1007
Butane	C_4H_{10}	106–97–8	*n*-Alkanes	830
Butanediamide	$C_4H_8N_2O_2$	110–14–5	Amides	1010
1,2-Butanediamine	$C_4H_{12}N_2$	4426–48–6	Amines	984
1,4-Butanedinitrile	$C_4H_4N_2$	110–61–2	Nitriles	996
Butanedioic acid	$C_4H_6O_4$	110–15–6	Acids	951
1,2-Butanediol	$C_4H_{10}O_2$	584–03–2	Alcohols	918
1,3-Butanediol	$C_4H_{10}O_2$	107–88–0	Alcohols	918
1,4-Butanediol	$C_4H_{10}O_2$	110–63–4	Alcohols	918
2,3-Butanediol	$C_4H_{10}O_2$	513–85–9	Alcohols	918
2,3-Butanedione	$C_4H_6O_2$	431–03–8	Ketones	942
1,4-Butanedithiol	$C_4H_{10}S_2$	1191–08–8	Thiols	1038
Butanenitrile	C_4H_7N	109–74–0	Nitriles	992,993
1,2,3,4-Butanetetrol	$C_4H_{10}O_4$	149–32–6	Alcohols	919
1-Butanethiol	$C_4H_{10}S$	109–79–5	Thiols	1036
2-Butanethiol	$C_4H_{10}S$	513–53–1	Thiols	1038
Butanoic acid	$C_4H_8O_2$	107–92–6	Acids	946
Butanol	$C_4H_{10}O$	71–36–3	Alcohols	910
2-Butanol	$C_4H_{10}O$	78–92–2	Alcohols	915

TABLE 56. Name and Formula Index – Continued

Name	Formula	CAS Registry No.	Family	Page
4-Butanolactone	$C_4H_6O_2$	96–48–0	Esters	975
Butanone	C_4H_8O	78–93–3	Ketones	938
Butanoyl chloride	C_4H_7ClO	141–75–3	Chloride	1084
trans-2-Butenal	C_4H_6O	4170–30–3	Aldehyde	936
1-Butene	C_4H_8	106–98–9	*n*-Alkenes	846
cis-2-Butene	C_4H_8	590–18–1	*n*-Alkenes	847
trans-2-Butene	C_4H_8	624–64–6	*n*-Alkenes	848
(E)-2-Butenedioic acid	$C_4H_4O_4$	110–17–8	Acids	951
(Z)-2-Butenedioic acid	$C_4H_4O_4$	110–16–6	Acids	951
cis-2-Butenenitrile	C_4H_5N	1190–76–7	Nitriles	994
trans-2-Butenenitrile	C_4H_5N	627–26–9	Nitriles	994
1-Buten-3-yne	C_4H_4	689–97–4	Alkynes	861
Butoxybutane	$C_8H_{18}O$	142–96–1	Ethers	927
2-Butoxy-2-butane	$C_8H_{18}O$	6863–58–7	Ethers	928
Butoxyethene	$C_6H_{12}O$	111–34–2	Ethers	929
N-Butylacetamide	$C_6H_{13}NO$	1119–49–9	Amides	1009
N-*tert*-Butylacetamide	$C_6H_{13}NO$	762–84–5	Amides	1009
Butyl acetate	$C_6H_{12}O_2$	123–86–4	Esters	969
tert-Butyl acetate	$C_6H_{12}O_2$	540–88–5	Esters	970
n-Butyl alcohol	$C_4H_{10}O$	71–36–3	Alcohols	910
sec-Butyl alcohol	$C_4H_{10}O$	78–92–2	Alcohols	915
tert-Butyl alcohol	$C_4H_{10}O$	75–65–0	Alcohols	916
n-Butyl amine	$C_4H_{11}N$	109–73–9	Amines	983
sec-Butyl amine	$C_4H_{11}N$	13952–84–6	Amines	984
tert-Butyl amine	$C_4H_{11}N$	75–64–9	Amines	984,985
Butylbenzene	$C_{10}H_{14}$	104–51–8	Aromat01	866
sec-Butylbenzene	$C_{10}H_{14}$	135–98–8	Aromat02	872
tert-Butylbenzene	$C_{10}H_{14}$	98–06–6	Aromat02	873
Butyl (E)-2-butenoate	$C_8H_{14}O_2$	7299–91–4	Esters	973
Butyl *trans*-2-butenoate	$C_8H_{14}O_2$	7299–91–4	Esters	973
Butyl chloroacetate	$C_6H_{11}ClO_2$	590–02–3	Chloride	1081
Butyl 2-chlorobutanoate	$C_8H_{15}ClO_2$	62108–74–1	Chloride	1083
Butyl 2-chloropropanoate	$C_7H_{13}ClO_2$	54819–86–2	Chloride	1082
Butyl 3-chloropropanoate	$C_7H_{13}ClO_2$	27387–79–7	Chloride	1082
Butylcyclohexane	$C_{10}H_{20}$	1678–93–9	Cyclic02	898
Butylcyclopentane	C_9H_{18}	2040–95–1	Cyclic02	893
N-Butyldiacetamide	$C_8H_{15}NO_2$	1563–86–6	Amides	1009
N-Butyldiacetylamine	$C_8H_{15}NO_2$	1563–86–6	Amides	1009
Butyl dichloroacetate	$C_6H_{10}Cl_2O_2$	29003–73–4	Chloride	1083
N-Butylethanamide	$C_6H_{13}NO$	1119–49–9	Amides	1009
Butyl ethanoate	$C_6H_{12}O_2$	123–86–4	Esters	969
Butyl ethyl sulfide	$C_6H_{14}S$	638–46–0	Sulfides	1042,1043
tert-Butyl ethyl sulfide	$C_6H_{14}S$	14290–92–7	Sulfides	1047
tert-Butyl ethyl sulfone	$C_6H_{14}O_2S$	34008–94–1	Sulfones	1051
tert-Butyl ethyl sulfoxide	$C_6H_{14}OS$	25432–20–6	Sulfoxides	1050
Butyl heptyl sulfide	$C_{11}H_{24}S$	40813–84–1	Sulfides	1045
tert-Butyl hydroperoxide	$C_4H_{10}O_2$	75–91–2	Hydroperoxides	979
n-Butylisobutylamine	$C_8H_{19}N$	20810–06–4	Amines	986
N-Butylisobutyleneimine	$C_8H_{17}N$	6898–75–5	Imines	992
Butyl methyl sulfide	$C_5H_{12}S$	628–29–5	Sulfides	1042
tert-Butyl methyl sulfide	$C_5H_{12}S$	6163–64–0	Sulfides	1046
Butyl methyl sulfone	$C_5H_{12}O_2S$	7560–59–0	Sulfones	1051
tert-Butyl methyl sulfone	$C_5H_{12}O_2S$	14094–12–3	Sulfones	1051
1-Butylnaphthalene	$C_{14}H_{16}$	1634–09–9	Aromat02	881
2-Butylnaphthalene	$C_{14}H_{16}$	1134–62–9	Aromat02	881
Butyl nonyl sulfide	$C_{13}H_{28}S$	66577–32–0	Sulfides	1046
Butyl pentadecyl sulfide	$C_{19}H_{40}S$	66359–42–0	Sulfides	1046
N-Butylpentanamide	$C_9H_{19}NO$	2763–67–9	Amides	1009
Butyl pentanoate	$C_9H_{18}O_2$	591–68–4	Esters	970
tert-Butyl perdecanoate	$C_{14}H_{28}O_3$	16474–36–5	Peroxyacids	981
tert-Butyl perdodecanoate	$C_{16}H_{32}O_3$	2123–88–8	Peroxyacids	981
tert-Butyl pertetradecanoate	$C_{18}H_{36}O_3$	59710–71–3	Peroxyacids	981
Butyl propyl sulfide	$C_7H_{16}S$	1613–46–3	Sulfides	1043
tert-Butyl-(1,1,3,3-tetramethylbutyl)diazene	$C_{12}H_{26}N_2$	57905–89–2	Diazene	999
N-*n*-Butylurea	$C_5H_{12}N_2O$	592–31–4	Ureas	1012
N-*sec*-Butylurea	$C_5H_{12}N_2O$	689–11–2	Ureas	1012

TABLE 56. Name and Formula Index – Continued

Name	Formula	CAS Registry No.	Family	Page
N-tert-Butylurea	$C_5H_{12}N_2O$	1118–12–3	Ureas	1012
Butyl valerate	$C_9H_{18}O_2$	591–68–4	Esters	970
n-Butyl vinyl ether	$C_6H_{12}O$	111–34–2	Ethers	929
1-Butyne	C_4H_6	107–00–6	Alkynes	858
2-Butyne	C_4H_6	503–17–3	Alkynes	860
2-Butyne-1,4-dinitrile	C_4N_2	1071–98–3	Nitriles	996
Butyraldehyde	C_4H_8O	123–72–8	Aldehyde	936
Butyramide	C_4H_9NO	541–35–5	Amides	1007
Butyric acid	$C_4H_8O_2$	107–92–6	Acids	946
γ-Butyrolactone	$C_4H_6O_2$	96–48–0	Esters	975
Butyronitrile	C_4H_7N	109–74–0	Nitriles	992,993
C				
Capric acid	$C_{10}H_{20}O_2$	334–48–5	Acids	947
Caprinitrile	$C_{10}H_{19}N$	1975–78–6	Nitriles	993
Caproic acid	$C_6H_{12}O_2$	142–62–1	Acids	946
Caprolactone	$C_6H_{10}O_2$	502–44–3	Esters	975
Caprylic acid	$C_8H_{16}O_2$	124–07–2	Acids	947
Capryonitrile	$C_8H_{15}N$	124–12–9	Nitriles	993
Catechol	$C_6H_6O_2$	120–80–9	Alcohols	924
Cetyl alcohol	$C_{16}H_{34}O$	36653–82–4	Alcohols	913
Chloroacetic acid	$C_2H_3ClO_2$	79–11–8	Chloride	1079
Chloroacetyl chloride	$C_2H_2Cl_2O$	79–04–9	Chloride	1084
2-Chlorobenzaldehyde	C_7H_5ClO	89–98–5	Chloride	1080
3-Chlorobenzaldehyde	C_7H_5ClO	587–04–2	Chloride	1080
4-Chlorobenzaldehyde	C_7H_5ClO	104–88–1	Chloride	1081
Chlorobenzene	C_6H_5Cl	108–90–7	Chloride	1072
2-Chloro-1,4-benzenediol	$C_6H_5ClO_2$	615–67–8	Chloride	1078
2-Chlorobenzoic acid	$C_7H_5ClO_2$	118–91–2	Chloride	1080
3-Chlorobenzoic acid	$C_7H_5ClO_2$	535–80–8	Chloride	1080
4-Chlorobenzoic acid	$C_7H_5ClO_2$	74–11–3	Chloride	1080
2-Chlorobenzoyl chloride	$C_7H_4Cl_2O$	609–65–4	Chloride	1085
3-Chlorobenzoyl chloride	$C_7H_4Cl_2O$	618–46–2	Chloride	1085
4-Chlorobenzoyl chloride	$C_7H_4Cl_2O$	122–01–0	Chloride	1085
1-Chlorobutane	C_4H_9Cl	109–69–3	Chloride	1066
2-Chlorobutane	C_4H_9Cl	78–86–4	Chloride	1067
2-Chlorobutanoic acid	$C_4H_7ClO_2$	4170–24–5	Chloride	1079
3-Chlorobutanoic acid	$C_4H_7ClO_2$	1951–12–8	Chloride	1079
4-Chlorobutanoic acid	$C_4H_7ClO_2$	627–00–9	Chloride	1079
Chlorocyclohexane	$C_6H_{11}Cl$	542–18–7	Chloride	1076
1-Chloro-1,1-difluoroethane	$C_2H_3ClF_2$	75–68–3	Mixed	1100
1-Chlorododecane	$C_{12}H_{25}Cl$	112–52–7	Chloride	1067
Chloroethane	C_2H_5Cl	75–00–3	Chloride	1066
1-Chloro-2-ethoxyethane	C_4H_9ClO	628–34–2	Chloride	1081
(1-Chloroethyl)benzene	C_8H_9Cl	672–65–1	Chloride	1073
1-Chloro-2-ethylbenzene	C_8H_9Cl	89–96–3	Chloride	1073
1-Chloro-4-ethylbenzene	C_8H_9Cl	622–98–0	Chloride	1073
Chloroethylene	C_2H_3Cl	75–01–4	Chloride	1071
2-Chloroethyl vinyl ether	C_4H_7ClO	110–75–8	Chloride	1081
1-Chloro-1-fluoroethane	C_2H_4ClF	1615–75–4	Mixed	1099
2-Chlorohexane	$C_6H_{13}Cl$	638–28–8	Chloride	1068
Chloromethane	CH_3Cl	74–87–3	Chloride	1066
1-Chloro-4-methylbenzene	C_7H_7Cl	106–43–4	Chloride	1072,1073
1-Chloro-3-methylbutane	$C_5H_{11}Cl$	107–84–6	Chloride	1067
2-Chloro-2-methylbutane	$C_5H_{11}Cl$	594–36–5	Chloride	1068
2-Chloro-3-methylbutane	$C_5H_{11}Cl$	631–65–2	Chloride	1068
1-Chloro-2-methylpropane	C_4H_9Cl	513–36–0	Chloride	1067
2-Chloro-2-methylpropane	C_4H_9Cl	507–20–0	Chloride	1068
1-Chloronaphthalene	$C_{10}H_7Cl$	90–13–1	Chloride	1073
2-Chloronaphthalene	$C_{10}H_7Cl$	91–58–7	Chloride	1074
1-Chlorooctadecane	$C_{18}H_{37}Cl$	3386–33–2	Chloride	1067
1-Chlorooctane	$C_8H_{17}Cl$	111–85–3	Chloride	1066
Chloropentafluorobenzene	C_6ClF_5	344–07–0	Mixed	1101
1-Chloro-1,1,3,3,3-pentafluoropropane	$C_3H_2ClF_5$	460–92–4	Mixed	1099
1-Chloropentane	$C_5H_{11}Cl$	543–59–9	Chloride	1066

TABLE 56. Name and Formula Index — Continued

Name	Formula	CAS Registry No.	Family	Page
3-Chlorophenol	C_6H_5ClO	108–43–0	Chloride	1076
4-Chlorophenol	C_6H_5ClO	106–48–9	Chloride	1076
1-Chloropropane	C_3H_7Cl	540–54–5	Chloride	1066
2-Chloropropane	C_3H_7Cl	75–29–6	Chloride	1067
3-Chloro-1,2-propanediol	$C_3H_7ClO_2$	96–24–2	Chloride	1076
2-Chloro-1,3-propanediol	$C_3H_7ClO_2$	497–04–1	Chloride	1076
2-Chloropropanoic acid	$C_3H_5ClO_2$	598–78–7	Chloride	1079
3-Chloropropanoic acid	$C_3H_5ClO_2$	107–94–8	Chloride	1079
2-Chloro-1-propene	C_3H_5Cl	557–98–2	Chloride	1071
3-Chloro-1-propene	C_3H_5Cl	107–05–1	Chloride	1071
1-Chloropropyne	C_3H_3Cl	7747–84–4	Chloride	1072
p-Chlorotoluene	C_7H_7Cl	106–43–4	Chloride	1072,1073
Chlorotrifluoroethylene	C_2ClF_3	79–38–9	Mixed	1101
1-Chloro-3,3,3-trifluoropropane	$C_3H_4ClF_3$	460–35–5	Mixed	1100
Chrysene	$C_{18}H_{12}$	218–01–9	Aromat02	885
Coronene	$C_{24}H_{12}$	191–07–1	Aromat02	886
m-Cresol	C_7H_8O	108–39–4	Alcohols	921
o-Cresol	C_7H_8O	95–48–7	Alcohols	921
p-Cresol	C_7H_8O	106–44–5	Alcohols	921
Crotonaldehyde	C_4H_6O	4170–30–3	Aldehyde	936
Cubane	C_8H_8	277–10–1	Cyclic03	904
Cubane 1,4-dimethyldicarboxylate	$C_{12}H_{12}O_4$	29412–62–2	Esters	977
Cumene	C_9H_{12}	92–82–8	Aromat02	872
Cumyl hydroperoxide	$C_9H_{12}O_2$	80–15–9	Hydroperoxides	980
Cyclobutane	C_4H_8	287–23–0	Cyclic01	887
Cyclobutane-1,3-dione	$C_4H_4O_2$	15506–53–3	Ketones	945
Cyclobutane Methyl Carboxylate	$C_6H_{10}O_2$	765–85–5	Esters	977
Cyclobutanenitrile	C_5H_7N	4426–11–3	Nitriles	995
Cyclobutene	C_4H_6	822–35–5	Cyclic01	889
Cyclobutylamine	C_4H_9N	2516–34–9	Amines	988
Cyclodecane	$C_{10}H_{20}$	293–96–9	Cyclic01	888
Cyclodecanone	$C_{10}H_{18}O$	1502–06–3	Ketones	943
Cyclododecane	$C_{12}H_{24}$	294–62–2	Cyclic01	888
Cyclododecanone	$C_{12}H_{22}O$	830–13–7	Ketones	943
Cycloheptadecane	$C_{17}H_{34}$	295–97–6	Cyclic01	888
Cycloheptadecanone	$C_{17}H_{32}O$	3661–77–6	Ketones	943
1,3-Cycloheptadiene	C_7H_{10}	4054–38–0	Cyclic01	890
Cycloheptane	C_7H_{14}	291–64–5	Cyclic01	887
Cycloheptanol	$C_7H_{14}O$	502–41–0	Alcohols	920
Cycloheptanone	$C_7H_{12}O$	502–42–1	Ketones	942
1,3,5-Cycloheptatriene	C_7H_8	544–25–2	Cyclic01	890
Cycloheptene	C_7H_{12}	628–92–2	Cyclic01	889
Cycloheptyl alcohol	$C_7H_{14}O$	502–41–0	Alcohols	920
Cyclohexadecane	$C_{16}H_{32}$	295–65–8	Cyclic01	888
1,3-Cyclohexadiene	C_6H_8	592–57–4	Cyclic01	889,890
1,4-Cyclohexadiene	C_6H_8	628–41–1	Cyclic01	890
Cyclohexane	C_6H_{12}	110–82–7	Cyclic01	887
Cyclohexanenitrile	$C_7H_{11}N$	766–05–2	Nitriles	995
Cyclohexanethiol	$C_6H_{12}S$	1569–69–3	Thiols	1040
Cyclohexanol	$C_6H_{12}O$	108–93–0	Alcohols	920
Cyclohexanone	$C_6H_{10}O$	108–94–1	Ketones	942
Cyclohexene	C_6H_{10}	110–83–8	Cyclic01	889
Cyclohexyl alcohol	$C_6H_{12}O$	108–93–0	Alcohols	920
Cyclohexylamine	$C_6H_{13}N$	108–91–8	Amines	989
3-Cyclohexyleicosane	$C_{26}H_{52}$	4443–57–6	Cyclic02	899
9-Cyclohexyleicosane	$C_{26}H_{52}$	4443–61–2	Cyclic02	899
11-Cyclohexylheneicosane	$C_{27}H_{54}$	6703–99–7	Cyclic02	899
13-Cyclohexylpentacosane	$C_{31}H_{62}$	6697–15–0	Cyclic02	900
Cyclononane	C_9H_{18}	293–55–0	Cyclic01	888
Cyclononanone	$C_9H_{16}O$	3350–30–9	Ketones	943
1,5-Cyclooctadiene	C_8H_{12}	111–78–4	Cyclic01	890
Cyclooctane	C_8H_{16}	292–64–8	Cyclic01	887
Cyclooctanone	$C_8H_{14}O$	502–49–8	Ketones	943
Cyclooctatetraene	C_8H_8	629–20–9	Cyclic01	890
Cyclooctene	C_8H_{14}	931–88–4	Cyclic01	889
Cyclopentadecane	$C_{15}H_{30}$	295–48–7	Cyclic01	888

TABLE 56. Name and Formula Index — Continued

TABLE 56. Name and Formula Index — Continued

TABLE 56. Name and Formula Index — Continued

Name	Formula	CAS Registry No.	Family	Page
cis-1,2-Diethylcyclopropane	C_7H_{14}	1192–18–3	Cyclic03	903
trans-1,2-Diethylcyclopropane	C_7H_{14}	822–50–4	Cyclic03	903
Diethyldiazene	$C_4H_{10}N_2$	821–14–7	Diazene	998
Diethyl disulfide	$C_4H_{10}S_2$	110–81–6	Disulfides	1048
N,N'-Diethyl-*N,N'*-diphenylurea	$C_{17}H_{20}N_2O$	85–98–3	Ureas	1013
Diethylene glycol	$C_4H_{10}O_3$	111–46–6	Ethers	932
Diethyl ethanedioate	$C_6H_{10}O_4$	95–92–1	Esters	974
Diethyl ether	$C_4H_{10}O$	60–29–7	Ethers	926
Diethyl ketone	$C_5H_{10}O$	96–22–0	Ketones	939
Diethyl malonate	$C_7H_{12}O_4$	105–53–3	Esters	974
Diethylnitramine	$C_4H_{10}N_2O_2$	7119–92–8	Nitramines	1034
Diethyl oxalate	$C_6H_{10}O_4$	95–92–1	Esters	974
3,3-Diethylpentane	C_9H_{20}	1067–20–5	*q*-Alkanes	845
Diethylperoxide	$C_4H_{10}O_2$	628–37–5	Peroxide	978
Diethyl phthalate	$C_{12}H_{14}O_4$	84–66–2	Esters	977
Diethyl o-phthalate	$C_{12}H_{14}O_4$	84–66–2	Esters	977
Diethyl 1,2-phthalate	$C_{12}H_{14}O_4$	84–66–2	Esters	977
Diethyl propanedioate	$C_7H_{12}O_4$	105–53–3	Esters	974
Diethyl succinate	$C_8H_{14}O_4$	123–25–1	Esters	974,975
2,2-Diethylsuccinic acid	$C_8H_{14}O_4$	5692–97–7	Acids	955
meso-2,3-Diethylsuccinic acid	$C_8H_{14}O_4$	35392–80–4	Acids	954
racemic-2,3-Diethylsuccinic acid	$C_8H_{14}O_4$	35392–77–9	Acids	954,955
2,2-Diethylsuccinic anhydride	$C_8H_{12}O_3$	2840–69–9	Anhydrides	965
Diethyl sulfate	$C_4H_{10}O_4S$	64–67–5	Sulfates	1055
Diethyl sulfide	$C_4H_{10}S$	352–93–2	Sulfides	1041,1042
Diethyl sulfite	$C_4H_{10}O_3S$	623–81–4	Sulfites	1055
Diethyl sulfone	$C_4H_{10}O_2S$	597–35–3	Sulfones	1051
Diethyl sulfoxide	$C_4H_{10}OS$	70–29–1	Sulfoxides	1049
Diethanoyl peroxide	$C_4H_6O_4$	110–22–5	Peroxide	978
N,N-Diethylurea	$C_5H_{12}N_2O$	634–95–7	Ureas	1012
1,2-Difluorobenzene	$C_6H_4F_2$	367–11–3	Fluoride	1061
1,3-Difluorobenzene	$C_6H_4F_2$	372–18–9	Fluoride	1061
1,4-Difluorobenzene	$C_6H_4F_2$	540–36–3	Fluoride	1061
2,2'-Difluorobiphenyl	$C_{12}H_8F_2$	388–82–9	Fluoride	1061
4,4'-Difluorobiphenyl	$C_{12}H_8F_2$	398–23–2	Fluoride	1061,1062
1,1-Difluoroethane	$C_2H_4F_2$	75–37–6	Fluoride	1059
1,1-Difluoroethylene	$C_2H_2F_2$	75–38–7	Fluoride	1059,1060
1,2-Difluorotetrachloroethane	$C_2Cl_4F_2$	76–12–0	Mixed	1100
Di-n-hexyl disulfide	$C_{12}H_{26}S_2$	10496–15–8	Disulfides	1049
Di-n-hexyl sulfide	$C_{12}H_{26}S$	6294–31–1	Sulfides	1045,1046
Dihyrofuran-2,5-dione	$C_4H_4O_3$	108–30–5	Anhydrides	964
2,3-Dihydrothiophene	C_4H_6S	1120–59–8	CyclCHS	1058
2,5-Dihydrothiophene	C_4H_6S	1708–32–3	CyclCHS	1058
2,3-Dihydroxynaphthalene	$C_{10}H_8O_2$	92–44–4	Alcohols	925
1,2-Diiodobenzene	$C_6H_4I_2$	615–42–9	Iodide	1096
1,3-Diiodobenzene	$C_6H_4I_2$	626–00–6	Iodide	1096
1,4-Diiodobenzene	$C_6H_4I_2$	624–38–4	Iodide	1096
1,2-Diiodobutane	$C_4H_8I_2$	53161–72–1	Iodide	1094
1,3-Diiodocyclobutane(*cis/trans*)	$C_4H_6I_2$	not available	Iodide	1096
1,3-Diiodocyclobutane (Z)	$C_4H_6I_2$	4934–57–0	Iodide	
1,3-Diiodocyclobutane (E)	$C_4H_6I_2$	4943–56–9	Iodide	
1,2-Diiodoethane	$C_2H_4I_2$	624–73–7	Iodide	1093
1,2-Diiodoethylene (E)	$C_2H_2I_2$	590–27–2	Iodide	1094
1,2-Diiodoethylene (Z)	$C_2H_2I_2$	590–26–1	Iodide	1094
1,2-Diiodopropane	$C_3H_6I_2$	598–29–8	Iodide	1093
Diisobutylamine	$C_8H_{19}N$	110–96–3	Amines	986
Diisobutyl sulfide	$C_8H_{18}S$	592–65–4	Sulfides	1044
Diisobutyl sulfone	$C_8H_{18}O_2S$	10495–45–1	Sulfones	1052
Diisopentyl sulfide	$C_{10}H_{22}S$	544–02–5	Sulfides	1044
Diisopropylamine	$C_6H_{15}N$	108–18–9	Amines	986
Diisopropyldiazene	$C_6H_{14}N_2$	3880–49–7	Diazene	999
Diisopropyl ether	$C_6H_{14}O$	108–20–3	Ethers	928
Diisopropyl ketone	$C_7H_{14}O$	565–80–0	Ketones	941
Diisopropyl sulfide	$C_6H_{14}S$	625–80–9	Sulfides	1043
1,2-Dimethoxybenzene	$C_8H_{10}O_2$	91–16–7	Ethers	934
1,1-Dimethoxyethane	$C_4H_{10}O_2$	25154–53–4	Ethers	930

TABLE 56. Name and Formula Index — Continued

Name	Formula	CAS Registry No.	Family	Page
Dimethoxymethane	$C_3H_8O_2$	109–87–5	Ethers	929
2,2-Dimethoxypropane	$C_5H_{12}O_2$	77–76–9	Ethers	930
N,N-Dimethylacetamide	C_4H_9NO	127–19–5	Amides	1010
Dimethylamine	C_2H_7N	124–40–3	Amines	985
N,N-Dimethylaniline	$C_8H_{11}N$	121–69–7	Amines	990
1,2-Dimethylbenzene	C_8H_{10}	95–47–6	Aromat01	863
1,3-Dimethylbenzene	C_8H_{10}	108–38–3	Aromat01	863
1,4-Dimethylbenzene	C_8H_{10}	106–42–3	Aromat01	863,864
2,3-Dimethyl benzoic acid	$C_9H_{10}O_2$	603–79–2	Acids	957
2,4-Dimethyl benzoic acid	$C_9H_{10}O_2$	611–01–8	Acids	957,958
2,5-Dimethyl benzoic acid	$C_9H_{10}O_2$	610–72–0	Acids	958
2,6-Dimethyl benzoic acid	$C_9H_{10}O_2$	632–46–2	Acids	958
3,4-Dimethyl benzoic acid	$C_9H_{10}O_2$	619–04–5	Acids	958
3,5-Dimethyl benzoic acid	$C_9H_{10}O_2$	499–06–9	Acids	958,959
trans-2,3-Dimethylbicyclo[2.2.1]heptane	C_9H_{16}	20558–16–1	Cyclic03	906
7,7-Dimethylbicyclo[2.2.1]heptane	C_9H_{16}	2034–53–9	Cyclic03	906
4,4′-Dimethylbiphenyl	$C_{14}H_{14}$	613–33–2	Aromat02	879
2,3-Dimethyl-1,3-butadiene	C_6H_{10}	513–81–5	*s*-Alkenes	858
2,2-Dimethylbutane	C_6H_{14}	75–83–2	*q*-Alkanes	842
2,3-Dimethylbutane	C_6H_{14}	79–29–8	*t*-Alkanes	841
2,2-Dimethyl-1,4-butanedioic acid	$C_6H_{10}O_4$	597–43–3	Acids	954
meso-2,3-Dimethyl-1,4-butanedioic acid	$C_6H_{10}O_4$	608–40–2	Acids	954
racemic-2,3-Dimethyl-1,4-butanedioic acid	$C_6H_{10}O_4$	608–39–9	Acids	954,955
2,3-Dimethyl-2-butanethiol	$C_6H_{14}S$	1639–01–6	Thiols	1040
3,3-Dimethyl-2-butanone	$C_6H_{12}O$	75–97–8	Ketones	941
2,3-Dimethyl-1-butene	C_6H_{12}	563–78–0	*s*-Alkenes	855
2,3-Dimethyl-2-butene	C_6H_{12}	563–79–1	*s*-Alkenes	855
3,3-Dimethyl-1-butene	C_6H_{12}	558–37–2	*s*-Alkenes	856
Dimethyl (Z)-2-butenedioate	$C_6H_8O_4$	624–48–6	Esters	974
3,3-Dimethyl-1-butyne	C_6H_{10}	693–02–7	Alkynes	862
1,1-Dimethylcyclohexane	C_8H_{16}	590–66–9	Cyclic02	897
trans-1,2-Dimethylcyclohexane	C_8H_{16}	6876–23–9	Cyclic02	897
trans-1,3-Dimethylcyclohexane	C_8H_{16}	2207–03–6	Cyclic02	897
trans-1,4-Dimethylcyclohexane	C_8H_{16}	2207–04–7	Cyclic02	897
1,1-Dimethylcyclopentane	C_7H_{14}	1638–26–2	Cyclic01	892
cis-1,2-Dimethylcyclopentane	C_7H_{14}	1192–18–3	Cyclic01	892
trans-1,2-Dimethylcyclopentane	C_7H_{14}	822–50–4	Cyclic01	892
trans-1,3-Dimethylcyclopentane	C_7H_{14}	1759–58–6	Cyclic01	892
Dimethyldiazene	$C_2H_6N_2$	503–28–6	Diazene	998
2,5-Dimethyldiphenylmethane	$C_{15}H_{16}$	13540–50–6	Aromat02	875
N,N′-Dimethyl-*N,N′*-diphenylurea	$C_{15}H_{16}N_2O$	611–92–7	Ureas	1013
Dimethyl disulfide	$C_2H_6S_2$	624–92–0	Disulfides	1048
N,N-Dimethylethanamide	C_4H_9NO	127–19–5	Amides	1010
Dimethyl ethanedioate	$C_4H_6O_4$	553–90–2	Esters	974
Dimethyl ether	C_2H_6O	115–10–6	Ethers	926
N,N-Dimethylformamide	C_3H_7NO	68–12–2	Amides	1008
2,6-Dimethyl-4-heptanone	$C_9H_{18}O$	108–83–8	Ketones	942
2,2-Dimethylhexane	C_8H_{18}	590–73–8	*q*-Alkanes	843
2,3-Dimethylhexane	C_8H_{18}	584–94–1	*t*-Alkanes	841
2,4-Dimethylhexane	C_8H_{18}	589–43–5	*t*-Alkanes	840
2,5-Dimethylhexane	C_8H_{18}	592–13–2	*t*-Alkanes	840
3,3-Dimethylhexane	C_8H_{18}	563–16–6	*q*-Alkanes	843
3,4-Dimethylhexane	C_8H_{18}	583–48–2	*t*-Alkanes	841
cis-2,2-Dimethyl-3-hexene	C_8H_{16}	690–92–6	*s*-Alkenes	854,855
trans-2,2-Dimethyl-3-hexene	C_8H_{16}	690–93–7	*s*-Alkenes	855
cis-2,5-Dimethyl-3-hexene	C_8H_{16}	10557–44–5	*s*-Alkenes	856
trans-2,5-Dimethyl-3-hexene	C_8H_{16}	692–70–6	*s*-Alkenes	857
1,1-Dimethylhydrazine	$C_2H_8N_2$	57–14–7	Hydrazines	997
1,2-Dimethylhydrazine	$C_2H_8N_2$	540–73–8	Hydrazines	998
Dimethyl isophthalate	$C_{10}H_{10}O_4$	1459–93–4	Esters	976,977
Dimethyl ketone	C_3H_6O	67–64–1	Ketones	938
Dimethyl maleate	$C_6H_8O_4$	624–48–6	Esters	974
N,N-Dimethylmethanamide	C_3H_7NO	68–12–2	Amides	1008
1,2-Dimethylnaphthalene	$C_{12}H_{12}$	573–98–8	Aromat02	881
1,3-Dimethylnaphthalene	$C_{12}H_{12}$	575–41–7	Aromat02	882
1,4-Dimethylnaphthalene	$C_{12}H_{12}$	571–58–4	Aromat02	882

TABLE 56. Name and Formula Index – Continued

Name	Formula	CAS Registry No.	Family	Page
1,5-Dimethylnaphthalene	$C_{12}H_{12}$	571–61–9	Aromat02	882
1,6-Dimethylnaphthalene	$C_{12}H_{12}$	575–43–9	Aromat02	882
1,7-Dimethylnaphthalene	$C_{12}H_{12}$	575–37–1	Aromat02	882
1,8-Dimethylnaphthalene	$C_{12}H_{12}$	569–41–5	Aromat02	883
2,3-Dimethylnaphthalene	$C_{12}H_{12}$	581–40–8	Aromat02	883
2,6-Dimethylnaphthalene	$C_{12}H_{12}$	581–42–0	Aromat02	883
2,7-Dimethylnaphthalene	$C_{12}H_{12}$	582–16–1	Aromat02	883
Dimethylnitramine	$C_2H_6N_2O_2$	4164–28–7	Nitramines	1033
Dimethylnitrosoamine	$C_2H_6N_2O$	62–75–9	Nitroso	1021
2,7-Dimethyloctane	$C_{10}H_{22}$	1072–16–8	*t*-Alkanes	842
Dimethyl oxalate	$C_4H_6O_4$	553–90–2	Esters	974
3,3-Dimethylpenta-1,4-diyne	C_7H_8	62496–43–9	Alkynes	862
2,2-Dimethylpentane	C_7H_{16}	590–35–2	*q*-Alkanes	842,843
2,3-Dimethylpentane	C_7H_{16}	565–59–3	*t*-Alkanes	841
2,4-Dimethylpentane	C_7H_{16}	108–08–7	*t*-Alkanes	840
3,3-Dimethylpentane	C_7H_{16}	562–49–2	*q*-Alkanes	843
2,2-Dimethyl-3-pentanone	$C_7H_{14}O$	564–04–5	Ketones	941
2,4-Dimethyl-3-pentanone	$C_7H_{14}O$	565–80–0	Ketones	941
2,4-Dimethyl-1-pentene	C_7H_{14}	2213–32–3	*s*-Alkenes	855
2,4-Dimethyl-2-pentene	C_7H_{14}	625–65–0	*s*-Alkenes	855
cis-4,4-Dimethyl-2-pentene	C_7H_{14}	762–63–0	*s*-Alkenes	856
trans-4,4-Dimethyl-2-pentene	C_7H_{14}	690–08–4	*s*-Alkenes	856
Dimethylperoxide	$C_2H_6O_2$	690–02–8	Peroxide	978
2,3-Dimethylphenol	$C_8H_{10}O$	526–75–0	Alcohols	922
2,4-Dimethylphenol	$C_8H_{10}O$	105–67–9	Alcohols	922
2,5-Dimethylphenol	$C_8H_{10}O$	95–87–4	Alcohols	923
2,6-Dimethylphenol	$C_8H_{10}O$	576–26–1	Alcohols	923
3,4-Dimethylphenol	$C_8H_{10}O$	95–65–8	Alcohols	923
3,5-Dimethylphenol	$C_8H_{10}O$	108–68–9	Alcohols	923
Dimethyl phthalate	$C_{10}H_{10}O_4$	131–11–3	Esters	976
Dimethyl m-phthalate	$C_{10}H_{10}O_4$	1459–93–4	Esters	976,977
Dimethyl o-phthalate	$C_{10}H_{10}O_4$	131–11–3	Esters	976
Dimethyl p-phthalate	$C_{10}H_{10}O_4$	120–61–6	Esters	977
Dimethyl 1,2-phthalate	$C_{10}H_{10}O_4$	131–11–3	Esters	976
Dimethyl 1,3-phthalate	$C_{10}H_{10}O_4$	1459–93–4	Esters	976,977
Dimethyl 1,4-phthalate	$C_{10}H_{10}O_4$	120–61–6	Esters	977
2,2-Dimethylpropanamide	$C_5H_{11}NO$	754–10–9	Amides	1007
N,N-Dimethylpropanamide	$C_5H_{11}NO$	758–96–3	Amides	1009
2,2-Dimethylpropane	C_5H_{12}	463–82–1	*q*-Alkanes	842
2,2-Dimethylpropane-1,3-dinitrile	$C_5H_6N_2$	7321–55–3	Nitriles	996
2,2-Dimethyl-1-propanethiol	$C_5H_{12}S$	1679–08–9	Thiols	1040
2,2-Dimethylpropanenitrile	C_5H_9N	630–18+2	Nitriles	995
2,2–Dimethylpropanoic acid	$C_5H_{10}O_2$	75-98-9	Acids	950
2,2–Dimethylpropanoic anhydride	$C_{10}H_{18}O_3$	1538–75-6	Anhydrides	964
N,N-Dimethylpropionamide	$C_5H_{11}NO$	758–96–3	Amides	1009
2,2-Dimethylpropyl ethanoate	$C_6H_{12}O_2$	540–88–5	Esters	970
2,3-Dimethylpyridine	C_7H_9N	583–61–9	CyclCHN	1004
2,4-Dimethylpyridine	C_7H_9N	108–47–4	CyclCHN	1005
2,5-Dimethylpyridine	C_7H_9N	589–93–5	CyclCHN	1005
2,6-Dimethylpyridine	C_7H_9N	108–48–5	CyclCHN	1005
3,4-Dimethylpyridine	C_7H_9N	583–58–4	CyclCHN	1005
3,5-Dimethylpyridine	C_7H_9N	591–22–0	CyclCHN	1005
2,5-Dimethylpyrrole	C_6H_9N	625–84–3	CyclCHN	1002
(*cis*–3,7a–H)–(*cis*–5,7a–H)–3,5–Dimethyl–pyrrolizidine	$C_9H_{17}N$	56160–71–5	CyclCHN	1006
2,2-Dimethylsuccinic acid	$C_6H_{10}O_4$	597–43–3	Acids	954
2,2-Dimethylsuccinic anhydride	$C_6H_8O_3$	17347–61–4	Anhydrides	964,965
meso-2,3-Dimethylsuccinic acid	$C_6H_{10}O_4$	608–40–2	Acids	954
racemic-2,3-Dimethylsuccinic acid	$C_6H_{10}O_4$	608–39–9	Acids	954,955
Dimethyl sulfate	$C_2H_6O_4S$	77–78–1	Sulfates	1055
Dimethyl sulfide	C_2H_6S	75–18–3	Sulfides	1041
Dimethyl sulfite	$C_2H_6O_3S$	616–42–2	Sulfites	1055
Dimethyl sulfone	$C_2H_6O_2S$	67–71–0	Sulfones	1050
Dimethyl sulfoxide	C_2H_6OS	67–68–5	Sulfoxides	1049
Dimethyl terephthalate	$C_{10}H_{10}O_4$	120–61–6	Esters	977
N,N-Dimethylurea	$C_3H_8N_2O$	598–94–7	Ureas	1011
1,2′-Dinaphthylmethane	$C_{21}H_{16}$	611–48–3	Cyclic03	909

TABLE 56. Name and Formula Index — Continued

TABLE 56. Name and Formula Index – Continued

Name	Formula	CAS Registry No.	Family	Page
Di-*n*-propyl ether	$C_6H_{14}O$	111–43–3	Ethers	926
Di-*n*-propyl sulfate	$C_6H_{14}O_4S$	598–05–0	Sulfates	1055
Di-*n*-propyl sulfide	$C_6H_{14}S$	111–47–7	Sulfides	1043
Di-*n*-propyl sulfite	$C_6H_{14}O_3S$	623–98–3	Sulfites	1055
Di-*n*-propyl sulfone	$C_6H_{14}O_2S$	598–03–8	Sulfones	1052
Di-*n*-propyl sulfoxide	$C_6H_{14}OS$	4253–91–2	Sulfoxides	1049,1050
Di-(1,1,3,3-tetramethylbutyl)diazene	$C_{16}H_{34}N_2$	39198–34–0	Diazene	999
Divinyl ether	C_4H_6O	109–93–3	Ethers	929
Divinyl sulfone	$C_4H_6O_2S$	77–77–0	Sulfones	1050
3,9-Dodecadiyne	$C_{12}H_{18}$	61827–89–2	Alkynes	862
5,7-Dodecadiyne	$C_{12}H_{18}$	1120–29–2	Alkynes	862
Dodecafluorocyclohexane	C_6F_{12}	355–68–0	Fluoride	1063
Dodecane	$C_{12}H_{26}$	112–40–3	*n*-Alkanes	831,832
Dodecanedioic acid	$C_{12}H_{22}O_4$	693–23–2	Acids	953
Dodecanoic acid	$C_{12}H_{24}O_2$	143–07–7	Acids	947
Dodecanol	$C_{12}H_{26}O$	112–53–8	Alcohols	911,912
n-Dodecyl alcohol	$C_{12}H_{26}O$	112–53–8	Alcohols	911,912
Dodecylbenzene	$C_{18}H_{30}$	123–01–3	Aromat01	868
Dodecylcyclohexane	$C_{18}H_{36}$	1795–17–1	Cyclic02	898
Dotriacontane	$C_{32}H_{66}$	544–85–4	*n*-Alkanes	834
E				
EGDN	$C_2H_4N_2O_6$	628–96–6	Nitrates	1032
Eicosane	$C_{20}H_{42}$	112–95–8	*n*-Alkanes	833
1-Eicosanethiol	$C_{20}H_{42}S$	13373–97–2	Thiols	1037
Eicosanoic acid	$C_{20}H_{40}O_2$	506–30–9	Acids	949,950
Eicosanol	$C_{20}H_{42}O$	629–96–9	Alcohols	914
n-Eicosanyl alcohol	$C_{20}H_{42}O$	629–96–9	Alcohols	914
Enanthonitrile	$C_7H_{13}N$	629–08–3	Nitriles	993
Enanthylic acid	$C_7H_{14}O_2$	111–14–8	Acids	946
Erythritol	$C_4H_{10}O_4$	149–32–6	Alcohols	919
Ethanal	C_2H_4O	75–07–0	Aldehyde	935
Ethanamide	C_2H_5NO	60–35–5	Amides	1006
Ethane	C_2H_6	74–84–0	*n*-Alkanes	830
Ethanedial	$C_2H_2O_2$	107–22–2	Aldehyde	935
1,2-Ethanediamine	$C_2H_8N_2$	107–15–3	Amines	983,984
Ethanedioic acid	$C_2H_2O_4$	144–62–7	Acids	951
1,2-Ethanediol	$C_2H_6O_2$	107–21–1	Alcohols	917
1,2-Ethanedithiol	$C_2H_6S_2$	540–63–6	Thiols	1037,1038
Ethanenitrile	C_2H_3N	75–05–8	Nitriles	992
Ethanethiol	C_2H_6S	75–08–1	Thiols	1035
Ethanoic acid	$C_2H_4O_2$	64–19–7	Acids	945
Ethanoic anhydride	$C_4H_6O_3$	108–24–7	Anhydrides	964
Ethanol	C_2H_6O	64–17–5	Alcohols	909
Ethenoxyethene	C_4H_6O	109–93–3	Ethers	929
Ethenylcyclopentane	C_7H_{12}	3742–34–5	Cyclic02	895
Ethenyl ethanoate	$C_4H_6O_2$	108–05–4	Esters	971
Ethoxybenzene	$C_8H_{10}O$	103–73–1	Ethers	934
Ethoxyethane	$C_4H_{10}O$	60–29–7	Ethers	926
2-Ethoxyethanol	$C_4H_{10}O_2$	110–80–5	Ethers	931
Ethoxyethene	C_4H_8O	109–92–2	Ethers	929
Ethoxypropane	$C_5H_{12}O$	628–32–0	Ethers	928
N-Ethylacetamide	C_4H_9NO	625–50–3	Amides	1008
Ethyl acetate	$C_4H_8O_2$	141–78–6	Esters	968,969
Ethyl alcohol	C_2H_6O	64–17–5	Alcohols	909
Ethyl amine	C_2H_7N	75–04–7	Amines	982
N-Ethylaniline	$C_8H_{11}N$	103–69–5	Amines	990
Ethylbenzene	C_8H_{10}	100–41–4	Aromat01	866
Ethyl benzoate	$C_9H_{10}O_2$	93–89–0	Esters	976
4-Ethyl benzophenone	$C_{15}H_{14}O$	18220–90–1	Ketones	944
Ethylbutanedioic acid	$C_6H_{10}O_4$	636–48–6	Acids	955
2-Ethyl-1-butene	C_6H_{12}	760–21–4	*s*-Alkenes	852,853
Ethyl (E)-2-butenoate	$C_6H_{10}O_2$	623–70–1	Esters	972
Ethyl *trans*-2-butenoate	$C_6H_{10}O_2$	623–70–1	Esters	972
Ethyl *tert*-butyl ketone	$C_7H_{14}O$	564–04–5	Ketones	941

TABLE 56. Name and Formula Index – Continued

Name	Formula	CAS Registry No.	Family	Page
Ethyl 4-chlorobutanoate	$C_6H_{11}ClO_2$	3153–36–4	Chloride	1082
Ethyl 2-chloropropanoate	$C_5H_9ClO_2$	535–13–7	Chloride	1081
Ethylcyclobutane	C_6H_{12}	4806–61–5	Cyclic01	891
Ethylcyclohexane	C_8H_{16}	1678–91–7	Cyclic02	897
1-Ethylcyclohexene	C_8H_{14}	1453–24–3	Cyclic02	899
Ethylcyclopentane	C_7H_{14}	1640–89–7	Cyclic01	892
1-Ethylcyclopentene	C_7H_{12}	2146–38–5	Cyclic02	896
Ethyl 2,3-dichloropropanoate	$C_5H_8Cl_2O_2$	6628–21–3	Chloride	1083
2-Ethyl-1,4-dimethylbenzene	$C_{10}H_{14}$	1758–88–9	Aromat01	870
2-Ethyl-1,3-dimethylbenzene	$C_{10}H_{14}$	2870–04–4	Aromat01	870
3-Ethyl-1,2-dimethylbenzene	$C_{10}H_{14}$	933–98–2	Aromat01	869
4-ethyl-1,2-dimethylbenzene	$C_{10}h_{14}$	934–80–5	Aromat01	870
4-Ethyl-1,3-dimethylbenzene	$C_{10}H_{14}$	874–41–9	Aromat01	870
5-Ethyl-1,3-dimethylbenzene	$C_{10}H_{14}$	934–74–7	Aromat01	870
N'-Ethyl-*N,N*-diphenylurea	$C_{15}H_{16}N_2O$	18168–01–9	Ureas	1013
Ethylene	C_2H_4	74–85–1	*n*-Alkenes	846
Ethylene carbonate	$C_3H_4O_3$	96–49–1	Carbonates	982
Ethylenediamine	$C_2H_8N_2$	107–15–3	Amines	983,984
Ethylenedinitramine	$C_2H_6N_4O_4$	26958–29–2	Nitramines	1033
Ethylene glycol	$C_2H_6O_2$	107–21–1	Alcohols	917
Ethylene glycol dinitrate	$C_2H_4N_2O_6$	628–96–6	Nitrates	1032
Ethyleneimine	C_2H_5N	151–56–4	CyclCHN	1001
Ethylene oxide	C_2H_4O	75–21–8	Ethers	932
N-Ethylethanamide	C_4H_9NO	627–45–2	Amides	1008
Ethyl ethanoate	$C_4H_8O_2$	141–78–6	Esters	968,969
Ethyl formate	$C_3H_6O_2$	109–94–4	Esters	968
3-Ethylheptane	C_9H_{20}	15869–80–4	*t*-Alkanes	839
4-Ethylheptane	C_9H_{20}	2216–32–2	*t*-Alkanes	839
2-Ethylhexanal	$C_8H_{16}O$	123–05–7	Aldehyde	937
3-Ethylhexane	C_8H_{18}	619–99–8	*t*-Alkanes	839
2-Ethyl-1-hexanol	$C_8H_{18}O$	104–76–7	Alcohols	915
Ethyl hexyl sulfide	$C_8H_{18}S$	7309–44–6	Sulfides	1045
Ethylidenecyclohexane	C_8H_{14}	1003–64–1	Cyclic02	899
Ethylidenecyclopentane	C_7H_{12}	2146–37–4	Cyclic02	894,895
Ethyl isopropyl ketone	$C_6H_{12}O$	565–69–5	Ketones	941
Ethyl methanoate	$C_3H_6O_2$	109–94–4	Esters	968
Ethyl 2-methylbutanoate	$C_7H_{14}O_2$	7452–79–1	Esters	971
1-Ethyl-1-methylcyclopentane	C_8H_{16}	16747–50–5	Cyclic03	905,906
cis-1-Ethyl-2-methylcyclopentane	C_8H_{16}	930–89–2	Cyclic03	905
trans-1-Ethyl-2-methylcyclopentane	C_8H_{16}	930–90–5	Cyclic03	905
cis-1-Ethyl-3-methylcyclopentane	C_8H_{16}	2613–66–3	Cyclic03	905
trans-1-Ethyl-3-methylcyclopentane	C_8H_{16}	2613–65–2	Cyclic03	905
2-Ethyl-3-methylnaphthalene	$C_{13}H_{14}$	31032–94–7	Aromat02	884
2-Ethyl-6-methylnaphthalene	$C_{13}H_{14}$	7372–86–3	Aromat02	884
2-Ethyl-7-methylnaphthalene	$C_{13}H_{14}$	17059–55–1	Aromat02	884
3-Ethyl-2-methylpentane	C_8H_{18}	609–26–7	*t*-Alkanes	841
3-Ethyl-3-methylpentane	C_8H_{18}	1067–08–9	*q*-Alkanes	845
Ethyl methyl sulfide	C_3H_8S	624–89–5	Sulfides	1041
Ethyl methyl sulfite	$C_3H_8O_3S$	10315–59–0	Sulfites	1055
Ethyl methyl sulfone	$C_3H_8O_2S$	594–43–4	Sulfones	1050
1-Ethylnaphthalene	$C_{12}H_{12}$	1127–76–0	Aromat02	880
2-Ethylnaphthalene	$C_{12}H_{12}$	939–27–5	Aromat02	880
Ethyl nitrate	$C_2H_5NO_3$	625–58–1	Nitrates	1032
Ethyl nitrite	$C_2H_5NO_2$	109–95–5	Nitrites	1031
3-Ethyloctane	$C_{10}H_{22}$	5881–17–4	*t*-Alkanes	839
4-Ethyloctane	$C_{10}H_{22}$	15869–86–0	*t*-Alkanes	839
Ethyl-2,4-pentadienoate	$C_7H_{10}O_2$	13038–12–5	Esters	973
3-Ethylpentane	C_7H_{16}	617–78–7	*t*-Alkanes	838
Ethyl pentanoate	$C_7H_{14}O_2$	539–82–2	Esters	970
Ethyl *cis*-2-pentenoate	$C_7H_{12}O_2$	27805–84–1	Esters	972
Ethyl *trans*-2-pentenoate	$C_7H_{12}O_2$	24410–84–2	Esters	972
Ethyl (E)-2-pentenoate	$C_7H_{12}O_2$	24410–84–2	Esters	972
Ethyl *cis*-3-pentenoate	$C_7H_{12}O_2$	27829–70–5	Esters	972
Ethyl *trans*-3-pentenoate	$C_7H_{12}O_2$	3724–66–1	Esters	972,973
Ethyl (E)-3-pentenoate	$C_7H_{12}O_2$	3724–66–1	Esters	972,973
Ethyl (Z)-2-pentenoate	$C_7H_{12}O_2$	27805–84–1	Esters	972

TABLE 56. Name and Formula Index — Continued

TABLE 56. Name and Formula Index – *Continued*

Name	Formula	CAS Registry No.	Family	Page
Heptadecane	$C_{17}H_{36}$	629–78–7	*n*-Alkanes	833
Heptadecanoic acid	$C_{17}H_{34}O_2$	506–12–7	Acids	949
Heptadecanol	$C_{17}H_{36}O$	123–24–0	Alcohols	913
n-Heptadecyl alcohol	$C_{17}H_{36}O$	123–24–0	Alcohols	913
2,2,3,3,4,4,4-Heptafluoro-1-butanol	$C_4H_3F_7O$	375–01–9	Fluoride	1064
Heptaldehyde	$C_7H_{14}O$	111–71–7	Aldehyde	936,937
Heptanal	$C_7H_{14}O$	111–71–7	Aldehyde	936,937
Heptane	C_7H_{16}	142–82–5	*n*-Alkanes	830,831
Heptanedioic acid	$C_7H_{12}O_4$	111–16–0	Acids	952
1-Heptanethiol	$C_7H_{16}S$	1639–09–4	Thiols	1036
Heptanenitrile	$C_7H_{13}N$	629–08–3	Nitriles	993
Heptanoic acid	$C_7H_{14}O_2$	111–14–8	Acids	946
Heptanol	$C_7H_{16}O$	111–70–6	Alcohols	910,911
1-Heptene	C_7H_{14}	592–76–7	*n*-Alkenes	846
cis-2-Heptene	C_7H_{14}	6443–92–1	*n*-Alkenes	849
trans-2-Heptene	C_7H_{14}	14686–13–6	*n*-Alkenes	849
cis-3-Heptene	C_7H_{14}	7642–10–6	*n*-Alkenes	850
trans-3-Heptene	C_7H_{14}	14686–14–7	*n*-Alkenes	850
n-Heptyl alcohol	$C_7H_{16}O$	111–70–6	Alcohols	910,911
Heptylbenzene	$C_{13}H_{20}$	1078–71–3	Aromat01	867
Heptylcyclohexane	$C_{13}H_{26}$	5617–41–4	Cyclic03	907
Heptylcyclopentane	$C_{12}H_{24}$	5617–42–5	Cyclic02	894
n-Heptyl-1-hydroperoxide	$C_7H_{16}O_2$	764–81–8	Hydroperoxides	979
n-Heptyl-2-hydroperoxide	$C_7H_{16}O_2$	762–46–9	Hydroperoxides	979
n-Heptyl-3-hydroperoxide	$C_7H_{16}O_2$	761–70–6	Hydroperoxides	980
n-Heptyl-4-hydroperoxide	$C_7H_{16}O_2$	761–40–0	Hydroperoxides	980
Heptyl methyl sulfide	$C_8H_{18}S$	20291–61–6	Sulfides	1045
1-Heptyne	C_7H_{12}	628–71–7	Alkynes	859
Hexachlorobenzene	C_6Cl_6	118–74–1	Chloride	1072
Hexachloroethane	C_2Cl_6	67–72–1	Chloride	1070
Hexacosane	$C_{26}H_{54}$	630–01–3	*n*-Alkanes	834
Hexadecafluoroheptane	C_7F_{16}	335–57–9	Fluoride	1059
Hexadecane	$C_{16}H_{34}$	544–76–3	*n*-Alkanes	832
1-Hexadecanethiol	$C_{16}H_{34}S$	2917–26–2	Thiols	1037
Hexadecanoic acid	$C_{16}H_{32}O_2$	57–10–3	Acids	948,949
Hexadecanol	$C_{16}H_{34}O$	36653–82–4	Alcohols	913
1-Hexadecene	$C_{16}H_{32}$	629–73–2	*n*-Alkenes	847
n-Hexadecyl alcohol	$C_{16}H_{34}O$	36653–82–4	Alcohols	913
1-Hexadecyne	$C_{16}H_{30}$	629–74–3	Alkynes	860
1,5-Hexadiyne	C_6H_6	628–16–0	Alkynes	861
Hexaethylbenzene	$C_{18}H_{30}$	604–88–6	Aromat02	872
Hexafluorobenzene	C_6F_6	392–56–3	Fluoride	1060
Hexafluoroethane	C_2F_6	76–16–4	Fluoride	1059
cis-Hexahydroindan	C_9H_{16}	4551–51–3	Cyclic02	900
trans-Hexahydroindan	C_9H_{16}	3296–50–2	Cyclic02	900
Hexaldehyde	$C_6H_{12}O$	66–25–1	Aldehyde	936
Hexamethylbenzene	$C_{12}H_{18}$	87–85–4	Aromat01	865
Hexamethyleneimine	$C_6H_{13}N$	111–49–9	CyclCHN	1003
Hexanal	$C_6H_{12}O$	66–25–1	Aldehyde	936
Hexanamide	$C_6H_{13}NO$	628–02–4	Amides	1007,1008
Hexane	C_6H_{14}	110–54–3	*n*-Alkanes	830
1,6-Hexanedinitrile	$C_6H_8N_2$	111–69–3	Nitriles	996
Hexanedioic acid	$C_6H_{10}O_4$	124–04–9	Acids	952
1,6-Hexanediol	$C_6H_{14}O_2$	629–11–8	Alcohols	919
1-Hexanethiol	$C_6H_{14}S$	111–31–9	Thiols	1036
Hexanoic acid	$C_6H_{12}O_2$	142–62–1	Acids	946
Hexanol	$C_6H_{14}O$	111–27–3	Alcohols	910
2-Hexanol	$C_6H_{14}O$	626–93–7	Alcohols	916
3-Hexanol	$C_6H_{14}O$	623–37–0	Alcohols	916
Hexanolactone	$C_6H_{10}O_2$	502–44–3	Esters	975
2-Hexanone	$C_6H_{12}O$	591–78–6	Ketones	939
3-Hexanone	$C_6H_{12}O$	589–38–8	Ketones	939
Hexaphenylethane	$C_{38}H_{30}$	17854–07–8	Cyclic03	908
1-Hexene	C_6H_{12}	592–41–6	*n*-Alkenes	846
cis-2-Hexene	C_6H_{12}	7688–21–3	*n*-Alkenes	848

TABLE 56. Name and Formula Index — Continued

TABLE 56. Name and Formula Index – Continued

TABLE 56. Name and Formula Index – Continued

Name	Formula	CAS Registry No.	Family	Page
2-Methylaniline	C_7H_9N	95–53–4	Amines	989
3-Methylaniline	C_7H_9N	108–44–1	Amines	989
4-Methylaniline	C_7H_9N	106–49–0	Amines	989
N-Methylaniline	C_7H_9N	100–61–8	Amines	990
Methyl azoethane	$C_3H_8N_2$	3880–48–6	Diazene	998
Methyl benzoate	$C_8H_8O_2$	93–58–3	Esters	976
2-Methyl benzoic acid	$C_8H_8O_2$	118–90–1	Acids	957
3-Methyl benzoic acid	$C_8H_8O_2$	99–04–7	Acids	957
4-Methyl benzoic acid	$C_8H_8O_2$	99–94–5	Acids	957
4-Methylbenzophenone	$C_{14}H_{12}O$	134–84–9	Ketones	944
Methyl benzyl ketone	$C_9H_{10}O$	103–79–7	Ketones	944
1-Methylbicyclo[4.1.0]heptane	C_8H_{14}	2439–79–4	Cyclic03	905
2-Methylbicyclo[2.2.1]hept-2-ene	C_8H_{12}	694–92–8	Cyclic03	904
1-Methylbicyclo[3.1.0]hexane	C_7H_{12}	4625–24–5	Cyclic03	903
2-Methylbiphenyl	$C_{13}H_{12}$	643–58–3	Aromat02	878
3-Methylbiphenyl	$C_{13}H_{12}$	643–93–6	Aromat02	878
4-Methylbiphenyl	$C_{13}H_{12}$	644–08–6	Aromat02	878
Methyl bromide	CH_3Br	74–83–9	Bromide	1086
2-Methyl-1,3-butadiene	C_5H_8	78–79–5	*s*-Alkenes	857
3-Methyl-1,2-butadiene	C_5H_8	598–25–4	*s*-Alkenes	858
2-Methylbutane	C_5H_{12}	78–78–4	*t*-Alkanes	835
Methylbutanedioic acid	$C_5H_8O_4$	498–21–5	Acids	954
2-Methyl-1-butanethiol	$C_5H_{12}S$	1878–18–8	Thiols	1040
2-Methyl-2-butanethiol	$C_5H_{12}S$	1679–09–0	Thiols	1039
3-Methyl-1-butanethiol	$C_5H_{12}S$	541–31–1	Thiols	1039
3-Methyl-2-butanethiol	$C_5H_{12}S$	2084–18–6	Thiols	1040
Methyl butanoate	$C_5H_{10}O_2$	623–42–7	Esters	966
2-Methylbutanoic acid	$C_5H_{10}O_2$	116–53–0	Acids	950
3-Methylbutanoic acid	$C_5H_{10}O_2$	503–74–2	Acids	950
2-Methyl-1-butanol	$C_5H_{12}O$	137–32–6	Alcohols	914
3-Methyl-1-butanol	$C_5H_{12}O$	123–51–3	Alcohols	914
2-Methyl-2-butanol	$C_5H_{12}O$	75–85–4	Alcohols	917
3-Methyl-2-butanone	$C_5H_{10}O$	563–80–4	Ketones	940
2-Methyl-1-butene	C_5H_{10}	563–46–2	*s*-Alkenes	852
2-Methyl-2-butene	C_5H_{10}	513–35–9	*s*-Alkenes	852
3-Methyl-1-butene	C_5H_{10}	563–45–1	*s*-Alkenes	853
Methyl (E)-2-butenoate	$C_5H_8O_2$	623–43–8	Esters	971
Methyl *trans*-2-butenoate	$C_5H_8O_2$	623–43–8	Esters	971
1-Methyl-4-(1-butenylsulfonyl)benzene	$C_{11}H_{14}O_2S$	111895–49–9	Sulfones	1054
1-Methyl-4-(2-butenylsulfonyl)benzene	$C_{11}H_{14}O_2S$	24931–66–6	Sulfones	1053
1-Methyl-4-(3-butenylsulfonyl)benzene	$C_{11}H_{14}O_2S$	17482–19–8	Sulfones	1053
3-Methylbutyl 2-chloropropanoate	$C_8H_{15}ClO_2$	62108–69–4	Chloride	1083
3-Methylbutyl 3-chloropropanoate	$C_8H_{15}ClO_2$	62108–70–7	Chloride	1083
Methyl-*n*-butyldiazene	$C_5H_{12}N_2$	4426–46–4	Diazene	998
3-Methylbutyl dichloroacetate	$C_7H_{12}Cl_2O_2$	37587–83–0	Chloride	1083
Methyl butyl ether	$C_5H_{12}O$	628–28–4	Ethers	927
Methyl *tert*-butyl ether	$C_5H_{12}O$	1634–04–4	Ethers	928
Methyl butyl ketone	$C_6H_{12}O$	591–78–6	Ketones	939
Methyl *tert*-butyl ketone	$C_6H_{12}O$	75–97–8	Ketones	941
3-Methyl-1-butyne	C_5H_8	598–23–2	Alkynes	860
Methyl butyrate	$C_5H_{10}O_2$	623–42–7	Esters	966
Methyl caprate	$C_{11}H_{22}O_2$	1623–43–8	Esters	967
Methyl caproate	$C_7H_{14}O_2$	106–70–7	Esters	966
Methyl caprylate	$C_9H_{18}O_2$	111–11–5	Esters	967
Methyl chloride	CH_3Cl	74–87–3	Chloride	1066
Methyl crotonate	$C_5H_8O_2$	623–43–8	Esters	971
Methylcyclobutane	C_5H_{10}	598–61–8	Cyclic01	891
Methylcyclohexane	C_7H_{14}	108–87–2	Cyclic02	896
1-Methylcyclohexene	C_7H_{12}	591–49–1	Cyclic02	898
Methylcyclopentane	C_6H_{12}	96–37–7	Cyclic01	891
1-Methylcyclopentene	C_6H_{10}	693–89–0	Cyclic02	895
3-Methylcyclopentene	C_6H_{10}	1120–62–3	Cyclic02	895,896
4-Methylcyclopentene	C_6H_{10}	1759–81–5	Cyclic02	896
2-Methyldecane	$C_{11}H_{24}$	6975–98–0	*t*-Alkanes	836
Methyl decanoate	$C_{11}H_{22}O_2$	110–42–9	Esters	967
Methyl decyl ether	$C_{11}H_{24}O$	7289–52–3	Ethers	927

TABLE 56. Name and Formula Index — Continued

Name	Formula	CAS Registry No.	Family	Page
Methyl 2,2-dimethylpropanoate	$C_6H_{12}O_2$	598–98–1	Esters	971
Methyldinitramine	$CH_3N_3O_4$	25346–05–8	Nitramines	1033
4-Methyldiphenylmethane	$C_{14}H_{14}$	620–83–7	Aromat02	875
N'-Methyl-*N,N*-diphenylurea	$C_{14}H_{14}N_2O$	13114–72–2	Ureas	1013
Methyl dodecanoate	$C_{13}H_{26}O_2$	111–82–0	Esters	967
Methyl *n*-dodecyl ketone	$C_{14}H_{28}O$	2345–27–9	Ketones	940
Methyl enanthate	$C_8H_{16}O_2$	106–73–0	Esters	967
2-Methylenebicyclo[2.2.1]heptane	C_8H_{12}	497–35–8	Cyclic03	904
N,N'-Methylene-bis-(*N,N'*-dimethylurea)	$C_7H_{16}N_4O_2$	60913–23–7	Ureas	1014
Methylenecyclobutane	C_5H_8	1120–56–5	Cyclic01	891
Methylenecyclohexane	C_7H_{12}	1192–37–6	Cyclic02	896
Methylenecyclopentane	C_6H_{10}	1528–30–9	Cyclic01	891
Methylenedinitramine	$CH_4N_4O_4$	14168–44–6	Nitramines	1033
Methyl ethanoate	$C_3H_6O_2$	79–20–9	Esters	966
1-Methyl-2-ethylbenzene	C_9H_{12}	611–14–3	Aromat01	868
1-Methyl-3-ethylbenzene	C_9H_{12}	620–14–4	Aromat01	868
1-Methyl-4-ethylbenzene	C_9H_{12}	622–96–8	Aromat01	868
3-Methyl-2-ethyl-1-butene	C_7H_{14}	7357–93–9	*s*-Alkenes	857
Methylethyldiazene	$C_3H_8N_2$	3880–48–6	Diazene	998
Methyl ethyl ether	C_3H_8O	540–67–0	Ethers	927
Methyl ethyl ketone	C_4H_8O	78–93–3	Ketones	938
2-Methyl-3-ethyl-1-pentene	C_8H_{16}	19780–66–6	*s*-Alkenes	857
Methyl fluoride	CH_3F	593–53–3	Fluoride	1058
N-Methylformamide	C_2H_5NO	123–39–7	Amides	1008
Methyl formate	$C_2H_4O_2$	107–31–3	Esters	966
N-Methylglycine	$C_3H_7NO_2$	107–97–1	Amino acids	1014
2-Methylheptane	C_8H_{18}	592–27–8	*t*-Alkanes	836
3-Methylheptane	C_8H_{18}	111002–96–1	*t*-Alkanes	837
4-Methylheptane	C_8H_{18}	589–53–7	*t*-Alkanes	838
Methyl heptanoate	$C_8H_{16}O_2$	106–73–0	Esters	967
Methyl hexadecanoate	$C_{17}H_{34}O_2$	112–39–0	Esters	968
2-Methylhexane	C_7H_{16}	591–76–4	*t*-Alkanes	836
3-Methylhexane	C_7H_{16}	589–34–4	*t*-Alkanes	837
Methyl hexanoate	$C_7H_{14}O_2$	106–70–7	Esters	966
3-Methyl-*cis*-3-hexene	C_7H_{14}	4914–89–0	*s*-Alkenes	853,854
3-Methyl-*trans*-3-hexene	C_7H_{14}	3899–36–3	*s*-Alkenes	854
Methyl hexyl ketone	$C_8H_{16}O$	111–13–7	Ketones	939
Methylhydrazine	CH_6N_2	60–34–4	Hydrazines	997
Methyl iodide	CH_3I	74–88–4	Iodide	1092
Methyl 2-iodobenzoate	$C_8H_7IO_2$	610–97–9	Iodide	1098
Methyl 3-iodobenzoate	$C_8H_7IO_2$	618–91–7	Iodide	1098
Methyl 4-iodobenzoate	$C_8H_7IO_2$	619–44–3	Iodide	1098
1-Methyl-2-isopropylbenzene	$C_{10}H_{14}$	527–84–4	Aromat01	869
1-Methyl-3-isopropylbenzene	$C_{10}H_{14}$	535–77–3	Aromat01	869
1-Methyl-4-isopropylbenzene	$C_{10}H_{14}$	99–87–6	Aromat01	869
Methyl isopropyl ether	$C_4H_{10}O$	598–53–8	Ethers	927,928
Methyl isopropyl ketone	$C_5H_{10}O$	563–80–4	Ketones	940
Methyl isovalerate	$C_6H_{12}O_2$	556–24–1	Esters	971
Methyl laurate	$C_{13}H_{26}O_2$	111–82–0	Esters	967
Methyl methacrylate	$C_5H_8O_2$	80–62–6	Esters	971
N-Methylmethanamide	C_2H_5NO	123–39–7	Amides	1008
Methyl methanoate	$C_2H_4O_2$	107–31–3	Esters	966
Methyl 2-methylbutanoate	$C_6H_{12}O_2$	868–57–5	Esters	970
Methyl 3-methylbutanoate	$C_6H_{12}O_2$	556–24–1	Esters	971
1-Methyl-4-(1-methylethenylsulfonyl)benzene	$C_{10}H_{12}O_2S$	67605–02–1	Sulfones	1053
Methyl 2-methylpropenoate	$C_5H_8O_2$	80–62–6	Esters	971
1-Methyl-4-(2-methyl-2-propenylsulfonyl)benzene	$C_{11}H_{14}O_2S$	16192–04–4	Sulfones	1054
Methyl myristate	$C_{15}H_{30}O_2$	124–10–7	Esters	968
1-Methylnaphthalene	$C_{11}H_{10}$	90–12–0	Aromat02	879
2-Methylnaphthalene	$C_{11}H_{10}$	91–57–6	Aromat02	879,880
Methyl nitrate	CH_3NO_3	598–58–3	Nitrates	1032
Methyl nitrite	CH_3NO_2	624–91–9	Nitrites	1031
1-Methyl-2-nitrobenzene	$C_7H_7NO_2$	88–72–2	Nitros	1026
1-Methyl-3-nitrobenzene	$C_7H_7NO_2$	99–08–1	Nitros	1026
1-Methyl-4-nitrobenzene	$C_7H_7NO_2$	99–99–0	Nitros	1026
2-Methyl-2-nitropropane	$C_4H_9NO_2$	594–70–7	Nitros	1024

TABLE 56. Name and Formula Index — Continued

Name	Formula	CAS Registry No.	Family	Page
N-Methyl-*N*-nitro-(2,4,6-trinitro)aniline	$C_7H_5N_5O_8$	479–45–8	Nitramines	1034
2-Methylnonane	$C_{10}H_{22}$	871–83–0	*t*-Alkanes	836
3-Methylnonane	$C_{10}H_{22}$	5911–04–6	*t*-Alkanes	837
4-Methylnonane	$C_{10}H_{22}$	17301–94–9	*t*-Alkanes	838
5-Methylnonane	$C_{10}H_{22}$	15869–85–9	*t*-Alkanes	838
Methyl nonanoate	$C_{10}H_{20}O_2$	1731–84–6	Esters	967
2-Methyloctane	C_9H_{20}	3221–61–2	*t*-Alkanes	836
3-Methyloctane	C_9H_{20}	2216–33–3	*t*-Alkanes	837
4-Methyloctane	C_9H_{20}	2216–34–4	*t*-Alkanes	838
Methyl octanoate	$C_9H_{18}O_2$	111–11–5	Esters	967
2-Methyloxirane	C_3H_6O	75–56–9	Ethers	933
Methyl palmitate	$C_{17}H_{34}O_2$	112–39–0	Esters	968
Methyl pentadecanoate	$C_{16}H_{32}O_2$	7132–64–1	Esters	968
Methyl pentadecylate	$C_{16}H_{32}O_2$	7132–64–1	Esters	968
N-Methylpentanamide	$C_6H_{13}NO$	6225–10–1	Amides	1009
Methyl pentanoate	$C_6H_{12}O_2$	624–24–8	Esters	966
2-Methylpentane	C_6H_{14}	107–83–5	*t*-Alkanes	835
3-Methylpentane	C_6H_{14}	96–14–0	*t*-Alkanes	837
2-Methyl-2-pentanethiol	$C_6H_{14}S$	1633–97–2	Thiols	1040
2-Methyl-3-pentanol	$C_6H_{14}O$	565–67–3	Alcohols	916
4-Methyl-2-pentanol	$C_6H_{14}O$	108–11–2	Alcohols	916
2-Methyl-3-pentanone	$C_6H_{12}O$	565–69–5	Ketones	941
3-Methyl-1-pentene	C_6H_{12}	29564–68–9	*s*-Alkenes	853
2-Methyl-1-pentene	C_6H_{12}	763–29–1	*s*-Alkenes	852
2-Methyl-2-pentene	C_6H_{12}	625–27–4	*s*-Alkenes	852
cis-3-Methyl-2-pentene	C_6H_{12}	922–61–2	*s*-Alkenes	853
trans-3-Methyl-2-pentene	C_6H_{12}	616–12–6	*s*-Alkenes	853
4-Methyl-1-pentene	C_6H_{12}	691–37–2	*s*-Alkenes	854
cis-4-Methyl-2-pentene	C_6H_{12}	691–38–3	*s*-Alkenes	854
trans-4-Methyl-2-pentene	C_6H_{12}	674–76–0	*s*-Alkenes	854
Methyl pentyl sulfide	$C_6H_{14}S$	1741–83–9	Sulfides	1043
Methyl perlargonate	$C_{10}H_{20}O_2$	1731–84–6	Esters	967
2-Methylphenol	C_7H_8O	95–48–7	Alcohols	921
3-Methylphenol	C_7H_8O	108–39–4	Alcohols	921
4-Methylphenol	C_7H_8O	106–44–5	Alcohols	921
3-Methylphenyl acetate	$C_9H_{10}O_2$	122–46–3	Esters	976
N-Methyl-*N*-phenylaniline	$C_{13}H_{13}N$	552–82–9	Amines	990
3-Methylphenyl ethanoate	$C_9H_{10}O_2$	122–46–3	Esters	976
Methyl phenyl ether	C_7H_8O	100–66–3	Ethers	934
1-Methyl-1-phenylethyl hydroperoxide	$C_9H_{12}O_2$	80–15–9	Hydroperoxides	980
Methyl phenyl ketone	C_8H_8O	98–86–2	Ketones	944
Methyl phenyl sulfide	C_7H_8S	100–68–5	Sulfides	1047
Methyl phenyl sulfone	$C_7H_8O_2S$	3112–85–4	Sulfones	1052
N-Methylpiperidine	$C_6H_{13}N$	626–67–5	CyclCHN	1003
2-Methylpiperidine	$C_6H_{13}N$	109–05–7	CyclCHN	1004
4-Methylpiperidine	$C_6H_{13}N$	626–58–4	CyclCHN	1004
Methyl pivalate	$C_6H_{12}O_2$	598–98–1	Esters	971
1-Methyl-4-(1,2-propadienylsulfonyl)benzene	$C_{10}H_{10}O_2S$	16192–08–8	Sulfones	1053
2-Methylpropanal	C_4H_8O	78–84–2	Aldehyde	937
N-Methylpropanamide	C_4H_9NO	1187–58–2	Amides	1009
2-Methylpropanamide	C_4H_9NO	563–83–7	Amides	1007
2-Methylpropane	C_4H_{10}	75–28–5	*t*-Alkanes	835
2-Methylpropanenitrile	C_4H_7N	78–82–0	Nitriles	994
2-Methyl-1-propanethiol	$C_4H_{10}S$	513–44–0	Thiols	1039
2-Methyl-2-propanethiol	$C_4H_{10}S$	75–66–1	Thiols	1039
Methyl propanoate	$C_4H_8O_2$	554–12–1	Esters	966
2-Methyl-1-propanol	$C_4H_{10}O$	78–83–1	Alcohols	914
2-Methyl-2-propanol	$C_4H_{10}O$	75–65–0	Alcohols	916,917
2-Methyl-1,2-propanediamine	$C_4H_{12}N_2$	811–93–8	Amines	985
2-Methyl-1,2-propanediol	$C_4H_{10}O_2$	558–43–0	Alcohols	918
2-Methylpropanoyl chloride	C_4H_7ClO	79–30–1	Chloride	1084
2-Methylpropene	C_4H_8	115–11–7	*s*-Alkenes	852
Methyl propenoate	$C_4H_6O_2$	96 33 3	Esters	971
1-Methyl-2-propenylbenzene	$C_{10}H_{12}$	934–10–1	Aromat02	874
1-Methyl-4-(2-propenylsulfonyl)benzene	$C_{10}H_{12}O_2S$	3112–87–6	Sulfones	1053

TABLE 56. Name and Formula Index — Continued

TABLE 56. Name and Formula Index – Continued

Name	Formula	CAS Registry No.	Family	Page
Nitrobenzene	$C_6H_5NO_2$	98–95–3	Nitros	1025
2-Nitrobenzoic acid	$C_7H_5NO_4$	552–16–9	Nitros	1030
3-Nitrobenzoic acid	$C_7H_5NO_4$	121–92–6	Nitros	1030,1031
4-Nitrobenzoic acid	$C_7H_5NO_4$	62–23–7	Nitros	1031
1-Nitrobutane	$C_4H_9NO_2$	627–05–4	Nitros	1023
2-Nitrobutane	$C_4H_9NO_2$	600–24–8	Nitros	1023,1024
Nitroethane	$C_2H_5NO_2$	79–24–3	Nitros	1023
Nitroglycerine	$C_3H_5N_3O_9$	55–63–0	Nitrates	1033
Nitromethane	CH_3NO_2	75–52–5	Nitros	1022
Nitromethylbenzene	$C_7H_7NO_2$	622–42–4	Nitros	1026,1027
1-Nitronaphthalene	$C_{10}H_7NO_2$	86–57–7	Nitros	1026
1-Nitropentane	$C_5H_{11}NO_2$	628–05–7	Nitros	1023
m-Nitrophenol	$C_6H_5NO_3$	554–84–7	Nitros	1027
o-Nitrophenol	$C_6H_5NO_3$	88–75–5	Nitros	1027
p-Nitrophenol	$C_6H_5NO_3$	100–02–7	Nitros	1027,1028
2-Nitrophenol	$C_6H_5NO_3$	88–75–5	Nitros	1027
3-Nitrophenol	$C_6H_5NO_3$	554–84–7	Nitros	1027
4-Nitrophenol	$C_6H_5NO_3$	100–02–7	Nitros	1027,1028
N-Nitropiperidine	$C_5H_{10}N_2O_2$	7119–94–0	Nitramines	1034
1-Nitropropane	$C_3H_7NO_2$	108–03–2	Nitros	1023
2-Nitropropane	$C_3H_7NO_2$	79–46–9	Nitros	1023
Nitrosobenzene	C_6H_5NO	586–96–9	Nitroso	1021
4-Nitroso-1-naphthol	$C_{10}H_7NO_2$	605–60–7	Nitroso	1021
N-Nitrosopiperidine	$C_5H_{10}N_2O$	100–75–4	Nitroso	1021
2-Nitrotoluene	$C_7H_7NO_2$	88–72–2	Nitros	1026
3-Nitrotoluene	$C_7H_7NO_2$	99–08–1	Nitros	1026
4-Nitrotoluene	$C_7H_7NO_2$	99–99–0	Nitros	1026
Nitrourea	$CH_3N_3O_3$	556–89–8	Nitramines	1033
Nonadecane	$C_{19}H_{40}$	629–92–5	*n*-Alkanes	833
Nonadecanoic acid	$C_{19}H_{38}O_2$	646–30–0	Acids	949
Nonadecanol	$C_{19}H_{40}O$	1454–84–8	Alcohols	913
n-Nonadecyl alcohol	$C_{19}H_{40}O$	1454–84–8	Alcohols	913
Nonadecylic acid	$C_{19}H_{38}O_2$	646–30–0	Acids	949
Nonaldehyde	$C_9H_{18}O$	124–19–6	Aldehyde	937
Nonanal	$C_9H_{18}O$	124–19–6	Aldehyde	937
Nonane	C_9H_{20}	111–84–2	*n*-Alkanes	831
Nonanedioic acid	$C_9H_{16}O_4$	123–99–9	Acids	953
1-Nonanethiol	$C_9H_{20}S$	1455–21–6	Thiols	1037
Nonanoic acid	$C_9H_{18}O_2$	112–05–0	Acids	947
Nonanol	$C_9H_{20}O$	143–08–8	Alcohols	911
5-Nonanone	$C_9H_{18}O$	502–56–7	Ketones	939,940
1-Nonene	C_9H_{18}	124–11–8	*n*-Alkenes	847
n-Nonyl alcohol	$C_9H_{20}O$	143–08–8	Alcohols	911
Nonylbenzene	$C_{15}H_{24}$	1081–77–2	Aromat01	867
Nonylcyclopentane	$C_{14}H_{28}$	2882–98–6	Cyclic02	894
1-Nonyne	C_9H_{16}	3452–09–3	Alkynes	859
Norbornadiene	C_7H_8	121–46–0	Cyclic03	902
Norbornane	C_7H_{12}	279–23–2	Cyclic03	903
Norbornene	C_7H_{10}	498–66–8	Cyclic03	903
Norleucine	$C_6H_{13}NO_2$	616–06–8	Amino acids	1016
O				
Octadecane	$C_{18}H_{38}$	593–45–3	*n*-Alkanes	833
Octadecanoic acid	$C_{18}H_{36}O_2$	57–11–4	Acids	949
Octadecanol	$C_{18}H_{38}O$	112–92–5	Alcohols	913
n-Octadecyl alcohol	$C_{18}H_{38}O$	112–92–5	Alcohols	913
1,7-Octadiyne	C_8H_{10}	871–84–1	Alkynes	862
2,2,3,3,4,4,5,5-Octafluoro-1,6-hexanediol	$C_6H_6F_8O_2$	355–74–8	Fluoride	1064
Octafluoropropane	C_3F_8	76–19–7	*Fluoride*	*1065*
Octahydroazocine	$C_7H_{15}N$	1121–92–2	CyclCHN	1005
Octaldehyde	$C_8H_{16}O$	124–13–0	Aldehyde	937
Octanal	$C_8H_{16}O$	124–13–0	Aldehyde	937
Octanamide	$C_8H_{17}NO$	629–01–6	Amides	1008
Octane	C_8H_{18}	111–65–9	*n*-Alkanes	831
Octanedioic acid	$C_8H_{14}O_4$	505–48–6	Acids	952

TABLE 56. Name and Formula Index — Continued

Name	Formula	CAS Registry No.	Family	Page
Octanenitrile	$C_8H_{15}N$	124–12–9	Nitriles	993
1-Octanethiol	$C_8H_{18}S$	111–88–6	Thiols	1036,1037
Octanoic acid	$C_8H_{16}O_2$	124–07–2	Acids	947
Octanol	$C_8H_{18}O$	111–87–5	Alcohols	911
2-Octanone	$C_8H_{16}O$	111–13–7	Ketones	939
1-Octene	C_8H_{16}	111–66–0	*n*-Alkenes	847
cis-2-Octene	C_8H_{16}	7642–04–8	*n*-Alkenes	849
trans-2-Octene	C_8H_{16}	13389–42–9	*n*-Alkenes	849
1-Octen-3-yne	C_8H_{12}	17679–92–4	Alkynes	861
Octogen	$C_4H_8N_8O_8$	2691–41–0	Nitramines	1034
n-Octyl alcohol	$C_8H_{18}O$	111–87–5	Alcohols	911
Octylbenzene	$C_{14}H_{22}$	2189–60–8	Aromat01	867
Octylcyclopentane	$C_{13}H_{26}$	1795–20–6	Cyclic02	894
1-Octyne	C_8H_{14}	629–05–0	Alkynes	859
DL-Ornithine	$C_5H_{12}N_2O_2$	616–07–9	Amino acids	1017
Oxalic acid	$C_2H_2O_4$	144–62–7	Acids	951
Oxane	$C_5H_{10}O$	142–68–7	Ethers	934
Oxetane	C_3H_6O	503–30–0	Ethers	933
2-Oxetanone	$C_3H_4O_2$	57–57–8	Esters	975
Oxirane	C_2H_4O	75–21–8	Ethers	932
Oxolane	C_4H_8O	109–99–9	Ethers	933
1,1′-Oxybisbenzene	$C_{12}H_{10}O$	101–84–8	Ethers	935
1,1′-Oxybisethene	C_4H_6O	109–93–3	Ethers	929
P				
Palmitic acid	$C_{16}H_{32}O_2$	57–10–3	Acids	948,949
2,2-Paracyclophane	$C_{16}H_{16}$	1633–22–3	Cyclic02	901
3,3-Paracyclophane	$C_{18}H_{20}$	2913–24–8	Cyclic02	901
Pelargonic acid	$C_9H_{18}O_2$	112–05–0	Acids	947
Pentachlorobenzene	C_6HCl_5	608–93–5	Chloride	1075,1076
Pentachloroethane	C_2HCl_5	76–01–7	Chloride	1070
Pentachlorophenol	C_6HCl_5O	87–86–5	Chloride	1078
Pentacosane	$C_{25}H_{52}$	629–99–2	*n*-Alkanes	834
Pentacyclo[4.2.0.0^2,5.0^3,8.0^4,7]octane	C_8H_8	277–10–1	Cyclic03	904
Pentadecane	$C_{15}H_{32}$	629–62–9	*n*-Alkanes	832
Pentadecanoic acid	$C_{15}H_{30}O_2$	1002–84–2	Acids	948
Pentadecanol	$C_{15}H_{32}O$	629–76–5	Alcohols	912
2-Pentadecanone	$C_{15}H_{30}O$	2345–28–0	Ketones	940
n-Pentadecyl alcohol	$C_{15}H_{32}O$	629–76–5	Alcohols	912
Pentadecylic acid	$C_{15}H_{30}O_2$	1002–84–2	Acids	948
1,2-Pentadiene	C_5H_8	591–95–7	*n*-Alkenes	850
cis-1,3-Pentadiene	C_5H_8	1574–41–0	*n*-Alkenes	850
trans-1,3-Pentadiene	C_5H_8	2004–70–8	*n*-Alkenes	851
1,4-Pentadiene	C_5H_8	591–93–5	*n*-Alkenes	851
2,3-Pentadiene	C_5H_8	591–96–8	*n*-Alkenes	851
Pentaerythritol	$C_5H_{12}O_4$	115–77–5	Alcohols	919
Pentaethylbenzene	$C_{16}H_{26}$	605–01–6	Aromat02	872
Pentafluorobenzene	C_6HF_5	363–72–4	Fluoride	1062,1063
Pentafluorobenzoic acid	$C_7HF_5O_2$	602–94–8	Fluoride	1064
Pentafluorophenol	C_6HF_5O	771–61–9	Fluoride	1064
2,2,3,3,3-Pentafluoro-1-propanol	$C_3H_3F_5O$	422–05–9	Fluoride	1064
2,3,4,5,6-Pentafluorotoluene	$C_7H_3F_5$	771–56–2	Fluoride	1063
Pentafluoro(trifluoromethyl)benzene	C_7F_8	434–64–0	Fluoride	1060
Pentaldehyde	$C_5H_{10}O$	110–62–3	Aldehyde	936
Pentamethyl benzoic acid	$C_{12}H_{16}O_2$	2243–32–5	Acids	961
Pentamethylbenzene	$C_{11}H_{16}$	700–12–9	Aromat01	865
Pentanal	$C_5H_{10}O$	110–62–3	Aldehyde	936
Pentanamide	$C_5H_{11}NO$	626–97–1	Amides	1007
Pentane	C_5H_{12}	109–66–0	*n*-Alkanes	830
1,5-Pentanedinitrile	$C_5H_6N_2$	544–13–8	Nitriles	996
Pentanedioic acid	$C_5H_8O_4$	110–94–1	Acids	952
1,5-Pentanediol	$C_5H_{12}O_2$	111–29–5	Alcohols	919
2,4-Pentanedione	$C_5H_8O_2$	123–54–6	Ketones	942
1,5-Pentanedithiol	$C_5H_{12}S_2$	928–98–3	Thiols	1038
Pentanenitrile	C_5H_9N	110–59–8	Nitriles	993

TABLE 56. Name and Formula Index — Continued

Name	Formula	CAS Registry No.	Family	Page
1-Pentanethiol	$C_5H_{12}S$	110–66–7	Thiols	1036
Pentanoic acid	$C_5H_{10}O_2$	109–52–4	Acids	946
Pentanol	$C_5H_{12}O$	71–41–0	Alcohols	910
2-Pentanol	$C_5H_{12}O$	6032–29–7	Alcohols	915
3-Pentanol	$C_5H_{12}O$	584–02–1	Alcohols	915
4-Pentanolactone	$C_5H_8O_2$	108–29–2	Esters	975
5-Pentanolactone	$C_5H_8O_2$	542–28–9	Esters	975
2-Pentanone	$C_5H_{10}O$	107–87–9	Ketones	938,939
3-Pentanone	$C_5H_{10}O$	96–22–0	Ketones	939
Pentanoyl chloride	C_5H_9ClO	638–29–9	Chloride	1084
Pentaphenylethane	$C_{32}H_{26}$	19112–42–6	Aromat02	877
1-Pentene	C_5H_{10}	109–67–1	*n*-Alkenes	846
cis-2-Pentene	C_5H_{10}	627–20–3	*n*-Alkenes	848
trans-2-Pentene	C_5H_{10}	646–04–8	*n*-Alkenes	848
trans-2-Pentenenitrile	C_5H_7N	26294–98–4	Nitriles	995
trans-3-Pentenenitrile	C_5H_7N	16529–66–1	Nitriles	995
cis-3-Penten-1-yne	C_5H_6	1574–40–9	Alkynes	861
trans-3-Penten-1-yne	C_5H_6	2004–69–5	Alkynes	861
2,2,3,4,4-Pentmethylpentane	$C_{10}H_{22}$	16747–45–8	*q*-Alkanes	845
n-Pentyl alcohol	$C_5H_{12}O$	71–41–0	Alcohols	910
n-Pentyl amine	$C_5H_{13}N$	110–58–7	Amines	983
Pentylbenzene	$C_{11}H_{16}$	700–12–9	Aromat01	866
Pentylcyclohexane	$C_{11}H_{22}$	4292–92–6	Cyclic02	898
Pentylcyclopentane	$C_{10}H_{20}$	3741–00–2	Cyclic02	893
1-Pentylnaphthalene	$C_{15}H_{18}$	86–89–5	Aromat02	881
2-Pentylnaphthalene	$C_{15}H_{18}$	93–22–1	Aromat02	881
1-Pentyne	C_5H_8	627–19–0	Alkynes	858,859
2-Pentyne	C_5H_8	627–21–4	Alkynes	860
Perbenzoic acid	$C_7H_6O_3$	93–59–4	Peroxyacids	980
Perdodecanoic acid	$C_{12}H_{24}O_3$	2388–12–7	Peroxyacids	980
Perfluoropropane	C_3F_8	76–19–7	Fluorides	1065
Perhexadecanoic acid	$C_{16}H_{32}O_3$	7311–29–7	Peroxyacids	981
Peroctadecanoic acid	$C_{18}H_{36}O_3$	5796–86–1	Peroxyacids	981
Peroxylauric acid	$C_{12}H_{24}O_3$	2388–12–7	Peroxyacids	980
Peroxymyristic acid	$C_{14}H_{28}O_3$	19816–73–0	Peroxyacids	980
Peroxypalmitic acid	$C_{16}H_{32}O_3$	7311–29–7	Peroxyacids	981
Peroxystearic acid	$C_{18}H_{36}O_3$	5796–86–1	Peroxyacids	981
Pertetradecanoic acid	$C_{14}H_{28}O_3$	19816–73–0	Peroxyacids	980
Perylene	$C_{20}H_{12}$	198–55–0	Aromat02	886
Phenanthrene	$C_{14}H_{10}$	85–01–8	Aromat02	885
Phenetole	$C_8H_{10}O$	103–73–1	Ethers	934
Phenol	C_6H_6O	108–95–2	Alcohols	921
N-Phenylacetamide	C_8H_9NO	103–84–4	Amides	1010
Phenyl acetate	$C_8H_8O_2$	122–79–2	Esters	976
DL-Phenylalanine	$C_9H_{11}NO_2$	150–30–1	Amino acids	1018
N-Phenylaniline	$C_{12}H_{11}N$	122–39–4	Amines	990
Phenylazide	$C_6H_5N_3$	622–37–7	Azides	1000
Phenyl benzoate	$C_{13}H_{10}O_2$	93–99–2	Esters	976
Phenylbutanedioic acid	$C_{10}H_{10}O_4$	635–51–8	Acids	963
1-Phenyl-1-butanone	$C_{10}H_{12}O$	495–40–9	Ketones	944
Phenylcarbinol	C_7H_8O	100–51–6	Alcohols	914
Phenylcyclopropane	C_9H_{10}	873–49–4	Cyclic03	906
N-Phenylethanamide	C_8H_9NO	103–84–4	Amides	1010
Phenyl ethanoate	$C_8H_8O_2$	122–79–2	Esters	976
2-Phenylethylamine	$C_8H_{11}N$	64–04–0	Amines	990
N-Phenylglycine	$C_8H_9NO_2$	103–01–5	Amino acids	1019
Phenylhydrazine	$C_6H_8N_2$	100–63–0	Hydrazines	998
N-(Phenylmethylene)benzenimine	$C_{13}H_{11}N$	538–51–2	Imines	992
Phenylnitromethane	$C_7H_7NO_2$	622–42–4	Nitros	1026,1027
1-Phenyl-1-propanone	$C_9H_{10}O$	93–55–0	Ketones	944
1-Phenyl-2-propanone	$C_9H_{10}O$	103–79–7	Ketones	944
trans-Phenyl β-styryl sulfone	$C_{14}H_{12}O_2S$	16212–06–9	Sulfones	1054
Phenylsuccinic acid	$C_{10}H_{10}O_4$	635–51–8	Acids	963
Phenyl *p*-tolyl ketone	$C_{14}H_{12}O$	134–84–9	Ketones	944
Phenylurea	$C_7H_8N_2O$	64–10–8	Ureas	1013
Phenyl vinyl sulfone	$C_8H_8O_2S$	5535–48–8	Sulfones	1052

TABLE 56. Name and Formula Index — Continued

TABLE 56. Name and Formula Index — Continued

Name	Formula	CAS Registry No.	Family	Page
N-Propylethanamide	$C_5H_{11}NO$	5331–48–6	Amides	1008
N-2-Propylethanamide	$C_5H_{11}NO$	1118–69–0	Amides	1008
Propyl ethanoate	$C_5H_{10}O_2$	109–60–4	Esters	969
4-Propylheptane	$C_{10}H_{22}$	3178–29–8	*t*-Alkanes	840
1-Propylnaphthalene	$C_{13}H_{14}$	2765–18–6	Aromat02	880
2-Propylnaphthalene	$C_{13}H_{14}$	2027–19–2	Aromat02	880
Propyl 2-pentenoate	$C_8H_{14}O_2$	62030–39–1	Esters	973,974
Propyl 3-pentenoate	$C_8H_{14}O_2$	62030–40–4	Esters	974
N-Propylpiperidine	$C_8H_{17}N$	5470–02–0	CyclCHN	1005,1006
n-Propyl nitrate	$C_3H_7NO_3$	627–13–4	Nitrates	1032
n-Propyl nitrite	$C_3H_7NO_2$	543–67–9	Nitrites	1031
Propyl pentanoate	$C_8H_{16}O_2$	141–06–0	Esters	970
Propyl phenyl ketone	$C_{10}H_{12}O$	495–40–9	Ketones	944
Propyl valerate	$C_8H_{16}O_2$	141–06–0	Esters	970
Propyne	C_3H_4	74–99–7	Alkynes	858
1-(Propynylsulfonyl)benzene	$C_9H_8O_2S$	2525–41–9	Sulfones	1052
2-(Propynylsulfonyl)benzene	$C_9H_8O_2S$	2525–40–8	Sulfones	1052
Pyrazine	$C_4H_4N_2$	290–37–9	CyclCHN	1003
Pyrene	$C_{16}H_{10}$	129–00–0	Aromat02	885
Pyridazine	$C_4H_4N_2$	289–80–5	CyclCHN	1002
Pyridine	C_5H_5N	110–86–1	CyclCHN	1001,1002
Pyrimidine	$C_4H_4N_2$	289–95–2	CyclCHN	1003
Pyrrole	C_4H_5N	109–97–7	CyclCHN	1002
Pyrrolidine	C_4H_9N	123–75–1	CyclCHN	1001
Pyrrolizidine	$C_7H_{13}N$	643–20–9	CyclCHN	1006
Q				
Quadricyclane	C_7H_8	278–06–8	Cyclic03	903
Quinoline	C_9H_7N	91–22–5	CyclCHN	1003
R				
RDX	$C_3H_6N_6O_6$	121–82–4	Nitramines	1034
Resorcinol	$C_6H_6O_2$	108–46–3	Alcohols	924
R-salt	$C_3H_6N_6O_3$	13980–04–6	Nitroso	1022
S				
Salicylic acid	$C_7H_6O_3$	69–72–7	Acids	961
Sarcosine	$C_3H_7NO_2$	107–97–1	Amino acids	1014
Sebacic acid	$C_{10}H_{18}O_4$	111–20–6	Acids	953
DL-Serine	$C_3H_7NO_3$	302–84–1	Amino acids	1017
Spiropentane	C_5H_8	157–40–4	Cyclic01	890,891
Stearic acid	$C_{18}H_{36}O_2$	57–11–4	Acids	949
cis-Stilbene	$C_{14}H_{12}$	645–49–8	Aromat02	876
trans-Stilbene	$C_{14}H_{12}$	103–30–0	Aromat02	876
Styrene	C_8H_8	100–42–5	Aromat02	873
cis-β-Styryl *p*-tolyl sulfone	$C_{15}H_{14}O_2S$	54897–33–5	Sulfones	1054
trans-β-Styryl *p*-tolyl sulfone	$C_{15}H_{14}O_2S$	16212–08–1	Sulfones	1054
Suberic acid	$C_8H_{14}O_4$	505–48–6	Acids	952
Succinamide	$C_4H_8N_2O_2$	110–14–5	Amides	1010
Succinic acid	$C_4H_6O_4$	110–15–6	Acids	951
Succinic anhydride	$C_4H_4O_3$	108–30–5	Anhydrides	964
Succinimide	$C_4H_5NO_2$	123–56–8	CyclCHNO	1035
Succinonitrile	$C_4H_4N_2$	110–61–2	Nitriles	996
T				
Terephthalic acid	$C_8H_6O_4$	100–21–0	Acids	962
ortho-Terphenyl	$C_{18}H_{14}$	84–15–1	Aromat02	879
2,3,5,6-Tetrachloro-1,4-benzenediol	$C_6H_2Cl_4O_2$	87–87–6	Chloride	1078
1,2,4,5-Tetrachloro-3,6-dimethylbenzene	$C_8H_6Cl_4$	877–10–1	Chloride	1075
1,1,2,2-Tetrachloroethane	$C_2H_2Cl_4$	79–34–5	Chloride	1070
Tetrachloroethylene	C_2Cl_4	127–18–4	Chloride	1071
1,1,1,3-Tetrachloropropane	$C_3H_4Cl_4$	1070–78–6	Chloride	1070

TABLE 56. Name and Formula Index — *Continued*

TABLE 56. Name and Formula Index – Continued

Name	Formula	CAS Registry No.	Family	Page
1,2,3-Tribromopropane	$C_3H_5Br_3$	96–11–7	Bromide	1090
Tri-*n*-butylamine	$C_{12}H_{27}N$	102–82–9	Amines	987
2,3,5-Trichloro-1,4-benzenediol	$C_6H_3Cl_3O_2$	608–94–6	Chloride	1078
2,2,3-Trichlorobutanal	$C_4H_5Cl_3O$	76–36–8	Chloride	1081
1,1,1-Trichloroethane	$C_2H_3Cl_3$	71–55–6	Chloride	1069
1,1,2-Trichloroethane	$C_2H_3Cl_3$	79–00–5	Chloride	1069
Trichloroethylene	C_2HCl_3	79–01–6	Chloride	1072
1,2,3-Trichloropropane	$C_3H_5Cl_3$	96–18–4	Chloride	1070
1,2,3-Trichloropropene	$C_3H_3Cl_3$	96–19–5	Chloride	1072
1,3,5-Trichloro-2,4,6-trifluorobenzene	$C_6Cl_3F_3$	319–88–0	Mixed	1101
1,1,1-Trichloro-3,3,3-trifluoropropane	$C_3H_2Cl_3F_3$	7125–83–9	Mixed	1100
1,1,2-Trichloro-1,2,2-trifluoroethane	$C_2Cl_3F_3$	76–13–1	Mixed	1099,1100
Tricyclo[2.2.1.0^{2,6}]heptane	C_7H_{10}	279–19–6	Cyclic03	903
Tricyclo[3.3.1.1^{3,7}]decane	$C_{10}H_{16}$	281–23–2	Cyclic02	901
Tricyclo[3.3.1.1^{3,7}]decane-1-carboxamide	$C_{11}H_{17}NO$	5511–18–2	Amides	1010
Tridecane	$C_{13}H_{28}$	629–50–5	*n*-Alkanes	832
Tridecanedioic acid	$C_{13}H_{24}O_4$	505–52–2	Acids	954
Tridecanoic acid	$C_{13}H_{26}O_2$	638–53–9	Acids	948
Tridecanol	$C_{13}H_{28}O$	112–70–9	Alcohols	912
n-Tridecyl alcohol	$C_{13}H_{28}O$	112–70–9	Alcohols	912
Tri-*n*-decylamine	$C_{30}H_{63}N$	1070–01–5	Amines	988
Tridecylic acid	$C_{13}H_{26}O_2$	638–53–9	Acids	948
Triethylamine	$C_6H_{15}N$	121–44–8	Amines	986,987
1,2,3-Triethylbenzene	$C_{12}H_{18}$	42205–08–3	Aromat02	871
1,2,4-Triethylbenzene	$C_{12}H_{18}$	877–44–1	Aromat02	871
1,3,5-Triethylbenzene	$C_{12}H_{18}$	102–25–0	Aromat02	871,872
Triethylbutanedioic acid	$C_{10}H_{18}O_4$	2103–18–6	Acids	956
Triethyleneglycol	$C_6H_{14}O_4$	112–27–6	Ethers	932
Triethylsuccinic acid	$C_{10}H_{18}O_4$	2103–18–6	Acids	956
1,1,1-Trifluoroethane	$C_2H_3F_3$	420–46–2	Fluoride	1059
1,1,2-Trifluoroethane	$C_2H_3F_3$	430–66–0	Fluoride	1059
2,2,2-Trifluoroethanol	$C_2H_3F_3O$	75–89–8	Fluoride	1063
Trifluoroethylene	C_2HF_3	359–11–5	Fluoride	1060
1,1,1-Trifluoro-2-iodoethane	$C_2H_2F_3I$	353–83–3	Mixed	1099
(Trifluoromethyl)benzene	$C_7H_5F_3$	98–08–8	Fluoride	1062
3,3,3-Trifluoro-1-propanol	$C_3H_5F_3O$	2240–88–2	Fluoride	1063
3,3,3-Trifluoropropene	$C_3H_3F_3$	677–21–4	Fluoride	1060
Tri-*n*-hexylamine	$C_{18}H_{39}N$	102–86–3	Amines	987
1,1,1-Trimethoxyethane	$C_5H_{12}O_3$	1445–45–0	Ethers	930
Trimethoxymethane	$C_4H_{10}O_3$	149–73–5	Ethers	929
Trimethylamine	C_3H_9N	75–50–3	Amines	986
1,2,3-Trimethylbenzene	C_9H_{12}	526–73–8	Aromat01	864
1,2,4-Trimethylbenzene	C_9H_{12}	95–63–6	Aromat01	864
1,3,5-Trimethylbenzene	C_9H_{12}	108–67–8	Aromat01	864
2,3,4-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	1076–47–7	Acids	959
2,3,5-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	2437–66–3	Acids	959
2,3,6-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	2529–39–7	Acids	959
2,4,5-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	528–90–5	Acids	959,960
2,4,6-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	480–63–7	Acids	960
3,4,5-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	1076–88–6	Acids	960
2,2,3-Trimethylbutane	C_7H_{16}	464–06–2	*q*-Alkanes	843
Trimethylbutanedioic acid	$C_7H_{12}O_4$	2103–16–4	Acids	955
2,3,3-Trimethyl-1-butene	C_7H_{14}	594–56–9	*s*-Alkenes	856
Trimethylene glycol	$C_3H_8O_2$	504–63–2	Alcohols	917
Trimethylene oxide	C_3H_6O	503–30–0	Ethers	933
Trimethyl isocyanurate	$C_6H_9N_3O_3$	827167	CyclCHN	1014
2,2,3–Trimethylpentane	C_8H_{18}	564–02-3	*q*-Alkanes	843,844
2,2,4-Trimethylpentane	C_8H_{18}	540–84–1	*q*-Alkanes	844
2,3,3-Trimethylpentane	C_8H_{18}	560–21–4	*q*-Alkanes	844
2,3,4-Trimethylpentane	C_8H_{18}	565–75–3	*t*-Alkanes	842
2,2,4-Trimethyl-3-pentanone	$C_8H_{16}O$	5857–36–3	Ketones	941
2,4,4-Trimethyl-1-pentene	C_8H_{16}	107–39–1	*s*-Alkenes	857
2,4,4-Trimethyl-2-pentene	C_8H_{16}	107–40–4	*s*-Alkenes	857
Trimethylsuccinic acid	$C_7H_{12}O_4$	2103–16–4	Acids	955
Trimethylurea	$C_4H_{10}N_2O$	632–14–4	Ureas	1011
2,4,6-Trinitroaniline	$C_6H_4N_4O_6$	489–98–5	Nitros	1030

TABLE 56. Name and Formula Index – Continued

Name	Formula	CAS Registry No.	Family	Page
1,3,5-Trinitrobenzene	$C_6H_3N_3O_6$	99–35–4	Nitros	1026
Trinitromethane	CHN_3O_6	517–25–9	Nitros	1022
2,4,6-Trinitrophenol	$C_6H_3N_3O_7$	29663–11–4	Nitros	1028
2,4,6-Trinitrotoluene	$C_7H_5N_3O_6$	118–96–7	Nitros	1027
Tri-*n*-nonylamine	$C_{27}H_{57}N$	2044–22–6	Amines	987,988
Tri-*n*-octylamine	$C_{24}H_{51}N$	1116–76–3	Amines	987
3,5,7-Trioxanonane	$C_6H_{14}O_3$	111–96–6	Ethers	930,931
Triphenylamine	$C_{18}H_{15}N$	603–34–9	Amines	988
Triphenylazidomethane	$C_{19}H_{15}N_3$	14309–25–2	Azides	1001
1,3,5-Triphenylbenzene	$C_{24}H_{18}$	612–71–5	Aromat02	879
Triphenylcarbinol	$C_{19}H_{16}O$	76–84–6	Alcohols	917
Triphenylene	$C_{18}H_{12}$	217–59–4	Aromat02	885
1,1,1-Triphenylethane	$C_{20}H_{18}$	5271–39–6	Aromat02	877
1,1,2-Triphenylethane	$C_{20}H_{18}$	1520–42–9	Aromat02	877
Triphenylethylene	$C_{20}H_{16}$	58–72–0	Aromat02	877
Triphenylmethane	$C_{19}H_{16}$	519–73–3	Aromat02	876
Triphenylmethanol	$C_{19}H_{16}O$	76–84–6	Alcohols	917
Triphenylmethylazide	$C_{19}H_{15}N_3$	14309–25–2	Azides	1001
Tri-*n*-propylamine	$C_9H_{21}N$	102–69–2	Amines	987
Tritriacontane	$C_{33}H_{68}$	630–05–7	*n*-Alkanes	835
L-Tyrosine	$C_9H_{11}NO_3$	60–18–4	Amino acids	1018
U				
Undecane	$C_{11}H_{24}$	1120–21–4	*n*-Alkanes	831
Undecanedioic acid	$C_{11}H_{20}O_4$	1852–04–6	Acids	953
Undecanenitrile	$C_{11}H_{21}N$	2244–07–7	Nitriles	993,994
Undecanoic acid	$C_{11}H_{22}O_2$	112–37–8	Acids	947
Undecanol	$C_{11}H_{24}O$	112–42–5	Alcohols	911
Undecanolactone	$C_{11}H_{20}O_2$	710–04–3	Esters	975
6-Undecanone	$C_{11}H_{22}O$	927–49–1	Ketones	940
Undecylbenzene	$C_{17}H_{28}$	6742–54–7	Aromat01	867
Undecylic acid	$C_{11}H_{22}O_2$	112–37–8	Acids	947
Undecylnitrile	$C_{11}H_{21}N$	2244–07–7	Nitriles	993,994
Urea	CH_4N_2O	57–13–6	Ureas	1011
V				
Valeric acid	$C_5H_{10}O_2$	109–52–4	Acids	946
γ-Valerolactone	$C_5H_8O_2$	108–29–2	Esters	975
δ-Valerolactone	$C_5H_8O_2$	542–28–9	Esters	975
Valeronitrile	C_5H_9N	110–59–8	Nitriles	993
L-Valine	$C_5H_{11}NO_2$	72–18–4	Amino acids	1016
Valylphenylalanine	$C_{14}H_{20}N_2O_3$	3918–92–1	Amino acids	1021
Vinyl acetate	$C_4H_6O_2$	108–05–4	Esters	971
Vinylcyclohexane	C_8H_{14}	695–12–5	Cyclic03	904
W,X,Y,Z				

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Appendix 1. Groups Derived from Thermodynamic Data for a Single Compound as Its Source

Groups which have emerged from a thermodynamic value for single compound and which are not cyclic structures are characterized by having residuals equal to zero and are listed below in Table 1–1. Cyclic compound which requires a ring strain correction and result in having zero residuals are excuded from this list but can be found in Table 2. Also excluded from this list are any molecular corrections, such as the *cis* correction, *ortho*, *meta*, and *para* corrections, and corrections for functional groups on adjacent carbon atoms. Compounds which can be described by a single group and cannot be estimated by group additivity, such as methane, formaldehyde, acetonitrile, nitromethane, methyl chloride, etc., are also found in Table 2.

TABLE 1–1. Groups derived from data on a single compound

Group	Source compound
$C-(H)(C)_2(C_t)$	3-Methyl-1-butyne
$C-(C)_2(C_t)_2$	3,3-Dimethylpenta-1,4-diyne
$C_d-(C)(C_B)$	α-Methylstyrene
$C-(H)_2(C_d)(C_B)$	2-Propenylbenzene
$C-(H)(C)(C_d)(C_B)$	1-Methyl-2-propenyl-benzene
$C-(O)_3(C)$	1,1,1-Trimethoxyethane
$CO-(H)(CO)$	Glyoxal
$CO-(H)(C_d)$	*trans*-2-Butenal
$CO-(H)(C_B)$	Benzaldehyde
$CO-(C_B)(CO)$	Benzil
$CO-(C)(CO)$	Biacetyl
$C-(C)_2(CN)_2$	2,2-Dimethylpropane-1,3-dinitrile
$C-(C)_3(CN)$	2,2-Dimethylpropanenitrile
$C-(C_B)_3(N_3)$	Triphenylmethyl azide
$C-(H)(C)_2(N_A)$	Diisopropyldiazene
$C_B-(CNO)$	1,4-Benzodinitrile *N*-oxide
$C-(H)_2(C_B)(NO_2)$	Nitromethylbenzene
$S-(H)(C_B)$	Benzenethiol
$C-(H)_2(C_B)(S)$	Benzyl mercaptan
$S-(C_B)_2$	Diphenyl sulfide
$S-(C_B)(S)$	Diphenyl disulfide
$C-(C)_3(SO)$	*tert*-Butyl ethyl sulfoxide
$SO_2-(C_d)_2$	Divinyl sulfone
$SO_2-(C_B)_2$	Diphenyl sulfone
$SO_2-(C_B)(SO_2)$	Diphenyl disulfone
$CO-(C)(F)$	Acetyl fluoride
$C_t-(Cl)$	1-Chloropropyne
$C-(H)_2(C_B)(Cl)$	Benzyl chloride
$CO-(C)(Cl)$	Acetyl chloride
$CO-(C_B)(Cl)$	Benzoyl chloride
$C_t-(Br)$	1-Bromopropyne
$C-(H)_2(C_B)(Br)$	Benzyl bromide
$CO-(C)(Br)$	Acetyl bromide
$C-(C)_3(I)$	2-Iodo-2-methylpropane
$C_t-(I)$	1-Iodopropyne
$C-(H)_2(C_B)(I)$	Benzyl iodide
$CO-(C)(I)$	Acetyl Iodide
$C-(H)(C)(Cl)(F)$	1-Chloro-1-fluoroethane
$C-(H)(C)(Br)(Cl)$	1,2-Dibromo-1,2-dichloro-ethane
$C-(C)(Br)(F)_2$	1,2-Dibromotetrafluoro-ethane
$C_d-(Cl)(F)$	Chlorotrifluoroethylene

Appendix 2. Comparison of Literature Data for Enthalpies and Entropies of Fusion and Enthalpies of Vaporization with the Estimated Differences for [$\Delta_f H°$(liq) – $\Delta_f H°$(g)], [$\Delta_f H°$(solid) – $\Delta_f H°$(liq)], and [$S°$(solid) – $S°$(liq)], at 298.15 K

We have shown that internal consistency exists when comparisons are made between literature data for enthalpies and entropies of fusion and vaporization and the estimated differences for [$\Delta_f H°$(liq) – $\Delta_f H°$(g)], [$\Delta_f H°$(solid) – $\Delta_f H°$(liq)], and [$S°$(solid) – $S°$(liq)], at 298.15 K.

Tables 2–1, 2–2, and 2–3 compare recommended values for the standard enthalpy of vaporization at 298.15 K from 85MAJ/SVO, and differences between [$\Delta_f H°$(liq) – $\Delta_f H°$(g)] from 86TRC and 69STU/WES with our estimated difference for [$\Delta_f H°$(liq) – $\Delta_f H°$(g)] for *n*-alkanes, thiols, and alkyl sulfides. General agreement is observed, usually within less than 1.0 kJ·mol^{-1}, and shows that $\Delta_{vap}H°$ = [$\Delta_f H°$(liq) – $\Delta_f H°$(g)] provides a measure of internal consistency for group additivity as applied to these homologous series.

Tables 2–4 and 2–5 compare literature data for 25 organic compounds with their enthalpies and entropies of fusion, corrected to 298.15 K, with our estimated differences for [$\Delta_f H°$(solid) – $\Delta_f H°$(liq)] and [$S°$(solid) – $S°$(liq)].

Equations used to correct $\Delta_{fus}H°$ and $\Delta_{fus}S°$ from the melting temperature (T_m) to 298.15 K are:

$$\Delta_{fus}H° \text{ at } 298.15\text{ K} = \Delta_{fus}H° \text{ at } T_m + (\Delta C_p)(298.15 - T_m)$$

$$\Delta_{fus}S° \text{ at } 298.15\text{ K} = \Delta_{fus}S° \text{ at } T_m + (\Delta C_p)\ln(298.15/T_m),$$

where ΔC_p is the difference between C_p(liq) and C_p(solid) over the temperature range from T_m to 298.15 K.

Comparison of $\Delta_{fus}H°$ corrected to 298.15 K with our estimated difference of [$\Delta_f H°$(solid) – $\Delta_f H°$(liq)] from the two columns on the right in Table 2–4 results in an average deviation of ±2.7 kJ·mol^{-1}. A similar comparison of $\Delta_{fus}S°$ corrected to 298.15 K with our estimated difference of [$S°$(solid) – $S°$(liq)] from the two columns on the right in Table 2–5 results in an average deviation of ±4.7 J·mol^{-1}·K^{-1}.

Table 2–6 gives a comparison of literature values for $\Delta_{vap}H°$ corrected to 298.15 K with our estimated difference of [$\Delta_f H°$(liq) $\Delta_f H°$(g)]; the two columns on the right of Table 2–6 should be compared, which result in an average deviation of ±1.6 kJ·mol^{-1}. The equation used tc correct data on $\Delta_{vap}H°$ at the boiling temperature (T_b) to 298.15 K is:

$$\Delta_{vap}H° \text{ at } 298.15\text{ K} = \Delta_{vap}H° \text{ at } T_b + (\Delta C_p)(298.15 - T_b),$$

where ΔC_p is the difference between C_p(liq) and C_p(g) over the temperature range from T_b to 298.15 K.

Please note that our estimated [$S°$(g) – $S°$(liq)] at 298.15 is not comparable to the entropy of vaporization corrected to 298.15 K because the former also contains conributions for the entropy of compression, $R\ln P$, and for the difference between the ideal and real gas entropies at 298.15 K.

Although the heat capacity in the gas, liquid, and solid phases appears to have a linear character within a given phase at 298.15 K, the experimental heat capacity difference between the liquid/solid phases does not correlate well with the estimated [C_p(liq) – C_p(solid)] at 298.15 K for several reasons, such as: (1) the inexactness of extrapolation of ΔC_p at the melting or boiling temperatures to 298.15 K, especially if T_m or T_b is signifcantly far from 298.15 K, (2) premelting phenomena in the region before reaching T_m, (3) solid/solid phase or lambda transitions near T_m, (4) the non-linearity of heat capacity with temperature in the condensed phase, and (5) minima or maxima in the heat capacity between T_m and T_b for some organic liquids.

TABLE 2–1. Comparison of literature data for $[\Delta_f H°(liq) - \Delta_f H°(g)]$ at 298.15 K and enthalpies of vaporization corrected to 298.15 K with estimated $[\Delta_f H°(liq) - \Delta_f H°(g)]$ for *n*-alkanes

n-Alkane	$\Delta_{vap}H°$ (85MAJ/SVO) kJ·mol^{-1}	$\Delta_f H°(l-g)$[a] (86TRC) kJ·mol^{-1}	$\Delta_f H°(l-g)$[a] (69STU/WES) kJ·mol^{-1}	$\Delta_f H°(l-g)$[a] (this work) kJ·mol^{-1}
Butane	19.99	21.74	21.46	20.90
Pentane	26.75	26.73	26.78	26.00
Hexane	31.73	31.74	31.63	31.10
Heptane	36.66	36.57	36.61	36.20
Octane	41.53	41.51	41.51	41.30
Nonane	46.43	46.44	46.44	46.40
Decane	51.39	51.37	51.38	51.50
Undecane	56.43	56.35	56.27	56.60
Dodecane	61.51	61.30	60.67	61.70
Tridecane	66.43	66.36	66.19	66.80
Tetradecane	71.30	71.09	71.13	71.90
Pentadecane	76.11	76.19	76.15	77.00
Hexadecane	81.38	81.38	83.01	82.10
Heptadecane	86.02	86.02	85.94	87.20
Octadecane	–	91.07	93.97	92.30

[a]$\Delta_f H°(l-g) = [\Delta_f H°(liq) - \Delta_f H°(g)]$

TABLE 2–2. Comparison of literature data for $[\Delta_f H°(liq) - \Delta_f H°(g)]$ at 298.15 K and enthalpies of vaporization corrected to 298.15 K with estimated $[\Delta_f H°(liq) - \Delta_f H°(g)]$ for *n*-alkanethiols

Thiol	$\Delta_{vap}H°$ (85MAJ/SVO) kJ·mol^{-1}	$\Delta_f H°(l-g)$[a] (86TRC) kJ·mol^{-1}	$\Delta_f H°(l-g)$[a] (69STU/WES) kJ·mol^{-1}	$\Delta_f H°(l-g)$[a] (this work) kJ·mol^{-1}
Methanethiol	–	23.80	23.81	23.93
Ethanethiol	27.52	27.30	27.53	27.53
Propanethiol	32.05	32.00	32.00	32.63
Butanethiol	37.70	36.50	36.57	36.73
Pentanethiol	41.26	42.00	41.13	42.83
Hexanethiol	–	45.80	46.61	47.93
Decanethiol	65.48	65.50	65.10	68.33

[a]$\Delta_f H°(l-g) = [\Delta_f H°(liq) - \Delta_f H°(g)]$

TABLE 2–3. Comparison of literature data for $[\Delta_f H°(liq) - \Delta_f H°(g)]$ at 298.15 K and enthalpies of vaporization corrected to 298.15 K with estimated $[\Delta_f H°(liq) - \Delta_f H°(g)]$ for alkyl sulfides

Sulfide	$\Delta_{vap}H°$ (85MAJ/SVO) kJ·mol^{-1}	$\Delta_f H°(l-g)$ (86TRC) kJ·mol^{-1}	$\Delta_f H°(l-g)$ (69STU/WES) kJ·mol^{-1}	$\Delta_f H°(l-g)$ (this work) kJ·mol^{-1}
Dimethyl	27.99	27.90	27.87	27.87
Methyl ethyl	31.99	31.90	31.97	31.47
Methyl propyl	36.31	36.30	36.28	36.57
Methyl *n*-butyl	41.50	40.70	40.71	40.67
Methyl *tert*-butyl	35.90	35.90	35.82	34.89
Methyl pentyl	45.25	45.00	45.19	46.77
Diethyl	35.88	35.90	35.86	35.07
Ethyl propyl	40.01	40.10	40.08	40.17
Ethyl *n*-butyl	45.25	45.20	45.10	45.27
Ethyl *tert*-butyl	–	39.90	39.33	38.48

[a]$\Delta_f H°(l-g) = [\Delta_f H°(liq) - \Delta_f H°(g)]$

TABLE 2-4. Comparison of literature data for enthalpies of fusion with estimated [$\Delta_f H°$(solid) − $\Delta_f H°$(liq)] at 298.15 K

Compound	$\Delta_{fus}H°$ at T_m kJ·mol⁻¹	Reference	$(\Delta C_p)(\Delta T)$ correction kJ·mol⁻¹	$\Delta_{fus}H°$ 298.15 K kJ·mol⁻¹	$\Delta_f H°(s-l)$[a] 298.15 K (this work) kJ·mol⁻¹
Hexane	13.08	46DOU/HUF	5.15	18.23	12.98
Heptane	14.04	61HUF/GRO	6.52	20.56	16.66
2,2,4-Trimethyl-pentane	9.21	40PIT	3.95	13.16	10.71
Hexadecane	53.36	54FIN/GRO	0.50	53.86	49.78
Octadecane	60.48	57MES/GUT	−0.23	60.25	57.14
Benzene	9.87	48OLI/EAT	0.06	9.93	9.78
Toluene	6.64	62SCO/GUT	5.50	12.14	12.16
Naphthalene	18.23	57MCC/FIN	−0.47	17.76	16.50
Butanol	9.37	65COU/HAL	4.32	13.69	11.85
Hexanol	15.38	29KEL2	3.08	18.46	19.21
Tetradecanol	49.40	91STE/CHI	−0.77	48.63	48.65
1,6-Hexanediol	22.60	91STE/CHI	−1.00	21.60	25.44
Phenol	11.51	63AND/COU	−1.03	10.48	9.04
Diphenyl ether	17.22	51FUR/GIN	−0.11	17.11	14.01
Benzophenone	18.19	83DEK/VAN	−1.66	16.53	18.00
Acetic acid	11.72	82MAR/AND	0.30	12.02	−0.13
Propionic acid	10.66	82MAR/AND	1.21	11.87	3.63
Tetradecanoic acid	45.10	82SCH/MIL2	−0.67	44.43	44.11
Hexadecanoic acid	53.71	82SCH/MIL2	−0.86	52.85	51.47
Benzoic acid	18.00	51FUR/MCC	−5.64	12.36	12.01
Aniline	10.54	62HAT/HIL	1.70	12.24	10.50
Benzonitrile	10.98	84LEB/BYK	0.73	11.71	9.33
Methyl phenyl sulfide	14.84	74MES/FIN	2.18	17.02	16.87
Chlorobenzene	9.56	37STU	1.28	10.84	7.95
Bromobenzene	10.70	75MAS/SCO	1.76	12.46	10.80

[a] $\Delta_f H°(s-l)$ = [$\Delta_f H°$(solid) − $\Delta_f H°$(liq)]

TABLE 2-5. Comparison of literature data for entropies of fusion with estimated [$S°$(solid) $S°$(liq)] at 298.15 K

Compound	$\Delta_{fus}S°$ at T_m J·mol⁻¹·K⁻¹	Reference	$(\Delta C_p)\ln(T/T_m)$ J·mol⁻¹·K⁻¹	$\Delta_{fus}S°$ 298.15 K J·mol⁻¹·K⁻¹	$S°(s-l)_a$ 298.15 K (this work) J·mol⁻¹·K⁻¹
Hexane	73.55	46DOU/HUF	21.97	95.52	90.70
Heptane	76.90	61HUF/GRO	27.64	104.54	100.07
2,2,4-Trimethyl-pentane	55.56	40PIT	17.51	73.07	69.96
Hexadecane	183.15	54FIN/GRO	1.70	184.85	184.40
Octadecane	204.60	57MES/GUT	−0.77	203.83	203.14
Benzene	35.40	48OLI/EAT	0.21	35.61	36.72
Toluene	37.25	62SCO/GUT	23.62	60.87	63.31
Naphthalene	51.57	57MCC/FIN	−1.45	50.12	49.88
Butanol	50.79	65COU/HAL	18.25	69.04	68.48
Hexanol	68.11	29KEL2	11.81	79.92	87.22
Tetradecanol	158.84	91STE/CHI	−2.52	156.32	162.18
1,6-Hexanediol	71.75	91STE/CHI	−3.26	68.49	71.78
Phenol	36.66	63AND/COU	−3.36	33.30	33.69
Diphenyl ether	57.38	51FUR/GIN	−0.32	57.06	57.01
Benzophenone	56.67	83DEK/VAN	−4.11	52.56	–
Acetic acid	40.46	82MAR/AND	1.03	41.49	43.70
Propionic acid	42.19	82MAR/AND	4.42	46.61	58.84
Tetradecanoic acid	137.79	82SCH/MIL2	−2.15	135.64	161.91
Hexadecanoic acid	160.02	82SCH/MIL2	−2.71	157.31	180.65
Benzoic acid	45.51	51FUR/MCC	−16.36	29.15	–
Aniline	39.46	62HAT/HIL	6.02	45.48	45.45
Benzonitrile	42.16	84LEB/BYK	2.62	44.78	44.90
Methyl phenyl sulfide	57.85	74MES/FIN	7.88	65.73	–
Chlorobenzene	41.93	37STU	4.90	46.83	42.70
Bromobenzene	44.15	75MAS/SCO	6.54	50.69	51.00

[a] $S°(s-l)$ = [$S°$(solid) − $S°$(liq)]

TABLE 2–6. Comparison of literature data for enthalpies of vaporization with estimated $[\Delta_f H°(liq) - \Delta_f H°(g)]$ at 298.15 K

Compound	$\Delta_{vap}H°$ at T_b kJ·mol^{-1}	Reference	$(\Delta C_p)(\Delta T)$ kJ·mol^{-1}	$\Delta_{vap}H°$ at 298 K kJ·mol^{-1}	$\Delta_f H°(l-g)$[a] at 298 K (this work) kJ·mol^{-1}
Hexane	–	47OSB/GIN	–	31.54	31.10
Heptane	–	47OSB/GIN	–	36.54	36.20
2,2,4-Trimethyl-pentane	31.00	40PIT	4.24	35.24	36.26
Hexadecane	–	72MOR	–	81.38	82.10
Octadecane	–	45PRO/ROS2	–	90.88	92.30
Benzene	–	47OSB/GIN	–	33.84	33.90
Toluene	–	45PRO/ROS2	–	37.99	38.08
Naphthalene[b]	–	63MIL	–	72.42	70.24
Butanol	–	66WAD2	–	52.30	50.62
Hexanol	–	66WAD2	–	61.63	60.82
Tetradecanol[b]	–	91STE/CHI	–	104.90	101.62
1,6-Hexanediol	–	91STE/CHI	–	102.90	90.54
Phenol[b]	45.69	60AND/BID	22.97	68.66	69.60
Diphenyl ether	–	72MOR2	–	65.98	65.83
Benzophenone	–	83DEK/VAN	–	76.68	75.50
Acetic acid	23.70	85MAJ/SVO	27.90	51.60	48.82
Propionic acid	–	85MAJ/SVO	–	55.00	51.00
Tetradecanoic acid[b]	141.00	61DAV/MAL	–	–	151.33
Hexadecanoic acid[b]	153.55	61DAV/MAL	–	–	168.89
Benzoic acid[b]	–	72MOR2	–	89.50	91.60
Aniline	42.44	85MAJ/SVO	13.39	55.83	55.70
Benzonitrile	–	59EVA/SKI	–	55.48	56.87
Methyl phenyl sulfide	–	72GOO2	–	54.31	52.47
Chlorobenzene	35.19	85MAJ/SVO	5.81	41.00	43.42
Bromobenzene	–	85MAJ/SVO	–	41.31	44.70

[a] $\Delta_f H°(s-l) = [\Delta_f H°(solid) - \Delta_f H°(liq)]$
[b] Sublimation (c/g)

Appendix 3. Comparison between Second-Order Group Additivity Approach (Benson) and the Extended Second-Order Group Additivity Approach (Pedley)

A group-additivity scheme has been developed for the estimation of enthalpies of formation in the gas phase at 298.15 K and 101.325 kPa by J. B. Pedley, R. D. Naylor, and S. P. Kirby (86PED/NAY, Chapters 2, 3, and 4) which extends the molecular parameterization of an organic compound in contrast to the limited parameterization used by Benson (76BEN). The more comprehensive account of nearest- and next-to-nearest-neighbor interactions by 86PED/NAY is expected to lead to smaller differences between experimental and estimated values. Because of a higher degree of parameterization and specificity, the scheme becomes more complex. An example of the more comprehensive parameterization can be shown in an examination of the $-CH_2-$ increment in hydrocarbons. The second-order approach of developed by Benson (76BEN) uses the notation: $C-(H)_2(C)_2$, which means that a carbon atom with two hydrogen atoms is also bonded to two other carbon atoms. No restriction is placed upon the kind of carbon atoms the $-CH_2-$ is bonded to in the Benson scheme's notation and there is only *one* assigned value for a given property for the gas phase. For example, a value of -20.63 kJ/mol has been used for $\Delta_f H°$ in the gas phase for $C-(H)_2(C)_2$ by 76BEN and also in this work.

The group additivity estimation scheme developed by (86PED/NAY) allows one to specify the nearest and next-to-nearest neighbors in an explicit manner and, hence, has the quality of an extended second-order or third-order approach. The codes used by (86PED/NAY) are different than those used by Benson and are shown in Table 3–1. In Table 3–2, one observes that groups other than $-CH_2-$ also have a significant number of extended parameters for their molecular description. Using the $-CH_2-$ increment as an example, one finds that 86PED/NAY uses the notation: 2(1 1) for $-CH_2-$ and has assigned 20 possible choices to it for hydrocarbons for estimating the enthalpy of formation in the gas phase. The 20 choices specify discrete carbon groups attached to the $-CH_2-$ group and are shown in Table 3–3. Each of the discrete values for the $-CH_2-$ has the intrinsic quality of accommodating the interactions between two- and three-centre groups, thus, accounting for their differences.

Table 3–4 compares estimated values for the enthalpy of formation of 20 hydrocarbons consisting of some alkanes, alkenes, and alkynes in the gas phase, using the Pedley estimation scheme and using the one in this work developed by Benson and co-workers, with experimentally determined values. Also, provided are selected enthalpies of formation from the tables of thermodynamic properties of hydrocarbons and related compounds compiled in the Thermodynamics Research Center (TRC) at Texas A&M University (86TRC) for comparison with the experimental values used in this work. The difference between the $\Delta_f H°$expt'l and $\Delta_f H°$est'd from (86PED/NAY) and this work shows average deviations of 0.6 and 0.5 kJ/mol, respectively. We feel that a different set of 20 or more hydrocarbons would give about the same kind of average deviations. We conclude from Table 3–4 that the Pedley approach with extended parameterization of groups and group values shows about the same overall differences in the estimated enthalpies of formation when compared to those calculated in this work.

Table 3–5 is similar to Table 3–4 except that alcohols, ethers, ketones, and acids form the basis of the comparison. In Table 3–5, the difference between the $\Delta_f H°$expt'l and $\Delta_f H°$est'd from 86PED/NAY and this work gives average deviations of 1.8 and 1.2 kJ/mol, respectively. Here again, in Table 3–5 the differences reflected in the average deviations suggest that about the same kind of general agreement between experimental and estimated $\Delta_f H°$'s are found as a result of extended parameterization of groups and group values.

The estimation method developed by (86PED/NAY) is clearly described, very systematic, and very scrupulous in its accounting of groups and group interactions. However, from the limited testing and comparisons which we have carried out, we do not see any significant improvement in the differences between experimental and estimated values for the enthalpies of formation in the gas phase. There are differences in the common base of comparison with respect to experimental values as listed in Tables 3–4 and 3–5, however, these tend to be generally small. We have retained any bias in the choice of experimental values used by 86PED/NAY and those used in this work. The selected values for $\Delta_f H°$'s from TRC (86TRC, 86TRC2) makes for another interesting comparison with both experimental and estimated values.

TABLE 3–1. Group and group codes for aliphatic hydrocarbons and aliphatic oxygen compounds (86PED/NAY)

Group name	Group	Pedley code
methyl	– CH_3	1
methylene	> CH_2	2
tertiary C	> CH-	3
quaternary C	> C <	4
ethenic C	= CH_2	5
subst. ethenic C	= CH–	6
acetylenic C	≡ CH	7
subst. acetylenic C	≡ C–	8
allenic	= C =	9
hydroxyl OH	– OH	O1
ether O	> O	O2
ketone CO	> CO	K2
acid COOH	– COOH	O1(K2)

TABLE 3–2. Group comparisons for aliphatic hydrocarbons and aliphatic organic oxygen compounds

Group	No. of groups needed		
	Benson	Pedley	This work
–CH_3	1	1	1
–CH_2–	1	24	1
–CH <	1	19	1
> C <	1	14	1
primary –OH	1	4	1
secondary –OH	1	4	1
tertiary –OH	1	2	1
ether O	1	12	1
ketone CO	1	10	1
acid –COOH	2	4	2
Corrections for:			
Alkane gauche	1	0	0
Alkene gauche	1	0	0
1,4 repulsion	0	0	1
1,5 repulsion	1	0	1
methyl group repulsion	0	0	4
alkene cis	1	0	1

TABLE 3–3. Group specificity and values for bonding of –CH_2– to two carbon atoms in aliphatic hydrocarbons (86PED/NAY)

Pedley notation for –CH_2–	specific group equivalent	group value (kJ/mol)
2(1 1)[a]	CH_3–CH_2–CH_3	–20.90
2(2 1)	–CH_2–CH_2–CH_3	–20.80
2(2 2)	–CH_2–CH_2–CH_2–	–20.80
2(3 1)	> CH–CH_2–CH_3	–20.20
2(3 2)[b]	> CH–CH_2–CH_2–	–20.10
2(3 3)	> CH–CH_2–CH <	–18.70
2(4 1)	⋗C–CH_2–CH_3	–19.60
2(4 2)	⋗C–CH_2–CH_2–	–16.80
2(4 3)	⋗C–CH_2–CH <	–7.50
2(4 4)	⋗C–CH_2–C⋖	4.00
2(6 1)	= CH–CH_2–CH_3	–20.40
2(6 2)	= CH–CH_2–CH_2–	–21.00
2(6 3)	= CH–CH_2–CH <	–22.10
2(6 4)[c]	= CH–CH_2–C⋖	–19.10
2(6 6)	= CH–CH_2–CH =	–19.20
2(7 1)	= C(–)–CH_2–CH_3	–19.60
2(7 2)	= C(–)–CH_2–CH_2–	–23.00
2(7 3)	= C(–)–CH_2–CH <	–18.50
2(7 4)	= C(–)–CH_2–C⋖	–12.00
2(9 1)	≡ C–CH_2–CH_3	–20.30

[a]2(1 1) means a methylene group (2) bonded to two methyl (1) groups. This group identifies propane explicitly.

[b]2(3 2) means a methylene group (2) bonded to a tertiary carbon atom (3) and another methylene group (2), as in 2-methylpentane.

[c]2(6 4) means a methylene group (2) bonded to a substituted ethenic group (6) and a quaternary carbon atom (4), as in 4,4-dimethylpentene-1.

TABLE 3–4. Comparison of enthalpies of formation in the gas phase at 298.15 K (in kJ/mol) (alkanes, alkenes, alkynes)

Compound	$\Delta_f H°$expt'l (86PED/NAY)	$\Delta_f H°$expt'l (this work)	$\Delta_f H°$selected (86TRC)	$\Delta_f H°$est'd (86PED/NAY)	$\Delta_f H°$est'd (this work)
ethane	−83.8	−83.85	−83.82	−83.8	−84.52
pentane	−146.9	−146.82	−146.76	−146.2	−146.41
2-methylpentane	−174.8	−174.77	−174.55	−174.4	−173.73
3-methylpentane	−172.1	−172.09	−171.97	−171.6	−171.47
2,2-dimethyl-pentane	−205.9	−205.85	−205.81	−204.4	−204.78
octane	−208.6	−208.27	−208.75	−208.6	−208.30
2-methylheptane	−215.4	−215.35	−215.35	−216.0	−214.99
decane	−249.5	−249.66	−249.46	−250.2	−249.56
dodecane	−289.7	−290.87	−290.72	−291.8	−290.82
hexadecane	−374.8	−374.76	−374.17	−375.0	−374.34
1-butene	0.1	−0.54	−0.54	0.1	−0.50
1-hexene	−43.5	−41.51	−41.5	−42.1	−41.76
trans-3-hexene	−54.4	−53.89	−52.3	−53.8	−53.39
trans-4,4-dimethyl-2-pentene	−88.8	−88.78	−90.2	−87.9	−87.95
1-octene	−81.4	−82.93	−83.6	−83.7	−83.02
2-methyl-3-ethyl-1-pentene	−100.3	−100.29	−100.7	−100.3	−101.47
1-decene	−123.4	−123.34	−124.7	−125.3	−124.28
1-hexadecene	−248.5	−249.16	−248.6	−250.1	−248.06
1-butyne	165.2	165.23	165.23	165.2	166.64
2-butyne	145.7	145.14	145.9	145.6	145.68
average deviation	0.55	0.47			

TABLE 3–5. Comparison of enthalpies of formation in the gas phase at 298.15 K (in kJ/mol) (alcohols, ethers, ketones, acids)

Compound	$\Delta_f H°$expt'l (86PED/NAY)	$\Delta_f H°$expt'l (this work)	$\Delta_f H°$selected (86TRC2)	$\Delta_f H°$est'd (86PED/NAY)	$\Delta_f H°$est'd (this work)
1-butanol	−275.0	−275.01	−274.60	−275.0	−275.75
2-butanol	−292.9	−292.90	−292.88	−292.9	−292.84
1-pentanol	−294.7	−294.70	−295.58	−295.8	−296.38
1-hexanol	−315.8	−315.90	−316.80	−316.6	−317.01
1-octanol	−355.5	−355.60	−357.00	−358.2	−358.27
1-decanol	−396.4	−396.60	−397.40	−399.8	−399.53
diethyl ether	−252.1	−252.10	−252.0	−252.1	−251.74
dipropyl ether	−292.9	−293.10	−293.1	−294.9	−293.00
diisopropyl ether	−319.2	−319.40	−319.4	−318.9	−318.42
di-*tert*-butyl ether	−362.0	−362.00	−362.0	−362.0	−363.34
2-pentanone	−259.0	−259.05	−258.9	−259.1	−259.66
2-hexanone	−279.8	−279.79	−279.0	−279.9	−280.29
2-methyl-3-pentanone	−286.1	−286.10	−286.1	−286.1	−286.06
5-nonanone	−344.9	−344.94	−344.9	−340.1	−343.39
6-undecanone	−387.4	−387.41	−385.1	−381.7	−384.65
propanoic acid	−453.5	−455.70	−452.8	−451.7	−455.64
butanoic acid	−475.8	−475.80	−473.6	−472.0	−476.27
pentanoic acid	−491.9	−496.30	−497.	−492.8	−496.90
octanoic acid	−554.3	−553.90	−553.	−555.2	−558.79
dodecanoic acid	−642.0	−642.00	−640.	−638.4	−641.31
average deviation	1.84	1.21			