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Estimation of the Thermodynamic Properties of Hydrocarbons at 298.15 K

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An estimation method 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 hydrocarbon compounds at 298.15 K. The second order approach which includes nearest neighbor interactions has been applied to the condensed phase. A total of 1311 comparisons are made between experimentally determined values and those calculated using additive group values. Of the 559 comparisons given for the enthalpy of formation ($\Delta_f H°$) in the gas, liquid, and solid phases, the average difference (residual), without regard to sign, is 2.6 kJ/mol. The average differences for 390 comparisons for the heat capacity ($C_p°$) and 352 comparisons for the entropy ($S°$) in the three phases are 1.9 and 2.3 J/mol·K, respectively. The good agreement between experimental and calculated values shows that the Benson group additivity approach to the estimation of thermodynamic properties of organic compounds is applicable to the liquid and solid phases as well as the gas phase. Appendices provide example calculations of the thermodynamic properties of selected hydrocarbon compounds, total symmetry numbers, and methyl repulsion corrections. Most of the 144 references listed offer an indication of the activity in the development of estimation methods for calculating thermodynamic properties since 1931.

Key words: condensed phase; enthalpy of formation; entropy; estimation methods; gas phase; heat capacity; hydrocarbons; thermodynamic properties.

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1. Introduction

For many years, thermodynamicists have been active in the development of numerical methods which correlate molecular structure and sub-structure with a corresponding energy contribution to a thermodynamic property. Some indication of this activity can be found by examining the 144 references at the end of this paper which primarily cover estimation methods and also identify some important reference sources of evaluated thermodynamic properties of hydrocarbon and related compounds. A variety of estimation schemes have emerged which demonstrate that good agreement can be achieved between calculated and experimentally measured thermodynamic properties. Of the estimation schemes which have been developed, the one put together by S.W. Benson and coworkers (58BEN/BUS, 68BEN, 69BEN/CRU, 69SHA, 71SHA, 73EIG/GOL, 76BEN, 77LUR/BEN, 77SHA/GOL, and 77STE/GOL) has the most desirable characteristics and appears to be generally acceptable to scientists within and between the disciplines of physical chemistry and chemical engineering. The attractive features of the Benson approach consist of simple additivity, clarity of notation, second order character, i.e., inclusion of nearest-neighbor interactions, ease of application, and satisfactory agreement between the estimated thermodynamic property and its experimentally determined value. Initially, focus was directed toward estimation of thermodynamic properties of organic compounds in the gas phase. The development of numerical methods oriented toward estimation of thermodynamic properties in the condensed phase has also been reported (69SHA, 71SHA, 77LUR/BEN), but primary attention has usually been placed upon gas phase processes. The estimation procedure developed by Benson and coworkers has been adopted into CHETAH, the ASTM Chemical Thermodynamic and Energy Release Evaluation Program (74SEA/FRE), for the estimation of thermodynamic properties of organic compounds in the gas phase and for the classification of chemical compounds or compositions according to whether they are likely to be impact sensitive.

The purpose of this paper is to extend the Benson group contribution values to the liquid and solid phases for hydrocarbon compounds, and when possible, to provide improved group contribution values for the gas phase. The thermodynamic properties at 298.15 K considered are: enthalpy of formation, heat capacity, and entropy. The approach taken in the evaluation of data and in the development of group values consisted of calculating and examining group increments in a systematic manner. This procedure was followed by the selection of group values which appeared to give minimum residuals between the calculated and experimental values. The development of groups and group values followed the path from alkanes to alkenes, alkynes, aromatic hydrocarbons, cycloalkanes, and other hydrocarbon derivatives. A global least squares, least sums, or regression-type fit of all the group values was not carried out because of differences in the quality of the data and because of the minimal amount of data available for certain group values. Computations were performed using a conventional desk-top electronic calculator. It is expected that the results we obtained are approximately equivalent to what would have been derived from a weighted regression analysis.

A companion document, 89DOM/HEA, is in preparation which describes a database and algorithm for calculating the enthalpy of formation, heat capacity, and entropy at 298.15 K of 1311 hydrocarbon compounds in the gas, liquid, and solid phases. The database includes the group contribution values used by the algorithm, the corresponding experimental and calculated data for the enthalpy of formation, heat capacity, and entropy of the hydrocarbon compounds, and the differences or residuals which result. The document, 89DOM/HEA, is also available on diskette and contains an interactive program which allows the user to carry out the calculation of the enthalpy of formation, heat capacity, or entropy for any hydrocarbon compound based on the assembly of the

corresponding group contribution values in a particular phase. Also calculated are 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.

The thermodynamic data used as the data-base for this study were obtained from the following reference sources: 53ROS/PIT, 69STU/WES, 70COX/PIL, 77PED/RYL, 84DOM/EVA, 86MAR, and 86PED/NAY. Differences between the enthalpy of formation, heat capacity, and entropy for the gas and liquid phases, and liquid and solid phases are related to the corresponding transition properties. For example, the difference between the enthalpies of formation at 298.15 K for the gas and liquids phases equals the enthalpy of vaporization at 298.15 K for that hydrocarbon. Similarly, the difference between the enthalpy of formation liquid and solid phases gives the transition property equal to the sum of the enthalpies of fusion and the enthalpies of the first-order crystal-crystal transitions at 298.15 K. In the tables containing data on hydrocarbon compounds in the solid phase, the experimental values for $\Delta_f H°$ were sometimes derived from a combination of $\Delta_f H°$(liquid), ΔH(fusion), and any ΔH(transition).

2. Discussion of Results

Group contribution values for hydrocarbons at 298.15 K are given for the enthalpy of formation, $\Delta_f H°$, heat capacity, $C_p°$, and entropy, $S°$, for the gas, liquid, and solid phases in Table 1 in joules. The superscript symbol, °, indicates that the substance is in its standard state. For a gaseous compound, the standard thermodynamic properties are for the pure compound at a pressure of 0.1 MPa (1 bar) and in a hypothetical state in which it exhibits ideal gas behavior. The heat capacity and enthalpy of the compound are those of the real gas extrapolated to zero pressure. For a liquid or solid compound, the standard thermodynamic properties are for the pure compound in the liquid or solid phase, respectively, under a pressure of 0.1 MPa (1 bar).

Ring strain corrections which are applicable to cycloalkanes and related compounds are shown in Table 2 and are also in joules. The joule is related to the thermochemical calorie through the definition: one thermochemical calories equals 4.1840 joules.

Recommendations by the IUPAC (82COX/ANG) to reference the standard state pressure as 100,000 Pa (1 bar) rather than 101,325 Pa (1 atmosphere) were examined. Calculations indicated that numerical changes to group contribution values were negligible when compared to the uncertainties the values themselves. Systematic differences imposed by a change in standard state pressure to 100,000 Pa were well below 0.4 kJ/mol (0.1 kcal/mol) for $\Delta_f H°$ and 0.4 J/mol·K (0.1 cal/mol·K) for $C_p°$ and $S°$ in most instances. Hence, no corrections to accommodate this change were deemed necessary.

Example calculations which give details of the additivity of the group values in the estimation of $\Delta_f H°$, $C_p°$, and $S°$ are provided for several hydrocarbon compounds in Appendix A. Appendix B shows a comparison of gas phase property data calculated from this study with that of 76BEN. Overall the residuals found between the two calculated values are small. Comparison to experimental values in other tables indicates that improvement takes place about half of the time.

2.1. *n*-Alkanes

Tables 3, 4, and 5 show the agreement between 122 experimental and calculated values for $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K for *n*-alkanes. In the gas phase, 50 comparisons were made between the experimental and calculated values for $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K; here, residuals do not exceed 1.5 kJ/mol for $\Delta_f H°$ or 1.5 J/mol·K for $C_p°$ or $S°$. In the liquid phase, 39 comparisons showed residuals for $\Delta_f H°$ of 1.6 kJ/mol or less and residuals for $S°$ of 0.4 J/mol·K or less. Residuals for liquid $C_p°$ result in only 3 of 14 exceeding 2.0 J/mol·K. In the solid phase, 17 comparisons between experimental and calculated values for $\Delta_f H°$ show 8 residuals below 2.0 kJ/mol. The development of group values for $C_p°$ and $S°$ in the solid phase for *n*-alkanes presented considerable difficulty. Data for $C_p°$ and $S°$ in the solid phase were not plentiful and some of the results reported are of dubious quality. For example, some (10) residuals for $C_p°$ and $S°$ in Table 5 appear to be unusually large, while others are quite satisfactory. In particular, the data on $C_p°$ and $S°$ for crystalline *n*-octadecane reported by 67MES/GUT and for crystalline *n*-hexacosane reported by 76AND/MAR were of high quality as were the extrapolated values for crystalline *n*-hexadecane derived from the liquid phase data of 67MES/GUT. However, data on $C_p°$ and $S°$ for solid phase *n*-alkanes reported before 1950 were considered unreliable because low temperature measurements did not extend below the boiling point of liquid nitrogen (~80 K). As a result of using the latter data, large residuals, shown in Table 5, were obtained for $C_p°$ and $S°$ for solid *n*-alkanes. In some of the reported studies, sample impurities may have introduced errors into the experimental data for $C_p°$ and $S°$. Additional experimental studies on solid *n*-alkanes in the C_{20} to C_{40} range are needed to improve the reliability of estimation of thermodynamic properties using group contribution values.

Although separate values for odd and even carbon containing homologues were developed for the calculation of values for the group C–(C)$_2$(H)$_2$ for $\Delta_f H$ in the solid phase for *n*-alkanes, this did not result in an improvement in the estimated values when compared to experimental data. Therefore, the separate values were discarded in preference for the single value listed in Table 1, C–(C)$_2$(H)$_2$ = −29.41 kJ/mol. Effects from odd and even numbers of carbon atoms in the data for $C_p°$ and $S°$ in *n*-alkanes were even less apparent and, hence, only a single value appears in Table 1 for the C–(C)$_2$(H)$_2$ group. It should also be mentioned that the value for the methyl group does not change, except for the physical phase, no matter to what structural entity it is attached, i.e., C–(H)$_3$(C) = C–(H)$_3$(X), where X is another carbon atom neighbor, such as C_d, C_t, or C_B.

2.2. Substituted Alkanes

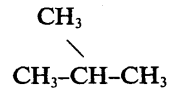
Tables 6 through 11 compare the experimental and calculated values for substituted or branched alkanes for $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K. During the evaluation of data on the enthalpies of formation of substituted alkanes, the Benson approach was modified for the treatment of gauche isomers. A new treatment was developed which corrects for the repulsive interaction of hydrogen atoms on methyl groups attached to tertiary or quaternary carbon atoms. A group value was assigned to a tertiary or quaternary carbon along with a group value for the number of methyl groups attached to the tertiary or quaternary carbon. For example, $\Delta_f H°$ for 2-methylpropane required 3 methyl repulsion correction values, 2-methylbutane required 2 methyl repulsion correction values, 3-methyl-pentane required 1 methyl repulsion correction value, and 3-ethyl- pentane needed no correction of this kind. $\Delta_f H°$ for the gas phase for these molecules is shown in the sample calculations below.

A similar rationale was applied to the methyl repulsion correction for a quaternary carbon atom. Molecules with quaternary carbon atoms which corresponded to the examples above were 2,2-dimethylpropane, 2,2-dimethylbutane, 3,3-dimethylpentane, 3-ethyl-3-methylpentane, and 3,3-diethylpentane and required 4, 3, 2, 1, and 0 methyl repulsion correction values, respectively, in the calculation of $\Delta_f H°$ at 298.15 K. In addition, different methyl repulsion correction values were required for quaternary carbon atoms which had a tertiary carbon atom adjacent to it and another such correction when an alkane had two quaternary carbon atoms in its structure. These additional methyl repulsion corrections have been developed for $\Delta_f H°$ in the gas and liquid phases, but not for the solid phase due to a lack of precise data on solid hydrocarbon compounds having the appropriate structures. The introduction of the methyl repulsion correction values was made because of the significant reduction observed in the differences in the experimental and calculated values for hydrocarbon compounds having tertiary and/or quaternary carbon atoms and because it appears simpler in both concept and application to the gauche correction developed earlier. Some further examples of the methyl repulsion corrections are provided in Appendix C.

Although the notion of methyl repulsion interactions in the arrays of data on $C_p°$ and $S°$ for substituted alkanes was examined carefully, correction terms did not emerge which brought about a reduction in the magnitude of the residuals for these hydrocarbons.

Among the substituted alkanes shown in Tables 6 through 11 for all three phases, 215 comparisons were made between experimental and calculated values. In the gas phase, out of a total of 117 comparisons, 101 show residuals of less than or equal to 4.0 kJ/mol for $\Delta_f H°$ and less than or equal to 4.0 J/mol·K for $C_p°$ and $S°$. In the liquid phase, 77 comparisons are listed. Of these, 42 show residuals of less than or equal to 4.0 kJ/mol for $\Delta_f H°$ and less than or equal to 4.0 J/mol·K for $C_p°$ and $S°$. In the solid phase, out of 19 comparisons for $\Delta_f H°$, 17 are less than or equal to 4.0 kJ/mol. Comparisons of $C_p°$ and $S°$ for solid substituted alkanes are virtually nonexistent. Experimental data are needed on key substituted alkanes to assist in the estimation of other family members.

2-Methylpropane



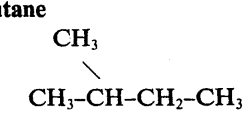
Enthalpy of formation (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
3	C-(C)(H)$_3$	−42.26	−126.78
1	C-(C)$_3$(H)	−1.17	−1.17
3	−CH$_3$ corr	−2.26	−6.78
			−134.73

Compare with experimental value: −134.18 kJ/mol (51PRO/MAR, 86PED/NAY).

Compare with estimated value from 76 BEN: −135.98 kJ/mol.

2-Methylbutane



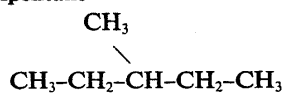
Enthalpy of formation (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
3	C-(C)(H)$_3$	−42.26	−126.78
1	C-(C)$_2$(H)$_2$	−20.63	−20.63
1	C-(C)$_3$(H)	−1.17	−1.17
2	−CH$_3$ corr	−2.26	−4.52
			−153.10

Compare with experimental value: −153.68 kJ/mol (70GOO, 86PED/NAY).

Compare with estimated value from 76BEN: −153.26 kJ/mol.

3-Methylpentane



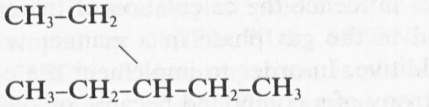
Enthalpy of formation (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
3	C-(C)(H)$_3$	−42.26	−126.78
2	C-(C)$_2$(H)$_2$	−20.63	−41.26
1	C-(C)$_3$(H)	−1.17	−1.17
1	-CH$_3$ corr	−2.26	−2.26
			−171.47

Compare with experimental value: −172.09 kJ/mol (41PRO/ROS, 86PED/NAY).

Compare with estimated value from 76BEN: −170.54 kJ/mol.

3-Ethylpentane



Enthalpy of formation (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
3	C-(C)(H)$_3$	−42.26	−126.78
3	C-(C)$_2$(H)$_2$	−20.63	−61.89
1	C-(C)$_3$(H)	−1.17	−1.17
			−189.84

Compare with experimental value: −189.62 kJ/mol (41PRO/ROS 2, 86PED/NAY).

Compare with estimated value from 76BEN: −187.82 kJ/mol.

2.3. *n*-Alkenes

Tables 12, 13, and 14 compare 154 experimental and calculated values for $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K for linear alkenes in the gas, liquid and solid phases. In the gas phase, 73 out of 83 comparisons show residuals of 2.0 kJ/mol or less for $\Delta_f H°$ and 2.0 J/mol·K or less for $C_p°$ and $S°$. In the liquid phase, 40 out of 54 comparisons show residuals of 2.0 kJ/mol or less for $\Delta_f H°$ and 2.0 J/mol·K or less for $C_p°$ and $S°$. In the solid phase, experimental data were unavailable for $C_p°$ and $S°$ on linear alkenes, suggesting the need for additional research. Data for $\Delta_f H°$ on solid linear alkene are derived from data on the liquid phase and data on enthalpies of fusion and transition. Here, 15 out of 17 comparisons show residuals of less than 2.0 kJ/mol. The residual for $\Delta_f H°$ of 1-hexadecene in the solid phase listed in Table 14 is large, 17.2 kJ/mol. Because the $\Delta_f H°$ residuals listed for most of the other linear alkenes are below 2.0 kJ/mol, it appears that the group contribution values are satisfactory. Low temperature heat capacity studies were performed on seven 1-olefins by 57MCC/FIN. The presence of a first order crystal-crystal transition in the temperature range between 200 K and the triple point of 1-decene and linear alkenes with higher carbon numbers was present, but not in 1-hexadecene, however, a lambda transition was observed. Also significant is the presence of a higher than normal impurity (1.3 mol%) in the 1-hexadecene sample studied by 57MCC/FIN. It is possible that the impurity in the 1-hexadecene has obscured a crystal-crystal transition near the lambda transition which is about the magnitude of the residual we find in Table 14, 17.2 kJ/mol. A careful phase transition study on a good quality sample would answer the question.

Attempts to extrapolate the low temperature data on $C_p°$ and $S°$ reported by 57MCC/FIN for 1-alkenes in the solid phase through the melting point to 298.15 K produced group values with large uncertainties and poor reliability, hence, such group values are not listed.

2.4. Substituted Alkenes

Tables 15, 16, and 17 show the agreement between 118 experimental and calculated values for substituted alkenes in the gas, liquid, and solid phases, respectively, for $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K. In the gas phase, 62 comparisons were made. Of these, 43 agreed within 4.0 kJ/mol or less for $\Delta_f H°$ and within 4.0 J/mol·K or less for $C_p°$ and $S°$. In the liquid phase, 47 comparisons were made of which 16 residuals were 4.0 kJ/mol or less for $\Delta_f H°$ and 12 residuals were 4.0 J/mol·K or less for $C_p°$ and $S°$. As with the data on solid linear alkenes, data are limited on solid substituted alkenes. Of the available data on $\Delta_f H°$, 5 out of 9 residuals were 4.0 kJ/mol or less.

We have examined the available data on the enthalpies of formation at 298.15 K for branched alkenes to determine whether a methyl repulsion correction could be derived which would be the counterpart of gauche alkene correction discussed in 69BEN/CRU. Our examination showed that a similar correction was needed for alkene groups which involved tertiary and quaternary carbon atoms. A cis correction for alkenes was also developed in the gas, liquid, and solid phases for $\Delta_f H°$, but for $C_p°$ and $S°$ in the gas phase only.

2.5. Alkynes

Tables 18, 19, and 20 give comparisons between 61 experimental and calculated values for alkynes in the gas, liquid, and solid phases, respectively, for $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K. In the gas phase, 41 comparisons were made of which 36 were 2.0 kJ/mol or less for $\Delta_f H°$ and 2.0 J/mol·K or less for $C_p°$ and $S°$. In the liquid phase, 18 comparisons were made of which 11 were 2.0 kJ/mol or less for $\Delta_f H°$ and 2.0 J/mol·K or less for $C_p°$ and $S°$. The solid phase is limited to 2 values of $\Delta_f H°$.

The experimental values for $C_p°$ and $S°$ for the alkynes in the gas phase were those calculated by 45WAG/KIL, using statistical thermodynamic procedures, and the methods established by 46TAY/WAG for calculating the regularities in gaseous thermodynamic functions for a homologous series. Those values were tabulated by 53ROS/PIT and 69STU/WES. The good agreement between the experimental and calculated values was expected because of the group additive features in both sets of values. Data for $C_p°$ and $S°$ for alkynes in the liquid phase were limited and those for the solid phase were absent.

2.6. Aromatic Hydrocarbons

Tables 21, 22, and 23 show the agreement between experimental and calculated values for aromatic hydrocarbons in the gas, liquid, and solid phases, respectively, for $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K. A total of 368 comparisons were made. In the gas phase, 135 out of 168 comparisons had residuals of 4.0 kJ/mol or less for $\Delta_f H°$, or 4.0 J/mol·K or less for $C_p°$ and $S°$. In the liquid phase, 80 out of 103 comparisons had residuals of 4.0 kJ/mol or less for $\Delta_f H°$, or 4.0 J/mol·K or less for $C_p°$ and $S°$. In the

solid phase, 57 out of 97 comparisons had residuals of 4.0 kJ/mol or less for $\Delta_f H°$, or 4.0 J/mol·K or less for $C_p°$ and $S°$.

The experimental values for $C_p°$ and $S°$ for benzene in the solid phase at 298.15 K which appeared in Table 23, were obtained by linear extrapolation of the data on the solid phase from the melting point to room temperature. Note that separate corrections were applicable for ortho substitution in the gas phase for $C_p°$ and $S°$ for naphthalene.

The experimental enthalpies of formation, heat capacities, and entropies of 1-methylnaphthalene and 2-methylnaphthalene in the gas, liquid, and solid phases have been based upon the data of 56MIL/BEC, 57MCC/FIN, 60SPE/ROS, and 74SAB/CHA. Although actual differences of 2.97, −6.39, and −0.58 kJ/mol can be calculated between the experimental enthalpies of formation of 1-methylnaphthalene and 2-methylnaphthalene for the gas, liquid, and solid phases, respectively, no correction to the calculated values has been applied because the experimental uncertainties in $\Delta_f H°$ for an isomer can be difficult to evaluate and the corresponding uncertainties for the calculated differences in $\Delta_f H°$ between isomers can become large.

2.7. Cycloalkanes and Related Hydrocarbons

The corrections listed in Table 2 are applicable to cycloalkanes and related compounds reflect the magnitude of the internal ring strain imposed for a given size ring. Note that somewhat different ring corrections were applied to substituted versus unsubstituted values for cyclopentane, cyclopentene, and cyclohexane.

Tables 24, 25, and 26 give comparisons between the experimental and calculated values for cycloalkanes, substituted cycloalkanes, and related compounds in the gas, liquid, and solid phases, respectively, for $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K. A total of 273 comparisons were made. Among the three phases, unsubstituted cycloalkanes showed equivalence between the experimental and calculated values, i.e., zero residual, since the ring corrections are derived from the differences which are found between the experimental and "strain-free" values. A total of 129 comparisons were made which gave zero residuals. For substituted cycloalkanes, a total 144 comparisons were made. In the gas phase, 44 out of 66 comparisons had residuals of 4.0 kJ/mol or less for $\Delta_f H°$ and 4.0 J/mol·K or less for $C_p°$ and $S°$. In the liquid phase, 50 out of 68 comparisons showed residuals of 4.0 kJ/mol or less for $\Delta_f H°$, or 4.0 J/mol·K or less for $C_p°$ and $S°$.

3. Symmetry Numbers and Entropy

In the calculation of the entropy of a gaseous molecule, it is important that proper symmetry contributions imposed by the presence of certain structural features are accounted for. Molecular symmetry is not a factor in the additive summation of group values in the calculation of the enthalpy of formation or heat capacity, but it does influence the calculation of the entropy of a compound in the gas phase in a manner which is not simply additive. In order to implement the contribution to the entropy of a compound because of symmetry features, the actual or real entropy, $S°$, is divided into two parts:

(1) intrinsic entropy, $S°$(group), which is the entropy contribution determined by adding the group values for the entropy of the structural parts of the compound; and,

(2) symmetry-related entropy, $S°$(sym), which is the entropy contribution determined from the symmetry features of the compound as a whole.

Hence, $S° = S°(\text{group}) + S°(\text{sym})$. The symmetry-related entropy is in turn divided into two parts:

(1) entropy due to optical isomerism in the molecule, $S°$(opt); and,

(2) entropy from the total symmetry number of the molecule, $S°$(tot), which is a reflection of how symmetrical the molecule is.

It therefore follows that: $S°(\text{sym}) = S°(\text{opt}) + S°(\text{tot})$, or $S°(\text{sym}) = R \ln N(\text{opt}) + R \ln N(\text{tot})$, where R is the gas constant, N(opt) is the number of optical isomers, N(tot) is the total symmetry number, and ln is the natural logarithm. Note that $R \ln N(\text{opt})$ is a positive quantity and that $R \ln N(\text{tot})$ is a negative quantity in the summation of the actual entropy, $S°$.

One of the ways in which a molecule may exhibit optical isomerism occurs when its mirror image cannot be superimposed upon itself as a result of simple molecular rotations. Such mirror images are called enantiomers and are said to be chiral. The two enantiomers have identical physical properties except for their interaction with transmitted polarized light. Other elements of optical isomerism require consideration in the calculation of $R \ln N(\text{opt})$, and discussions can be found in textbooks on organic chemistry and stereoisomerism.

A discussion of how to calculate the total symmetry number as well as several sample calculations for selected hydrocarbon compounds is given in Appendix D. Any of the tables which show gas phase comparisons between experimental and calculated entropies, also contains a column entry on the extreme right giving the value for N(tot) for that hydrocarbon molecule.

4. Summary and Conclusions

A series of group contribution values has been developed which permits the estimation of the enthalpy of formation, heat capacity, and entropy at 298.15 K for hydrocarbon compounds in the gas, liquid, and solid-phases. The set of group values which has been pro-

vided in the gas phase for $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K are comparable in accuracy of prediction to the group values developed by 58BEN/BUS, 68BEN, 69BEN/CRU, and 76BEN. This comparison is shown in Appendix B for the gas phase. The present set of group values have the advantage of including experimental data on hydrocarbon compounds which were reported over the period 1975–1987. The evaluation of thermodynamic data on gaseous hydrocarbon compounds also provided group values which have internal consistency with the corresponding values for the liquid and solid phases.

A total of 1311 comparisons have been made between an experimentally determined value and one calculated using the additive group contribution values reported here for $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K. From the total, 559 comparisons are listed for $\Delta_f H°$ among the three phases and have an average residual, calculated without regard to sign, of 2.6 kJ/mol. Similarly, the average residuals obtained for the 390 comparisons made for $C_p°$ and the 352 comparisons made for $S°$ are 1.9 and 2.3 J/mol·K, respectively. Here also, the average residuals were calculated without regard to sign, and the unusually large residuals found for $C_p°$ and $S°$ for five n-alkanes in the solid phase in Table 5 have been omitted. The average residuals calculated for $\Delta_f H°$, $C_p°$, and $S°$ are comparable to what are often reported for corresponding experimental uncertainties. These results demonstrate the general applicability of the Benson second order group additivity approach to the estimation of thermodynamic properties in the liquid and solid phases.

An approach has been developed which corrects for the repulsive interactions of hydrogen atoms on methyl groups in branched hydrocarbon compounds. Different methyl repulsion correction values are needed for branching to a tertiary carbon, a quaternary carbon, a tertiary or quaternary carbon atom adjacent to quaternary carbon atom, and for two non-adjacent quaternary carbon atoms. These corrections are applicable not only to branched hydrocarbon groups which are present in saturated hydrocarbons, but to those present in unsaturated, alicyclic, or aromatic hydrocarbon compounds.

Plans are underway to develop the Benson approach of group value additivity to the estimation of $\Delta_f H°$, $C_p°$, and $S°$ at 298.15 K for organic compounds containing the elements CHO, CHN, CHNO, CHS, and CHSO in the gas, liquid, and solid phases.

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Appendix A. Example Calculations of Enthalpy of Formation, Heat Capacity, and Entropy at 298.15 K for Some Hydrocarbon Compounds

n-Hexane

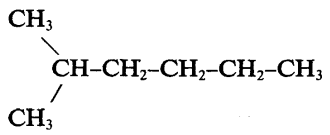
$CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$

Enthalpy of formation (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
2	$C-(C)(H)_3$	−42.26	−84.52
4	$C-(C)_2(H)_2$	−20.63	−82.52
			−167.04

Compare with experimental value: −167.11 kJ/mol (44PRO/ROS, 69GOO/SMI, 86PED/NAY).

2-Methylhexane

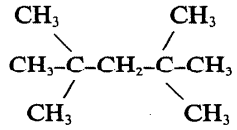


Enthalpy of formation (liquid phase)

No. of groups	Group	Group value	Sum (kJ/mol)
3	$C-(C)(H)_3$	−47.61C	−142.83
3	$C-(C)_2(H)_2$	−25.73	−77.19
1	$C-(C)_3(H)$	−4.77	−4.77
2	$-CH_3$ corr	−2.18	−4.36
			−229.15

Compare with experimental value: −229.49 kJ/mol (45PRO/ROS 2, 86PED/NAY).

2,2,4,4-Tetramethylpentane

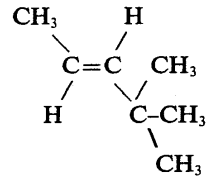


Enthalpy of formation (liquid phase)

No. of groups	Group	Group value	Sum (kJ/mol)
6	$C-(C)(H)_3$	−47.61	−285.66
1	$C-(C)_2(H)_2$	−25.73	−25.73
2	$C-(C)_4$	17.99	35.98
6	$-CH_3$ corr	−0.64	−3.84
			−279.25

Compare with experimental value: −279.99 kJ/mol (47JOH/PRO, 86PED/NAY).

trans-4,4-Dimethylpentene-2

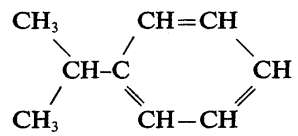


Enthalpy of formation (liquid phase)

No. of groups	Group	Group value	Sum (kJ/mol)
3	$C-(C)(H)_3$	−47.61	−142.83
1	$C-(C_d)(H)_3$	−47.61	−47.61
2	$Cd-(C)(H)$	31.05	62.10
1	$C-(C_d)(C)_3$	20.79	20.79
3	$-CH_3$ corr	−4.39	−13.17
			−120.72

Compare with experimental value: −121.71 kJ/mol (61ROC/ROS, 86PED/NAY).

Isopropylbenzene



Enthalpy of formation (solid phase)

No. of groups	Group	Group value	Sum (kJ/mol)
2	$C-(C)(H)_3$	−46.74	−93.48
1	$C-(C)_2(C_B)(H)$	−3.50	−3.50
1	$C_B-(C)(C_B)_2$	13.90	13.90
5	$C_B-(H)(C_B)_2$	6.53	32.65
2	$-CH_3$ corr.	−2.34	−4.68
			−55.11

Compare with experimental value: −48.45 kJ/mol (45JOH/PRO, 73KIS/SUG).

1-Octyne

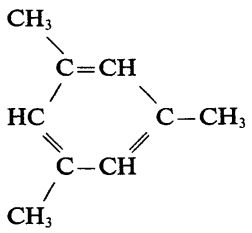
$CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-C\equiv CH$

Heat capacity (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
1	$C-(C)(H)_3$	25.73	25.73
4	$C-(C)_2(H)_2$	22.89	91.56
1	$C-(C_t)(C)(H)_2$	20.97	20.97
1	$C_t-(C)$	13.22	13.22
1	$C_t-(H)$	22.55	22.55
			174.03

Compare with experimental value: 173.97 J/mol·K (69STU/WES).

1,3,5-Trimethylbenzene

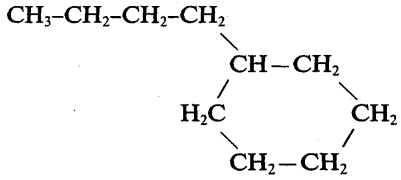


Heat capacity (liquid phase)

No. of groups	Group	Group value	Sum (kJ/mol)
3	$C-(C_B)(H)_3$	36.48	109.44
3	$C_B-(H)(C_B)_2$	22.68	68.04
3	$C_B-(C)(C_B)_2$	10.10	30.30
			207.78

Compare with experimental value: 209.33 J/mol·K (55TAY/KIL, 84DOM/EVA).

n-Butylcyclohexane

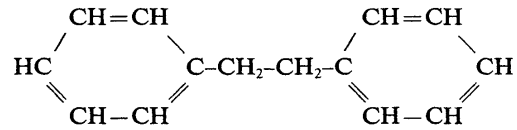


Heat capacity (liquid phase)

No. of groups	Group	Group value	Sum (kJ/mol)
1	$C-(C)(H)_3$	36.48	36.48
8	$C-(C)_2(H)_2$	30.42	243.36
1	$C-(C)_3(H)$	21.38	21.38
1	Ring corr.	−26.21	−26.21
			275.01

Compare with experimental value: 271.04 J/mol·K (65FIN/MES, 84DOM/EVA).

1,2-Diphenylethane



Heat capacity (solid phase)

No. of groups	Group	Group value	Sum (kJ/mol)
10	$C_B-(H)(C_B)_2$	20.13	201.30
2	$C_B-(C)(C_B)_2$	−23.26	−46 52
2	$C-(C_B)(C)(H)_2$	49.38	98.76
			253.54

Compare with experimental value: 253.55 J/mol·K (31SMI/AND, 84DOM/EVA).

n-Hexadecane

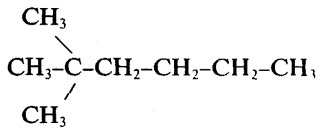
$CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-$
$CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_3$

Entropy (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
2	$C-(C)(H)_3$	127.32	254.64
14	$C-(C)_2(H)_2$	39.16	548.24
1	$-R\ln[N(\mathrm{tot})]$	−24.03	−24 03
			778 85

Compare with experimental value: 778.31 J/mol·K (69STU/WES)

2,2-Dimethylhexane

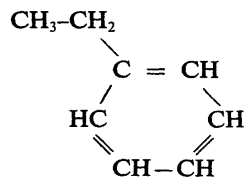


Entropy (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
4	$C-(C)(H)_3$	127.32	509.28
3	$C-(C)_2(H)_2$	39.16	117.48
1	$C-(C)_4$	−149.49	−149.49
1	$-R\ \ln[N(\mathrm{tot})]$	−45.67	−45.67
			431.60

Compare with experimental value: 431.20 J/mol·K (69STU/WES).

Ethylbenzene

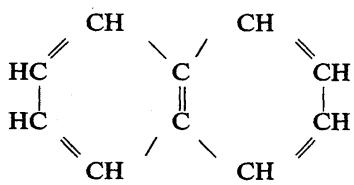


Entropy (liquid phase)

No. of groups	Group	Group value	Sum (kJ/mol)
1	C–(C)(H)$_3$	83.30	83.30
1	C–(C)(C$_B$)(H)$_2$	47.40	47.40
1	C$_B$–(C)(C$_B$)$_2$	−19.50	−19.50
5	C$_B$–(H)(C$_B$)$_2$	28.87	144.35
			255.55

Compare with experimental value: 255.01 J/mol·K (44GUT/SPI, 84DOM/EVA).

Naphthalene



Entropy (solid phase)

No. of groups	Group	Group value	Sum (kJ/mol)
8	C$_B$–(H)(C$_B$)$_2$	22.75	182.00
2	C$_{BF}$–(C$_{BF}$)(C$_B$)$_2$	−6.00	−12.00
			170.00

Compare with experimental value: 167.40 J/mol·K (57MCC/FIN, 84DOM/EVA).

Appendix B. Comparison of Calculated Thermodynamic Properties in the Gas Phase with Benson's Values at 298.15 K

Enthalpy of formation

Compound	$\Delta_f H°$ (This work)	$\Delta_f H°$ (76BEN)	Residual
		kJ/mol	
propane	−105.15	−105.98	0.83
2-methylbutane	−153.10	−153.26	0.16
trans-2-hexene	−53.39	−54.02	0.63
p-xylene	18.00	15.98	2.02
n-butylbenzene	−12.17	−12.18	0.01

Heat capacity

Compound	$C_p°$ (This work)	$C_p°$ (76BEN)	Residual
		J/mol·K	
n-hexane	143.02	143.85	−0.83
2,5-dimethylhexane	188.86	187.61	−1.25
cis-3-hexene	122.17	123.85	−1.68
ethylbenzene	129.14	129.29	−0.15
cyclopentane	83.01	87.86	−4.85

Entropy

Compound	$S°$ (This work)	$S°$ (76BEN)	Residual
		J/mol·K	
n-pentane	348.09	348.69	−0.60
2-methylpropane	291.82	294.68	−2.86
1-hexene	383.28	386.81	3.53
benzene	269.20	268.78	0.42
methylcyclohexane	344.36	343.34	1.02

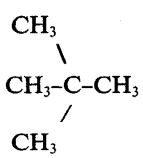
Comparison of the small data set in Appendix B to corresponding experimental values for these compounds shows that residual for $\Delta_f H°$ are less than 4 kJ/mol and those for $C_p°$ and S° are below 4 J/mol·K. An improvement on the part of our group contribution values for the gas phase over those of Benson *et al.*, is demonstrated about half of the time.

Appendix C. Methyl Repulsion Corrections for Branched Hydrocarbons

Methyl Repulsion Corrections in Branched Alkane Hydrocarbons with Quaternary Carbon Atoms

Several examples of application of the methyl repulsion corrections to the calculation of $\Delta_f H°$ in the gas phase for hydrocarbons which contain quaternary carbon atoms are given below.

2,2-Dimethylpropane

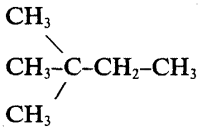


Enthalpy of formation (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
4	C-(C)(H)$_3$	−42.26	−169.04
1	C-(C)$_4$	19.20	19.20
4	Quat. CH$_3$ corr	−4.56	−18.24
			−168.08

Compare with experimental value: −167.99 kJ/mol (70GOO, 86PED/NAY).
Compare with estimated value from 76BEN: −168.62 kJ/mol.

2,2-Dimethylbutane

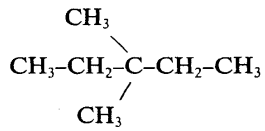


Enthalpy of formation (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
4	C-(C)(H)$_3$	−42.26	−169 04
1	C-(C)$_2$(H)$_2$	−20.63	−20 63
1	C-(C)$_4$	19.20	19 20
3	Quat. CH$_3$ corr	−4 56	−13 68
			−184 15

Compare with experimental value. −186 10 kJ/mol (41PRO/ROS, 86PED/NAY).
Compare with estimated value from 76BEN: −182.55 kJ/mol

3,3-Dimethylpentane

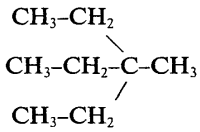


Enthalpy of formation (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
4	C-(C)(H)$_3$	−42 26	−169.04
2	C-(C)$_2$(H)$_2$	−20.63	−41.26
1	C-(C)$_4$	19.20	19.20
2	Quat. CH$_3$ corr	−4.56	−9.12
			−200.22

Compare with experimental value: −201.17 kJ/mol (41PRO/ROS 2, 86PED/NAY).
Compare with estimated value from 76BEN: −196.48 kJ/mol.

3-Ethyl-3-methylpentane

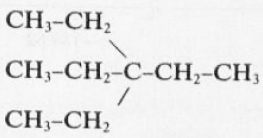


Enthalpy of formation (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
4	C-(C)(H)$_3$	−42.26	−169 04
3	C-(C)$_2$(H)$_2$	−20.63	−61 89
1	C-(C)$_4$	19.20	19.20
1	Quat. CH$_3$ corr	−4.56	−4 56
			−216 29

Compare with experimental value: −214 85 kJ/mol (45PRO/ROS, 86PED/NAY).
Compare with estimated value from 76BEN −210 41 kJ/mol

3,3-Diethylpentane



Enthalpy of formation (gas phase)

No. of groups	Group	Group value	Sum (kJ/mol)
4	C-(C)(H)$_3$	−42.26	−169.04
4	C-(C)$_2$(H)$_2$	−20.63	−82.52
1	C-(C)$_4$	19.20	19.20
			−232.36

Compare with experimental value: −232.34 kJ/mol (47JOH/PRO, 86PED/NAY).
Compare with estimated value from 76BEN: −224.35 kJ/mol.

Comparison of the methyl repulsion correction and Benson's gauche — correction in branched alkane hydrocarbons (gas phase)

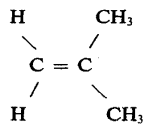
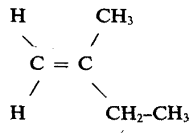
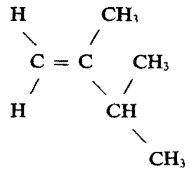
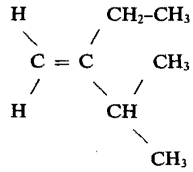
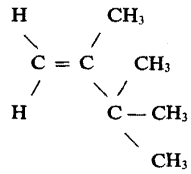
Compound name and formula	Gauche isomers (76BEN)	Benson method (76 BEN) $\Delta_f H°$ (kJ/mol)			Methyl repulsion method (This work) $\Delta_f H°$ (kJ/mol)		
		expt	calc	resd	expt	calc	resd
2-Methylpropane CH_3 \ CH_3–CH / CH_3	0	−134.18	−135.98	1.80	−134.18	−134.73	0.55
2,2-Dimethylpropane CH_3 \ CH_3–C–CH_3 / CH_3	0	−167.99	−168.62	0.63	−167.99	−168.08	0.09
2-Methylbutane CH_3 \ CH_3–CH–CH_2–CH_3	1	−153.63	−153.26	−0.37	−153.63	−153.10	−0.53
3-Methylpentane CH_3 \ CH_3–CH_2–CH–CH_2–CH_3	2	-172.09	-170.54	-1.55	-172.09	-171.47	-0.62
2,2-Dimethylbutane CH_3 \ CH_3–C–CH_2–CH_3 / CH_3	2	−186.10	−182.55	−3.55	−186.10	−184.15	−1.95
2,3-Dimethylbutane CH_3 CH_3 \ / CH_3–CH–CH–CH_3	2	−178.28	−179.91	1.63	−178.28	−180.42	2.14
3-Ethylpentane CH_3–CH_2 \ CH_3–CH_2–CH / CH_3–CH_2	3	−189.62	−187.82	-1.80	−189.62	−189.84	0.22
2,2,3-Trimethylbutane CH_3 CH_3 \ / CH_3–C–CH–CH_3 / CH_3	5	−204.47	−202.51	−1.97	−204.47	−202.27	−2.20

Comparison of the methyl repulsion correction and Benson's gauche — correction in branched alkane hydrocarbons (gas phase) — Continued

Compound name and formula	Gauche isomers (76BEN)	Benson method (76 BEN) $\Delta_f H°$ (kJ/mol)			Methyl repulsion method (This work) $\Delta_f H°$ (kJ/mol)		
		expt	calc	resd	expt	calc	resd
3,3-Diethylpentane CH_3-CH_2 CH_3-CH_2-C-CH_2-CH_3 CH_3-CH_2	8	−232.34	−224.35	−7.99	−232.34	−232.36	0.02
2,2,3,3-Tetramethylbutane CH_3 CH_3 CH_3-C-C-CH_3 CH_3 CH_3	6	−225.60	−231.79	−6.23	−225.60	−219.00	−6.60
2,2,3,3-Tetramethyl-pentane CH_3 CH_3 CH_3-C-C-CH_2-CH_3 CH_3 CH_3	8	−236.69	−245.73	9.04	−236.69	−238.99	2.30
2,2,3,4-Tetramethyl-pentane CH_3 CH_3 CH_3-C-CH-CH-CH_3 CH_3 CH_3	6	−236.86	−249.78	12.92	−236.86	−247.50	10.64
2,3,3,4-Tetramethyl-pentane CH_3 CH_3 CH_3-CH-C-CH-CH_3 CH_3 CH_3	6	−236.10	−249.78	13.68	−236.10	−247.50	11.40
2,2,4,4-Tetramethyl-pentane CH_3 CH_3 CH_3-C-CH_2-C-CH_3 CH_3 CH_3	4	−241.63	−252.84	11.21	−241.63	−239.63	−2.00

Examination of the residuals found above show that the methyl repulsion approach gives better agreement most of the time in contrast to the gauche correction developed by Benson *et al.*, for branched alkane hydrocarbons. Residuals are smaller in 10 out of the above 14 cases when the methyl repulsion approach is used.

Comparison of the methyl repulsion correction and Benson's gauche — correction in branched alkene hydrocarbons (gas phase)

Compound name and formula	Gauche isomers (76BEN)	Benson method (76BEN) $\Delta_f H^\circ$ (kJ/mol)			Methyl repulsion method (This work) $\Delta_f H^\circ$ (kJ/mol)		
		expt	calc	resd	expt	calc	resd
2-Methylpropene	0	−16.90	−15.90	−1.00	−16.90	−18.58	1.68
							
2-Methyl-1-butene	0	−35.31	−35.82	0.51	−35.31	−37.20	1.89
							
2,3-Dimethyl-1-butene	1	−62.38	−62.67	0.04	−62.38	−64.73	2.35
							
3-Methyl-2-ethyl-1-butene	1	−79.54	−82.59	3.05	−79.54	−83.35	3.81
							
2,3,3-Trimethyl-1-butene	2	−85.48	−90.04	4.56	−85.48	−92.39	6.91
							

Calculation of the enthalpies of formation at 298.15 K in the gas phase using either group values developed in this work or those reported by 76BEN yield $\Delta_f H^\circ$'s of about the same magnitudes. For this reason, residuals are also about the same magnitudes from both approaches.

Appendix D. Example Calculations of Total Symmetry Number for Some Hydrocarbon Compounds

The total symmetry number of the molecule, N(tot), is composed of two parts: the internal symmetry number and the external symmetry number. Both are defined below.

(1) The internal symmetry number, N(int), is determined when a terminal rotator has more than one indistinguishable conformation as it makes one complete rotation about an axis colinear with the single bond linking it to the rest of the molecule. If there are n such conformations, then the axis is called an n-fold axis of symmetry and N(int) for that rotor will be equal to n. For example, a methyl group has three such conformations, and therefore, a three-fold axis of symmetry and N(int) equal to 3. The phenyl group has two indistinguishable conformations as it makes one complete rotation about an axis through the bonding carbon atom of the aromatic ring and carbon atom in the para position to it, thus exhibiting two-fold symmetry.

Although nonsymmetrical terminal rotors do not affect N(tot) of a molecule, they need to be considered in determining the symmetry of compound rotors and N(ext) for a molecule.

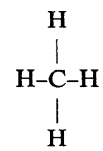
Several example calculations are provided below within a format which allows for an examination of the internal and external symmetry elements in a molecule followed by a final calculation of the total symmetry number. Using this approach, the symmetries of the terminal rotors are noted. They are then conceptually spun to yield time-averaged symmetry similar to that of a single atom. The time-averaged rotor is called a pseudo-atom and the resulting molecule is called a pseudo-molecule. This process is continued until there are no further terminal rotors and the molecule becomes rigid. The value for N(int) will be the product of the symmetry numbers of all of the rotors.

(2) external symmetry number, N(ext), which is determined when a rigid molecule or a pseudo-molecule, derived from the spinning process, shows additional symmetry. N(ext) is defined as the total number of independent permutations of identical atoms (or pseudo-atoms) in a molecule that can be arrived at by rigid rotations of the entire molecule (or pseudo-molecule).

The value of N(tot) is equal to the product of all N(int) and N(ext).

Example Calculations for Several Hydrocarbon Compounds

methane



Symmetrical terminal rotors: None.
Pseudo-molecule representation: Y.
Internal symmetry: Methane has no internal symmetry.
External symmetry: Methane exhibits tetrahedral symmetry and has four three-fold symmetry axes. Each axis goes through a different C–H bond and includes the rotation of the remaining CH_3 group about this bond. Twelve unique rotational permutations of the methane molecule can be drawn, consequently, N(ext) = 12.
Total symmetry : Methane has N(tot) = N(ext) = 12.

ethane

CH_3–CH_3

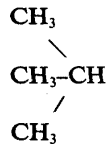
Symmetrical terminal rotors: Ethane has two terminal methyl groups each of which have three-fold symmetry.
Pseudo-molecule representation: Y–Y.
Internal symmetry: Ethane has N(int) = 3×3 = 9.
External symmetry: End-to-end symmetry can be visualized in the structural formula or the pseudo-molecule resulting in N(ext) = 2.
Total symmetry: N(tot) = N(int)$\times N$(ext) = $3\times3\times2$ = 18. The value of N(tot) is the same for all of the n-alkanes.

***n*-butane**

CH_3–CH_2–CH_2–CH_3

Symmetrical terminal rotors: n-Butane has two methyl groups each of which have three-fold symmetry. N(int) = 3×3 = 9.
Pseudo-molecule representation: Y–CH_2–CH_2–Y.
Internal symmetry: Spinning of the Y–CH_2 groups in the pseudo-molecule does not result in any change in internal symmetry, hence, N(int) = 9.
External symmetry: End-to-end symmetry can be visualized in either the structural formula or the pseudo-molecule resulting in N(ext) = 2.
Total symmetry: N(tot) = N(int)$\times N$(ext) = $3\times3\times2$ = 18. The value of n(tot) is the same for all of the n-alkanes.

2-Methylpropane



Symmetrical terminal rotors: 2-Methylpropane has three methyl groups each of which have three-fold symmetry. $N(\text{int}) = 3\times3\times3 = 27$.

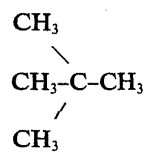
Pseudo-molecule representation: Y_3–CH.

Internal symmetry: The Y_3–CH pseudo-molecule itself has three-fold symmetry and contributes an additional $N(\text{int}) = 3$. The final $N(\text{int})$ for the molecule is $N(\text{int}) = 27\times3 = 81$.

External symmetry: Spinning of either the structural formula or the pseudo-molecule shows no end-to-end symmetry, hence, $N(\text{ext}) = 1$.

Total symmetry: $N(\text{tot}) = N(\text{int})\times N(\text{ext}) = 81\times1 = 81$.

2,2-Dimethylpropane



Symmetrical terminal rotors: 2,2-Dimethylpropane has four methyl groups each of which have three-fold symmetry. $N(\text{int}) = 3\times3\times3\times3 = 81$.

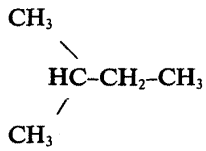
Pseudo-molecule representation: CY_4.

Internal symmetry: The CY_4 pseudo-molecule offers no additional elements of internal symmetry, hence, $N(\text{int}) = 81$.

External symmetry: The external symmetry for the CY_4 pseudo-molecule is the same as that for the methane molecule because 12 unique rotational permutations can be drawn for CY_4, giving $N(\text{ext}) = 12$.

Total symmetry: $N(\text{tot}) = N(\text{int})\times N(\text{ext}) = 81\times12 = 972$.

2-Methylbutane



Symmetrical terminal rotors: 2-Methylbutane has three terminal methyl groups each of which have three-fold symmetry. $N(\text{int}) = 3\times3\times3 = 27$.

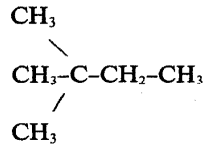
Pseudo-molecule representation: Y_2CH–CH_2Y.

Internal symmetry: Examination of the pseudo-molecule does not result in any additional internal symmetry contributions. $N(\text{int}) = 27$.

External symmetry: Rotation of the pseudo-molecule about the central bond give no contribution to external symmetry. $N(\text{ext}) = 1$.

Total symmetry: $N(\text{int})\times N(\text{ext}) = 27\times1 = 27$.

2,2-Dimethylbutane



Symmetrical terminal rotors: 2,2-Dimethylbutane has four methyl groups each of which have three-fold symmetry. $N(\text{int}) = 3\times3\times3\times3 = 81$.

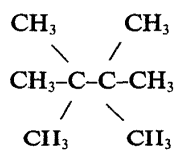
Pseudo-molecule representation: Y_3C–CH_2Y.

Internal symmetry: Examination of the pseudo-molecule shows that the CY_3 group exhibits an additional amount of three-fold symmetry so that $N(\text{int})$ is now $3\times3\times3\times3\times3$ or 243.

External symmetry: Rotation of the pseudo-molecule does not yield any extra elements of external symmetry, hence, $N(\text{ext}) = 1$.

Total symmetry: $N(\text{int})\times N(\text{ext}) = 243\times1$ or 243.

2,2,3,3-Tetramethylbutane



Symmetrical terminal rotors: 2,2,3,3-Tetramethylbutane has six methyl groups each of which have three-fold symmetry, giving $N(\text{int}) = 3\times3\times3\times3\times3\times3$ or 729.

Pseudo-molecule representation: Y_3C–CY_3.

Internal symmetry: Each CY_3 group of the pseudo-molecule exhibits three-fold symmetry enhancing $N(\text{int})$ to $729\times3\times3$ or 6561.

External symmetry: Rotation of the pseudo-molecule about the central bond shows it to have two-fold symmetry, hence, $N(\text{ext}) = 2$.

Total symmetry: $N(\text{int})\times N(\text{ext}) = 6561\times2 = 13122$.

Ethylene

$$H_2C{=}CH_2$$

Symmetrical terminal rotors: None.

Pseudo-molecule representation: Y=Y.

Internal symmetry: Ethylene does not exhibit internal symmetry because the double bond prevents internal rotation.

External symmetry: Ethylene has two two-fold rotational axes, one horizontally through the two carbon atoms and the other vertically bisecting the two carbon atoms. From this one obtains $N(\text{ext}) = 2\times2$ or 4.

Total symmetry: $N(\text{tot}) = N(\text{ext}) = 4$.

Propylene

$$CH_3\text{–}CH_2{=}CH_2$$

Symmetrical terminal rotors: Propylene has one methyl group which has three-fold symmetry giving N(int) = 3.

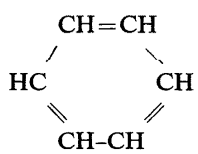
Pseudo-molecule representation: $YCH{=}CH_2$.

Internal symmetry: The pseudo-molecule does not provide any additional elements of internal symmetry, hence, N(int) = 3.

External symmetry: Rotation of the pseudo-molecule does not provide any additional elements of external symmetry, hence, N(ext) = 1.

Total symmetry: $N(\text{tot}) = N(\text{int}) \times N(\text{ext}) = 3 \times 1 = 3$. The latter value for N(tot) is applicable to all 1-olefinic hydrocarbons.

Benzene



Symmetrical terminal rotors: None.

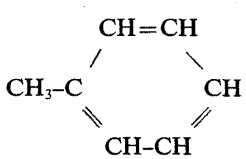
Pseudo-molecule representation: Z.

Internal symmetry: Benzene has no internal symmetry.

External symmetry: Benzene has a six-fold rotational axis perpendicular to the ring which also passes through the center of the ring. Perpendicular to the six-fold axis, there are six two-fold axes through the opposite carbon atoms or bisecting the opposite carbon-carbon bonds, hence, $N(\text{ext}) = 2 \times 6 = 12$.

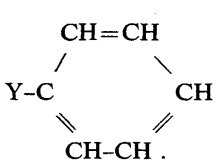
Total symmetry: $N(\text{tot}) = N(\text{ext}) = 12$.

Toluene



Symmetrical terminal rotors: Toluene has one methyl group which exhibits three-fold symmetry and the phenyl group which shows two-fold symmetry, giving $N(\text{int}) = 3 \times 2 = 6$.

Pseudo-molecule representation: Y–Z or,

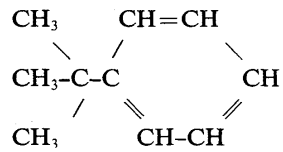


Internal symmetry: Further examination of the pseudo-molecule does not give any additional elements of internal symmetry, hence, N(int) = 6.

External symmetry: Rotation of the pseudo-molecule does not give any additional elements of external symmetry, hence, N(ext) = 1.

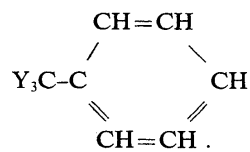
Total symmetry: $N(\text{tot}) = N(\text{int}) \times N(\text{ext}) = 6 \times 1 = 6$.

***t*-Butylbenzene**



Symmetrical terminal rotors: *t*-Butylbenzene has three methyl groups each of which have three-fold symmetry. This gives $N(\text{int}) = 3 \times 3 \times 3 = 27$. The phenyl group has two-fold symmetry for which N(int) = 2.

Pseudo-molecule representation: $Y_3C\text{–}Z$ or,



Internal symmetry: Examination of the pseudo-molecule shows that the CY_3 group exhibits three-fold symmetry resulting in another N(int) = 3. A final overall N(int) results which is equal to $27 \times 2 \times 3$ or 162.

External symmetry: Rotation of the pseudo-molecule does not provide any additional elements of external symmetry, hence, N(ext) = 1.

Total symmetry: $N(\text{tot}) = N(\text{int}) \times N(\text{ext}) = 162 \times 1 = 162$.

TABLE 1. Additive group contribution values for hydrocarbons at 298.15 K

Groups	Gas phase			Liquid phase			Solid phase		
	$\Delta_f H°$ kJ/mol	$C_p°$ J/mol·K	$S°$ J/mol·K	$\Delta_f H°$ kJ/mol	$C_p°$ J/mol·K	$S°$ J/mol·K	$\Delta_f H°$ kJ/mol	$C_p°$ J/mol·K	$S°$ J/mol·K
Alkane 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		
-CH$_3$ corr[a]	−2.26			−2.18			−2.34		
C-(C)$_4$	19.20	16.53	−149.49	17.99	10.24	−98.65	12.47	−83.63[j]	−33.19[j]
-CH$_3$ corr[b]	−4.56			−4.39			−4.35		
-CH$_3$ corr[c]	−1.80			−1.77			−2.70		
-CH$_3$ corr[d]	−0.64			−0.64			−2.24		
Alkene Groups									
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$_B$)][e]									
C$_d$-(C)(C$_B$)	37.95	15.90	−51.97	38.58					
[C$_d$-(H)(C$_t$)][f]									
C$_d$-(C$_B$)$_2$	32.88			30.83	25.10		49.90	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[a]	−2.26			−2.18			−2.34		
C-(C)$_3$(C$_d$)	22.13	9.16	−150.23	20.79	28.74	−108.20	12.51		
-CH$_3$ corr[a]	−4.56			−4.39			−4.35		
C-(H)(C)(C$_d$)$_2$	−1.00								
C-(H)$_2$(C$_d$)$_2$	−19.79	24.77	42.08	−25.27	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-correction[g]	4.85	−8.03	5.06	5.27			5.73		
Alkyne groups									
C$_t$-(H)	113.50	22.55	101.96	104.47	39.96	67.57	110.34		
C$_t$-(C)	115.10	13.2	226.32	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[a]	−2.26			−2.18			−2.34		
C-(C)$_3$(C$_t$)				22.83					
-CH$_3$ corr[b]	−4.56			−4.39			−4.35		
C-(H)$_2$(C$_t$)$_2$	−41.14			−39.08					
C-(C)$_2$(C$_t$)$_2$				20.67					

TABLE 1. Additive group contribution values for hydrocarbons at 298.15 K — Continued

Groups	Gas phase			Liquid phase			Solid phase		
	$\Delta_f H°$ kJ/mol	$C_p°$ J/mol·K	$S°$ J/mol·K	$\Delta_f H°$ kJ/mol	$C_p°$ J/mol·K	$S°$ J/mol·K	$\Delta_f H°$ kJ/mol	$C_p°$ J/mol·K	$S°$ J/mol·K
				Allenic group					
C_a	142.67	15.86	26.28	134.68	30.04	14.39	131.08		
				Aromatic groups					
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)$_2$][h]									
C_B-(C_B)$_3$	21.66	13.12	−36.57	17.21	17.07		17.03	−1.72	−6.00
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)							67.20	39.83	
C-(C_B)$_4$							64.89	58.74	
C_{BF}-(C_{BF})(C_B)$_2$	20.10	[i]	[i]	15.83	9.52	−5.54	14.10	2.30	−6.00
C_{BF}-(C_B)(C_{BF})$_2$	16.00			1.50			12.00	5.77	2 00
C_{BF}-(C_{BF})$_3$	3.59			−0.90			1.94	8.00	7.00
ortho corr	1.26	6.40	−2.50	3 26	3.50	0.00	5.00	0.00	0.00
meta corr	−0.63	0.71	0.00	0.00	0.00	0.00	2.00	0.00	0.00

[a]Use for each adjacent methyl group.
[b]Use for each adjacent methyl group when one C-(C)$_4$ is present.
[c]Use for each adjacent methyl group when there is a C-(C)$_4$ and a C-(C)$_3$(H) group present in the longest carbon chain.
[d]Use for each adjacent methyl group when there are two C-(C)$_4$ groups present in the longest carbon chain.
[e]C_d-(H)(C_B) = C_d-(H)(C_d)
[f]C_d-(H)(C_t) = C_d-(H)(C_d)
[g]When one of the groups is t-butyl, apply the following *cis* correction: $\Delta_f H°$(g) = 17.24; $\Delta_f H°$(liq) = 17.48; $\Delta_f H°$(solid) = 17 57
[h]C_B-(C_t)(C_B)$_2$ = C_B-(C_d)(C_B)$_2$.
[i]C_{BF}-(C_B)2(C_{BF})· Do not use ortho, meta corrections for naphthalenes
Use: 1. 0 substitution $C_p°$(g) = 11.83; $S°$(g) = −19.66
Use: 2 1 substitution $C_p°$(g) = 14 39; $S°$(g) = −21 50
Use: 3. 2 substitutions $C_p°$(g) = 16.48; $S°$(g) = −23.00.
[j]Group value calculated from experimental data on solid 2,2,3,3-tetramethylbutane (52SCO/DOU)

TABLE 2. Ring strain corrections to be applied to cycloalkanes and related hydrocarbons

Rings	Gas phase			Liquid phase			Solid phase		
	$\Delta_f H°$ kJ/mol	$C_p°$ J/mol·K	$S°$	$\Delta_f H°$ kJ/mol	$C_p°$ J/mol·K	$S°$	$\Delta_f H°$ kJ/mol	$C_p°$ J/mol·K	$S°$
cyclopropane	115.15	−12.73	134.86						
cyclobutane	110.89	−19.34	126.04	106.64	−10.68	51.48			
cyclopentane[a]	26.75	−31.44	116.22	23.59	−23.32	42.24	34.00		
cyclohexane[a]	0.39	−31.07	78.18	−2.06	−26.21	10.07	10.30		
cycloheptane	26.34	−37.14	73.97	23.50	−32.19	15.89			
cyclooctane	40.63	−43.17	70.78	38.10	−27.88	2.96			
cyclononane	52.91			50.40					
cyclodecane	43.63			50.61					
cycloundecane	47.56			47.55					
cyclododecane	17.31						46.27		
cyclotridecane	21.84			24.83					
cyclotetradecane	49.58						37.74		
cyclopentadecane	8.03						65.09		
cyclohexadecane	8.41						67.14		
cycloheptadecane	−13.59						69.56		
cyclopropene	224.21								
cyclobutene	125.81	−11.67	126.77						
cyclopentene[a]	24.31	−26.53	113.76	19.82	−15.82	48.37			
cyclohexene	5.36	−19.50	95.69	2.33	−20.26	29.34			
cycloheptene	21.81								
cyclooctene	24.65			18.26					
1,3-cyclo-pentadiene	24.94			24.79					
1,3-cyclo-hexadiene	18.79			18.18	−26.56	50.18			
1,4-cyclo-hexadiene					−34.22	36.41			
1,3-cyclo-heptadiene	27.54								
1,5-cyclo-octadiene	9.58			9.01	−7.45	23.35			
1,3,5-cyclo-heptatriene	14.90	−18.63	102.26	16.62	−54.00	84.96			
cyclo-octatetraene	69.61	−26.31	116.38	77.07	−68.18	113.89			
spiropentane	248.50	−19.97	286.59	242.58	2.60	162.81			
***cis*-decalin**				−4.02	−54.12	53.75			
***trans*-decalin**				−15.22	−57.63	53.67			
***cis*-hexahydroindan**				16.55	−41.52	86.59			
***trans*-hexahydroindan**				16.45	−46.00	79.98			
2,2-metacyclophane							55.06		
2,2-metaparacyclophane							109.46	−4.02	
2,2-paracyclophane							125.66	−13.18	−1.92
3,3-paracyclophane							65.68	14.90	
adamantane	−6.14						6.28		
bicyclo[2.2.2]octane	27.12				−67.59	−63.45	41.52		
bicyclo[3.3.3]undecane	99.06						124.10		

[a] Values given are for unsubstituted rings. When the ring is substituted, use the following values:
cyclopentane: $C_p°$, gas = -27.87, $S°$, gas = 118.39, liq = 56.65.
cyclohexane: $C_p°$, gas = -22.82, $S°$, gas = 83.97, liq = 25.10.
cyclopentene: $C_p°$, gas = -24.50, S°, gas = 117.11.

TABLE 3 n-Alkane hydrocarbons in the gas phase at 298.15 K

Name	$\Delta_f H°$(kJ/mol) expt	calc	resd	$C_p°$(J/mol·K) expt	calc	resd	$S°$(J/mol·K) expt	calc	resd	N(tot)
ethane	−83.85	−84.52	0.67	52.63	51.46	1.17	229 49	230.61	−1.12	18
propane	−104.68	−105.15	0.47	73.51	74.35	−0.84	269.91	269.77	0.14	18
butane	−125 65	−125.78	0.13	97.45	97.24	0.21	310.12	308.93	1.19	18
pentane	−146.82	−146.41	−0.41	120 21	120.13	0.08	348.95	348.09	0.86	18
hexane	−167.11	−167 04	−0.07	143.09	143.02	0.07	388.40	387.25	1 15	18
heptane	−187.65	−187.67	0.02	165.98	165 91	0.07	427.90	426.41	1.49	18
octane	−208.57	−208.30	−0.27	188.87	188.80	0.07	466.73	465.57	1.16	18
nonane	−228.24	−228.93	0.69	211.71	211.69	0.02	505.68	504.73	0.95	18
decane	−249.49	−249.56	0.07	234 60	234.58	0.02	544.63	543.89	0.74	18
undecane	−270.91	−270.19	−0.72	257 44	257.47	−0.03	583.58	583.05	0.53	18
dodecane	289.66	290.82	1.16	280.33	280.36	−0.03	622.50	622.21	0 29	18
tridecane				303.21	303.25	−0.04	661.45	661 37	0 08	18
tetradecane				326.06	326.14	−0.08	700.40	700.53	−0.13	18
pentadecane				348.95	349.03	−0.08	739 35	739.69	−0.34	18
hexadecane	−374.76	−373.34	−1.42	371.79	371.92	−0.13	778.31	778.85	−0.54	18
heptadecane				394.68	394.81	−0.13	817.26	818.01	−0.75	18
octadecane				417.56	417.70	−0.14	856.21	857.17	−0.96	18
nonadecane				440.41	440.59	−0 18	895.17	896.33	−1.16	18
eicosane				463 29	463.48	−0.19	934 12	935 49	−1.37	18

TABLE 4. n-Alkane hydrocarbons in the liquid phase at 298.15 K

Name	$\Delta_f H°$(kJ/mol) expt	calc	resd	$C_p°$(J/mol·K) expt	calc	resd	$S°$(J/mol·K) expt	calc	resd
propane	−119.75	−120.95	1.20						
butane	−146.65	−146.68	0.03	135.00[a]	133.80	1.20	231.00	231.36	−0.36
pentane	−173.47	−172.41	−1 06	167.19	164.22	2.97	263.47	263.74	−0.27
hexane	−198.66	−198.14	−0.52	194.97	194.64	0.33	296.06	296.12	−0.06
heptane	−224.22	−223.87	−0.35	224.93	225.06	−0.13	328.57	328.50	0.07
octane	−250.08	−249.60	−0.48	254.14	255.48	−1.34	361.20	360.88	0.32
nonane	−274.68	−275.33	0.65	284.39	285.90	−1.51	393.67	393.26	0.41
decane	−300.87	−301.06	0.19	314.47	316.32	−1.85	425.89	425.64	0.25
undecane	−327.23	−326.79	−0.44	345.05	346.74	−1.69	458.15	458.02	0.13
dodecane	−350.91	−352.52	1.61	375.97	377.16	−1.19	490.66	490.40	0.26
tridecane				406.89	407.58	−0.69	522.87	522.78	0.09
tetradecane				438.44	438.00	0.44	555.43	555.16	0.27
pentadecane				470.07	468.42	1.65	587.52	587.54	−0.02
hexadecane	−456.14	−455.44	−0.70	501.45	498.84	2.61	619.65	619.92	−0.27
heptadecane				534.34	529.26	5.08	652.24	652.30	−0.06

[a]Obtained from extrapolation of experimental data of 40AST/MES to 298 15 K

TABLE 5. n-Alkane hydrocarbons in the solid phase at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
propane	−123.30	−122.89	−0.41						
butane	−153.39	−152.30	−1.09						
pentane	−181.46	−181.71	0.25						
hexane	−211.71	−211.12	−0.59						
heptane	−238.24	−240.53	2.29						
octane	−270.83	−269.94	−0.89						
nonane	−296.44	−299.35	2.91						
decane	−329.57	−328.76	−0.81						
undecane	−356.27	−358.17	1.90						
dodecane	−387.73	−387.58	−0.15						
tridecane	−414.43	−416.99	2.56						
tetradecane	−449.07	−446.40	−2.67						
pentadecane	−473.50	−475.81	2.31						
hexadecane	−509.49	−505.22	−4.27	441.79[a]	441.78	0.01	434.84[a]	435.52	−0.68
heptadecane	−532.33	−534.63	2.30						
octadecane	−567.43	−564.04	−3.39	485.64	485.62	0.02	480.20	481.54	−1.34
eicosane				(479.90)	529.46	−49.56	(558.56)	527.56	31.00
tetracosane				(730.94)	617.14	113.80	(651.03)	619.60	31.43
pentacosane				(769.02)	639.06	129.96	(671.11)	642.61	28.50
hexacosane				661.20	660.98	0.22	667.01	665.62	1.39
dotriacontane	−968.34	−975.78	7.44	(877.38)	792.50	84.88	(851.44)	803.68	47.76
tritriacontane				(900.82)	814.42	86.40	(877.80)	826.69	51.11

[a]Obtained from extrapolation of experimental data of 54FIN/GRO to 298.15 K.

TABLE 6. Substituted alkane hydrocarbons (tertiary carbon) in the gas state 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
2-methylpropane	−134.18	−134.73	0.55	96.82	97.27	−0.45	294.64	291.82	2.82	81
2-methylbutane	−153.63	−153.10	−0.53	118.78	120.16	−1.38	343.59	340.12	3.47	27
2-methylpentane	−174.77	−173.73	−1.04	144.18	143.05	1.13	380.53	379.28	1.25	27
2-methylhexane	−194.64	−194.36	−0.28	165.98	165.94	0.04	419.99	418.44	1.55	27
2-methylheptane	−215.35	−214.99	−0.36	188.87	188.83	0.04	455.26	457.60	−2.34	27
2-methyloctane				217.07	211.72	5.35	495.89	496.76	−0.87	27
2-methylnonane				242.09	234.61	7.48	534.46	535.92	−1.46	27
3-methylpentane	−172.09	−171.47	−0.62	143.09	143.05	0.04				
3-methylhexane	−191.33	−192.10	0.77	165.98	165.94	0.04				
3-methylheptane	−212.51	−212.73	0.22	188.87	188.83	0.04	461.58	463.36[a]	−1.78	27
3-methyloctane				212.59	211.72	0.87				
3-methylnonane				237.61	234.61	3.00				
4-methylheptane	−211.96	−212.73	0.77	188.87	188.83	0.04	453.34	451.83	1.51	54
4-methyloctane				212.59	211.72	0.87				
4-methylnonane				237.61	234.61	3.00				
5-methylnonane				237.61	234.61	3.00				
3-ethylpentane	−189.62	−189.84	0.22	165.98	165.94	0.04	411.50	412.67	−1.17	54
3-ethylhexane	−210.71	−210.47	−0.24	188.87	188.83	0.04	458.19	457.60	0.59	27
3-ethylheptane				208.11	211.72	−3.61				
3-ethyloctane				233.13	234.61	−1.48				

TABLE 6 Substituted alkane hydrocarbons (tertiary carbon) in the gas state 298.15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
4-ethylheptane				208.11	211.72	−3.61				
4-ethyloctane				233.13	234.61	−1.48				
4-propylheptane				233.13	234.61	−1.48				
4-isopropylheptane				231.00	234.64	−3.64				
2,4-dimethylpentane	−201.71	−201.05	−0.66	165.98	165 97	0.01	396.64	398.94	−2.30	162
2,4-dimethylhexane	−219.24	−219.42	0.18	188.87	188.86	0.01	445.64	449.63[a]	−3.99	81
2,5-dimethylhexane	−222 51	−221.68	−0.83	188.87	188 86	0.01	439.03	438.10	0 93	162
2,3-dimethylbutane	−178.28	−180.42	2.14	140.54	143 08	−2.54	365.77	359.78	5 99	162
2,3-dimethylpentane	−198.87	−198.79	−0.08	165.98	165.97	0.01	414.05	410.47[a]	3.58	81
2,3-dimethylhexane	−213.80	−219.42	5.62	188.87	188.86	0.01	443.96	443.86	0.10	81
3,4-dimethylhexane	−212.84	−217.16	4.32	188 87	188.86	0.01	448.32	449.63[a]	−1 31	81
3-ethyl-2-methylpentane	−211 04	−217 16	6.12	188.87	188.86	0.01	441.12	443.86	−2 74	81
2,3,4-trimethylpentane	−217 32	−226.11	8.79	188 87	188 89	−0 02	428 07	430 13	−2 06	243

[a]Includes correction to entropy for optical isomerism, $R \ln 2$.

TABLE 7 Substituted alkane hydrocarbons (tertiary carbon) in the liquid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
2-methylpropane	−153.47	−154.14	0.67						
2-methylbutane	−178.57	−177.69	−0.88						
2-methylpentane	−204.64	−203.42	−1.22	193.72	191.66	2.06	290.58	290.77	−0.19
2-methylhexane	−229.49	−229.15	−0.34	222.92	222.08	0.84	323.34	323.15	0.19
2-methylheptane	−255.01	−254.88	−0.13	252.00	252.50	−0.50	356.39	355.53	0.86
2-methylnonane				313.30	313.34	−0.04	420.07	420.29	−0.22
2-methyldecane				341.21	343.76	−2.55	453.80	452.67	1.13
3-methylpentane	−202.38	−201.24	−1.14	190.66	191.66	−1.00			
3-methylhexane	−226.44	−226.97	0.53	214.51	222.08	−7.57	327.31	323.15	4.16
3-methylheptane	−252.34	−252.70	0.36	250.20	252.50	−2.30			
3-methylnonane				308.99	313.34	−4.35	427.19	420.29	6.90
4-methylheptane	−251.63	−252.70	1.07	251.09	252.50	−1.41			
4-methylnonane				317.36	313.34	4.02	425.51	420.29	5.22
5-methylnonane				314.43	313.34	1.09	423.84	420.29	3.55
3-ethylpentane	−224.89	−224.79	−0.10	219.58	222.08	−2.50	314.55	323.15	−8.60
3-ethylhexane	−250.41	−250.52	0.11						
2,4-dimethylpentane	−234.60	−234.43	−0.17	224.22	219.10	5.12	303.17	317.80	−14.63
2,4-dimethylhexane	−257.02	−257.98	0.96						
2,5-dimethylhexane	−260.37	−260.16	−0.21	249.20	249.52	−0.32			
2,3-dimethylbutane	−207.40	−208.70	1.30						
2,3-dimethylpentane	−233.09	−232.25	−0.84	215.89	219.10	−3.21	319.11	317.80	1.31
2,3-dimethylhexane	−252.59	−257.98	5.39						
2,7-dimethyloctane				301.67	310.36	−8.69			
3,4-dimethylhexane	−251.83	−255.80	3.97						
3-ethyl-2-methylpentane	−249.58	−255.80	6.22						
2,3,4-trimethylpentane	−255.01	−263.26	8.25	246.23	246.54	−0.31	329.32	344.83	−15.51

TABLE 8. Substituted alkane hydrocarbons (tertiary carbon) in the solid state at 198.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
2-methylpropane	−157.99	−153.22	−4.77						
2-methylbutane	−183.72	−180.29	−3.43						
2-methylpentane	−210.92	−209.70	−1.22						
2-methylhexane	−238.66	−239.11	0.45						
2-methylheptane	−266.94	−268.52	1.58						
3-methylpentane	−207.69	−207.36	−0.33						
3-methylhexane	−234.93	−236.77	1.84						
3-methylheptane	−264.01	−266.18	2.17						
3-ethylpentane	−234.43	−234.43	0.00						
4-methylheptane	−262.46	−266.18	3.72						
2,4-dimethylpentane	−241.46	−237.69	−3.77						

TABLE 9. Substituted alkane hydrocarbons (quaternary carbon) in the gas state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
2,2-dimethylpropane	−167.99	−168.08	0.09	121.63	119.45	2.18	306.39	302.59	3.80	972
2,2-dimethylbutane	−186.10	−184.15	−1.95	141.88	142.34	−0.46	358.23	353.28	4.95	243
2,2-dimethylpentane	−205.85	−204.78	−1.07	165.98	165.23	0.75	392.88	392.44	0.44	243
2,2-dimethylhexane	−224.60	−225.41	0.81	188.87	188.12	0.75	431.20	431.60	−0.40	243
3,3-dimethylpentane	−201.17	−200.22	−0.95	165.98	165.23	0.75	399.70	395.81	3.89	162
3,3-dimethylhexane	−219.99	−220.85	0.86	188.87	188.12	0.75	438.06	440.73	−2.67	81
2,2,3-trimethylbutane	−204.47	−202.27	−2.20	164.56	165.26	−0.70	383.60	378.70	4.90	729
2,2,3-trimethylpentane	−219.99	−221.10	1.11	188.87	188.15	0.72	425.18	417.86	7.32	729
2,2,4-trimethylpentane	−224.01	−222.90	−1.11	188.87	188.15	0.72	423.21	417.86	5.35	729
2,3,3-trimethylpentane	−216.27	−221.10	4.83	188.87	188.15	0.72	431.54	427.00	4.54	243
2,2,3,3-tetramethylbutane	−225.60	−219.00	−6.60	192.59	187.44	5.15	389.36	386.10	3.26	13,122
2,2,3,3-tetramethylpentane	−236.69	−238.99	2.30	212.09	210.33	1.76				
2,2,4,4-tetramethylpentane	−241.63	−239.63	−2.00	211.63	210.33	1.30				
2,2,3,4,4-pentamethylpentane				234.43	233.25	1.18				
3-ethyl-3-methylpentane	−214.85	−216.29	1.44	188.87	188.12	0.75	432.96	431.60	1.36	243
3,3-diethylpentane	−232.34	−232.36	0.02	204.18	211.01	−6.83	461.54	459.23	2.31	972

TABLE 10. Substituted alkane hydrocarbons (quaternary carbon) in the liquid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
2,2-dimethylpropane	−190.33	−190.01	−0.32						
2,2-dimethylbutane	−213.80	−211.35	−2.45	183.18	186.58	−3.40	272.00	266.93	5.07
2,2-dimethylpentane	−238.28	−237.08	−1.20	221.12	217.00	4.12	300.29	299.31	0.98
2,2-dimethylhexane	−261.88	−262.81	0.93						
3,3-dimethylpentane	−234.18	−232.69	−1.49	211.71	217.00	−5.29	293.30	299.31	−6.01
3,3-dimethylhexane	−257.94	−258.42	0.48	246.60	247.42	−0.82			
2,2,3-trimethylbutane	−236.52	−233.68	−2.84	213.51	214.02	−0.51	292.25	293.96	−1.71
2,2,3-trimethylpentane	−256.90	−257.94	0.74						
2,2,4-trimethylpentane	−259.16	−259.41	0.25	238.57	244.44	−5.87	328.03	326.34	1.69
2,3,3-trimethylpentane	−253.51	−257.64	4.13	245.56	244.44	1.14			

TABLE 10 Substituted alkane hydrocarbons (quaternary carbon) in the liquid state at 298.15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
2,2,3,3-tetramethyl-pentane	−278.28	−278.61	0.33						
2,2,4,4-tetramethyl-pentane	−279.99	−279.25	−0.74						
3-ethyl-3-methylpentane	−252.84	−254.03	1.19						
3,3-diethylpentane	−275.39	−275 37	−0.02						

TABLE 11. Substituted alkane hydrocarbons (quaternary carbon) in the solid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
2,2-dimethylpropane	−196 15	−191 89	−4.26						
2,2-dimethylbutane	−220.08	−216.95	−3.13						
2,2-dimethylpentane	−244.14	−246.36	2.22						
3,3-dimethylpentane	−241 25	−242 01	0 76						
2,2,3-trimethylbutane	−241.08	−240.71	−0.37						
3-ethyl-3-methylpentane	−267.48	−267.07	−0 41						
3,3-diethylpentane	−292.13	−292.13	0.00						
2,2,3,3-tetramethyl-butane	−268.95	−268.94	−0.01	237 44	237.44	0.00	273.76	273.76	0.00

TABLE 12. *n*-Alkene hydrocarbons in the gas state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
ethylene	52.47	52.64	−0.17	43.56	42.76	0.80	219.45	219.51	−0.06	4
propylene	20.00	20.38	−0.38	63.89	65.85	−1.96	266.94	266.76	0.18	3
1-butene	0.21	−0 50	0.71	85.65	86.48	−0.83	305.60	304.96	0.64	3
1-pentene	−21.59	−21.13	−0.46	109.58	109.37	0.21	345.81	344.12	1.69	3
1-hexene	−41.67	−41.76	0.09	132.34	132.26	0.08	384.64	383.28	1.36	3
1-heptene	−62.30	−62.39	0 09	155.23	155.15	0.08	423.59	422.44	1.15	3
1-octene	−82.93	−83.02	0.09	178.07	178.04	0.03	462.54	461.60	0.94	3
1-nonene	−103.51	−103.65	0.14	200.96	200.93	0.03	501.49	500.76	0.73	3
1-decene	−124.14	−124.28	0.14	223.80	223.82	−0.02	540.45	539.92	0.53	3
1-hexadecene	−247.82	−248 06	0.24	361.04	361.16	−0.12	774.12	774.88	−0.76	3
cis-2-butene	−7.07	−7.03	−0.04	78.91	80.91	−2.00	300.83	301.77	−0.94	18
***trans*-2-butene**	−11.51	−11.88	0.37	87.82	88.94	−1.12	296.48	296.71	−0.23	18
***cis*-2-pentene**	−28 49	−27.91	−0 58	101.75	101.54	0.21	346.27	345.73	0.54	9
***trans*-2-pentene**	−32.38	−32 76	0 38	108.45	109.57	−1.12	340.41	340.67	−0.26	9
***cis*-2-hexene**	−52 34	−48 54	−3 80	125.69	124.43	1.26	386.48	384.89	1.59	9
***trans*-2-hexene**	−53 89	53 39	0 50	132.38	132.46	−0.08	380.62	379.83	0.79	9
***cis*-3-hexene**	−47 61	−48 79	1 18	123.64	122.17	1.47	379.61	378.17	1.44	18
***trans*-3-hexene**	−54 43	53 64	0 79	132.84	130.20	2.64	374.84	373.11	1.73	18
***cis*-2-heptene**	−69 16	−69 17	0 01							
***trans*-2-heptene**	−73 55	−74 02	0 47							

TABLE 12. *n*-Alkene hydrocarbons in the gas state at 298.15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
cis-3-heptene	−68.78	−69.42	0.64							
trans-3-heptene	−73.76	−74.27	0.51							
1,2-butadiene	162.26	163.05	−0.79	80.12	81.71	−1.59	293.01	293.04	−0.03	3
1,2-pentadiene	140.71	142.17	−1.46	105.44	102.34	3.10	333.46	331.24	2.22	3
1,3-butadiene	109.96	109.20	0.76	79.54	79.84	−0.30	278.74	280.76	−2.02	2
cis-1,3-pentadiene	81.25	81.79	−0.54	94.56	94.90	−0.34	324.26	327.30	−3.04	3
trans-1,3-pentadiene	76.07	76.94	−0.87	103.34	102.93	0.41	319.66	322.24	−2.58	3
1,4-pentadiene	105.48	105.49	−0.01	105.02	105.01	0.01	333.46	333.46	0.00	2
1,5-hexadiene	84.06	83.52	0.54							
2,3-pentadiene	133.05	130.79	2.26	101.25	104.80	−3.55	324.68	322.99	1.69	18
allene	190.46	195.31	−4.85	59.25	58.62	0.63	243.93	245.79	−1.86	4

TABLE 13. *n*-Alkene hydrocarbons in the liquid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
ethylene		43.50			56.74			172.38	
propylene		5.19			89.45			198.07	
1-butene	−20.38	−20.54	0.16	121.85[a]	118.74	3.11	227.63[b]	229.74	−2.11
1-pentene	−47.03	−46.27	−0.76	155.31	149.16	6.15	262.55	262.12	0.43
1-hexene	−72.38	−72.00	−0.38	183.30	179.58	3.72	295.18	294.50	0.68
1-heptene	−98.03	−97.73	−0.30	211.79	210.00	1.79	327.65	326.88	0.77
1-octene	−123.51	−123.46	−0.05	241.21	240.42	0.79	360.45	359.26	1.19
1-nonene	−149.03	−149.19	0.16						
1-decene	−174.60	−174.92	0.32	300.33	301.26	−0.93	425.01	424.02	0.99
1-hexadecene	−328.70	−329.30	0.60						
cis-2-butene	−29.66	−27.85	−1.81	126.15	122.16	3.99	219.91	223.76	−3.85
trans-2-butene	−33.10	−33.12	0.02	125.90[c]	122.16	3.74	221.25[c]	223.76	−2.51
cis-2-pentene	−54.52	−53.58	−0.94	151.71	151.45	0.26	258.61	255.43	3.18
trans-2-pentene	−58.83	−58.85	0.02	156.98	151.45	5.53	256.52	255.43	1.09
cis-2-hexene	−83.89	−79.31	−4.58						
trans-2-hexene	−85.52	−84.58	−0.94						
cis-2-heptene	−105.14	−105.04	−0.10						
trans-2-heptene	−109.54	−110.31	0.77						
cis-2-octene	−135.69	−130.77	−4.92						
trans-2-octene	−135.69	−136.04	0.35						
cis-3-hexene	−78.95	−79.31	0.36						
trans-3-hexene	−86.06	−84.58	−1.48						
cis-3-heptene	−104.31	−105.04	0.73						
trans-3-heptene	−109.33	−110.31	0.98						
1,2-butadiene	138.99	139.87	−0.88						
1,2-pentadiene	150.83	148.78	2.05	244.97	244.13	0.84			
1,3-butadiene	87.91	87.86	0.05	123.65	120.08	3.57	198.99	198.98	0.01
1,4-pentadiene	80.33	80.33	0.00	146.82	146.82	0.00	248.86	248.86	0.00
2,3-pentadiene	152.42	152.20	0.22	237.32	238.15	−0.83			
1,5-hexadiene	54.10	54.14	−0.04						

[a]Obtained from extrapolation of experimental data of 46AST/FIN to 298.15 K.
[b]Calculated from table XI in 46AST/FIN.
[c]Obtained from extrapolation of experimental data of 45GUT/PIT to 298.15 K.

TABLE 14. *n*-Alkene hydrocarbons in the solid state at 298 15

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
propylene		1.17							
1-butene	−24.23	−23.18	−1.05						
1-pentene	−52.84	−52.59	−0.25						
1-hexene	−82.13	−82.00	−0.13						
1-heptene	−110.58	−111.41	0.83						
1-octene	−138.83	−140.82	1.99						
1-decene	−196.36	−199.64	3.28						
1-hexadecene	−358.90	−376 10	17.20						
***cis*-2-butene**	−36.99	−36.79	−0.20						
***trans*-2-butene**	−42.84	−42.52	−0.32						
***cis*-2-pentene**	−61.63	−61.14	−0.49						
***trans*-2-pentene**	−67.20	−66.87	−0.33						
2-hexene[a]	−97.78	−96.28	−1.50						
2-heptene[a]	−124.68	−125.69	1.01						
2-octene[a]	−153.64	−155.10	1.46						
1,2-butadiene	132.05	132.25	−0.20						
1,3-butadiene	79.91	79.92	−0.01						
1,4-pentadiene	74.22	74.22	0.00						

[a]Assumed to be the *trans* isomer.

TABLE 15. Substituted alkene hydrocarbons in the gas state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
2-methylpropene	−16.90	−18.58	1.68	89.12	87.94	1.18	293.59	295.29	−1.70	18
2-methyl-1-butene	−35.31	−37.20	1.89	111.63	108.57	3.06	339.53	339.25	0.28	9
2-methyl-1-pentene	−59.37	−57.83	−1.54	135.60	131.46	4.14	382.17	378.41	3.76	9
2-methyl-2-butene				105.02	111.03	−6.01	338.57	345.90	−7.33	9
2-methyl-2-pentene				126.61	131.66	−5.05	378.44	384.10	−5.66	9
2-ethyl-1-butene	−56.02	−55.82	−0.20	133.55	129.20	4.35	376.60	371.69	4.91	18
3-methyl-1-butene	−27.45	−28.03	0.58	118.62	119.07	−0.45	333.46	334.56	−1.10	9
3-methyl-1-pentene	−49.50	−48.66	−0.84	142.42	141.96	0.46	376.81	373.72	3.09	9
***cis*-3-methyl-2-pentene**	−62.30	−64.61	2.31	126.61	123.63	2.98	378.44	380.03	−1.59	27
***trans*-3-methyl-2-pentene**	−63.14	−69.46	6.32	126.61	131.66	−5.05	381.83	374.97	6.86	27
3-methyl-*cis*-3-hexene	−79.41	−85.49	6.08							
3-methyl-*trans*-3-hexene	−76.82	−90.34	13.52							
4-methyl-1-pentene				126.48	132.29	−5.81	367.73	369.54	−1.81	9
***cis*-4-methyl-2-pentene**	−57.49	−55.44	−2.05	133.55	134.13	−0.58	373.34	375.34	−2.00	27
***trans*-4-methyl-2-pentene**	−61.50	−60.29	−1.21	141.42	142.16	−0.74	368.28	370.28	−2.00	27
***cis*-2,2-dimethyl-3-hexene**	−89.29	−91.59	2.30							
***trans*-2.2-dimethyl-3-hexene**	−107.65	−108.83	1.18							
2,3-dimethyl-1-butene	−62.38	−64.73	2.35	143.47	141.16	2.31	365.64	368.86	−3.22	27
2,3-dimethyl-2-butene				123.60	133.12	−9.52	364.64	365.30	−0.66	162
2,4-dimethyl-1-pentene	−83.81	−85.15	1.34							
2,4-dimethyl-2-pentene	−88.70	−99.25	10.55							
3,3-dimethyl-1-butene	−60.67	−55.69	−4.98	126.48	126.47	0.01	343.76	343.76	0.00	81
***cis*-4,4-dimethyl-2-pentene**	−72.63	−70.71	−1.92							
***trans*-4,4-dimethyl-2-pentene**	−88.78	−87.95	−0.83							
2,3,3-trimethyl-1-butene	−85.48	−92.39	6.91							

TABLE 15. Substituted alkene hydrocarbons in the gas state at 298.15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
2,4,4-trimethyl-1-pentene	−110.37	−116.20	5.83							
2,4,4-trimethyl-2-pentene	−104.89	−126.91	22.02							
2-methyl-3-ethyl-1-pentene	−100.29	−101.47	1.18							
3-methyl-2-ethyl-1-butene	−79.54	−83.35	3.81							
2-methyl-1,3-butadiene	75.44	73.18	2.26	104.60	104.60	0.00	315.64	315.64	0.00	3
3-methyl-1,2-butadiene				105.44	103.80	1.64	319.66	321.57	−1.91	18

TABLE 16. Substituted alkene hydrocarbons in the liquid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
2-methylpropene		−34.31			124.55				
2-methyl-1-butene	−61.13	−60.04	1.09	157.19	153.84	3.35	253.97	254.63	−0.66
2-methyl-1-pentene	−89.96	−87.95	−2.01						
2-methyl-2-butene	−68.58	−76.98	8.40	152.80	157.26	−4.46	251.04	248.65	2.39
2-ethyl-1-butene	−87.11	−85.77	−1.34						
3-methyl-1-butene	−51.38	−51.80	0.42	156.06	156.05	0.01	253.30	253.30	0.00
3-methyl-1-pentene	−78.16	−77.53	−0.63						
***cis*-3-methyl-2-pentene**	−94.47	−95.26	0.79						
***trans*-3-methyl-2-pentene**	−94.56	−100.53	5.97						
***cis*-4-methyl-2-pentene**	−87.03	−84.84	−2.19						
***trans*-4-methyl-2-pentene**	−91.55	−90.11	−1.44						
3-methyl-*cis*-3-hexene	−115.94	−120.99	5.05						
3-methyl-*trans*-3-hexene	−112.72	−126.26	13.54						
***cis*-2,2-dimethyl-3-hexene**	−126.44	−128.97	2.53						
***trans*-2,2-dimethyl-3-hexene**	−144.93	−146.45	1.52						
2,3-dimethyl-1-butene	92.63	93.48	0.85						
2,3-dimethyl-2-butene	−101.46	−120.84	19.38	174.68	192.36	−17.68	270.20	273.54	−3.34
2,4-dimethyl-1-pentene	−116.98	−118.96	1.98						
2,4-dimethyl-2-pentene	−123.09	−133.97	10.88						
3,3-dimethyl-1-butene	−87.40	−82.41	−4.99	191.17	191.15	0.02	256.50	256.47	0.03
***cis*-4,4-dimethyl-2-pentene**	−105.31	−103.24	−2.07						
***trans*-4,4-dimethyl-2-pentene**	−121.71	−120.72	−0.99						
***cis*-2,5-dimethyl-3-hexene**	−151.04	−141.83	−9.21						
***trans*-2,5-dimethyl-3-hexene**	−159.24	−147.10	−12.14						
2,3,3-trimethyl-1-butene	−117.70	−124.09	6.39						
2,4,4-trimethyl-1-pentene	−146.15	−152.62	6.47	240.20	237.04	3.16	311.71	322.58	−10.87
2,4,4-trimethyl-2-pentene	−142.42	−164.58	22.16						
2-methyl-3-ethyl-1-pentene	−136.36	−140.58	4.22						
3-methyl-2-ethyl-1-butene	−114.06	−117.03	2.97						

TABLE 16. Substituted alkene hydrocarbons in the liquid state at 298.15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
2-methyl-1,3-butadiene	48.49	46.31	2.18	151.08	151.08	0.00	228.28	227.06	1.22
3-methyl-1,2-butadiene	101 17	96.01	5.16	152.42	154.59	−2.17	231.79	237.35	−5 56
2,3-dimethyl-1,3-butadiene	14.14	4.76	9.38						

TABLE 17. Substituted alkene hydrocarbons in the solid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
2-methylpropene		−38.08							
2-methyl-1-butene	−69.04	−64.77	−4.27						
2-methyl-2-butene	−76.44	−86.45	10.01						
3-methyl-1-butene	−56.74	−56.74	0.00						
2,3-dimethyl-2-butene	−111.13	−130.38	19.25						
3,3-dimethyl-1-butene	−92.84	−92.85	0.01						
2,4,4-trimethyl-1-pentene	−154.89	−158.83	3.94						
2,4,4-trimethyl-2-pentene	−149.16	−180.47	31.31						
2-methyl-1,3-butadiene	43.56	41.22	2.34						
3-methyl-1,2-butadiene	93.22	88.32	4.90						

TABLE 18. Alkyne hydrocarbons in the gas state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
acetylene	228.24	227.00	1.24	43.93	45 10	−1.17	200.83	198.16	2.67	2
propyne	184.93	186.34	−1.41	60.67	61.50	−0.83	248.11	246.47	1.64	3
1-butyne	165 23	166 64	−1.41	81.42	82.47	−1.05	290 83	289.27	1.56	3
1-pentyne		146.01		106.69	105.36	1.33	329.78	328.43	1 35	3
1-hexyne		125.38		128.24	128.25	−0.01	368.74	367.59	1 15	3
1-heptyne		104.75		151 08	151.14	−0.06	407 69	406 75	0 94	3
1-octyne		84.12		173.97	174.03	−0.06	446 64	445 91	0 73	3
1-nonyne		63.49		196.82	196.92	−0.10	485 60	485 07	0 53	3
1-decyne		42.86		219.70	219.81	−0.11	524 51	524 23	0 28	3
1-hexadecyne		−80.92		356.94	357.15	−0.21	758 22	759 19	−0 97	3
2-butyne	145.69	145.68	0.01	77.95	77.90	0 05	283 30	283 25	0 05	18
2-pentyne	128.87	125.98	2.89	98 70	98.87	−0 17	331 79	331 81	−0 02	9
3-methyl-1-butyne	136.40	136.40	0.00	104.68	104 68	0 00	318 95	318 96	−0 01	9
1-buten-3-yne				73 18	73 18	0 00	279 37	279 38	−0 01	2
***cis*-3-penten-1-yne**	253 55	262.11	−8.56							
***trans*-3-penten-1-yne**	254.89	257 26	−2.37							
***cis*-3-decen-1-yne**	151.67	158.71	−7 04							
***trans*-3-decen-1-yne**	154.60	153 86	0.74							
butadiyne				73 64	73 64	0 00	250 04	250.04	0.00	2
1,5-hexadiyne	416.06	416.06	0 00							

TABLE 19. Alkyne hydrocarbons in the liquid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
1-butyne	141.88	141.88	0.00	132.42	132.42	0.00	197.48	197.48	0.00
2-butyne	119.08	119.08	0.00	124.14	124.14	0.00	195.10	195.10	0.00
***cis*-3-penten-1-yne**	226.48	230.13	−3.65						
***trans*-3-penten-1-yne**	228.15	224.86	3.29						
1-octene-3-yne	140.71	144.65	−3.94						
***cis*-3-decen-1-yne**	99.20	101.48	−2.28						
***trans*-3-decen-1-yne**	100.46	96.21	4.25						
1,5-hexadiyne	384.17	384.16	0.01						
1,7-octadiyne	334.43	327.52	6.91						
3,9-dodecadiyne	197.82	193.40	4 42						
5,7-dodecadiyne	181.50	181.50	0.00						
3,3-dimethyl-1-butyne	78.45	78.45	0.00						
3,3-dimethylpenta-1,4-diyne	348.69	348.69	0.00						
3,3,6,6-tetramethyl-octa-1,7-diyne	211.08	209.44	1.64						

TABLE 20. Alkyne hydrocarbons in the solid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
1-butyne	135.85	135.85	0.00						
2-butyne	109.85	109.84	0.01						

TABLE 21. Aromatic hydrocarbons in the gas state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
benzene	82.89	82.86	0.03	81.67	81.66	0.01	269.20	269.20	0.00	12
toluene	50.17	50.43	−0.26	103.64	103.53	0.11	320.66	318.36	2.30	6
1,2-dimethylbenzene (o-xylene)	19.08	19.26	−0.18	133.26	131.80	1.46	352.75	350.13	2.62	18
1,3-dimethylbenzene (m-xylene)	17.32	17.37	−0.05	127.57	126.11	1.46	357.69	352.63	5.06	18
1,4-dimethylbenzene (p-xylene)	18.03	18.00	0.03	126.86	125.40	1.46	352.42	352.63	−0.21	18
1,2,3-trimethylbenzene	−9.46	−12.54	3.08	154.18	160.78	−6.60	384.84	381.89	2.95	54
1,2,4-trimethylbenzene	−13.85	−13.80	−0.05	154.01	154.38	−0.37	395.76	390.16	5.60	27
1,3,5-trimethylbenzene	−15.94	−16.32	0.38	150.25	149.40	0.85	385.30	377.76	7.54	162
1,2,3,4-tetramethyl benzene				189.58	189.76	−0.18	416.52	413.66	2.86	162
1,2,3,5-tetramethyl-benzene				185.73	183.36	2.37	422.54	416.16	6.38	162
1,2,4,5-tetramethyl-benzene				186.52	183.36	3.16	418.53	410.40	8.13	324
pentamethylbenzene				216.48	219.45	−2.97	443.88	445.47	−1.54	486
hexamethylbenzene	−86.82	−107.31	20.49	248.61	254.83	−6.22	452.37	459.79	−7.42	8,748
ethylbenzene	29.92	29.09	0.83	128.41	129.14	−0.73	360.45	360.95	−0.50	6
propylbenzene	7.91	8.46	−0.55	152.34	152.03	0.31	400.66	400.11	0.55	6

TABLE 21. Aromatic hydrocarbons in the gas state at 298 15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
butylbenzene	−13.05	−12.17	−0.88	175.10	174 92	0.18	439.49	439.27	0.22	6
pentylbenzene				197.99	197.81	0 18	478.94	478.43	0.51	6
hexylbenzene				220.87	220.70	0 17	517.90	517.59	0.31	6
heptylbenzene				243 72	243 59	0 13	556.85	556.75	0 10	6
octylbenzene				266 60	266 48	0.12	595 80	595 91	−0.11	6
nonylbenzene				289.45	289.37	0.08	634.75	635.07	−0 32	6
decylbenzene				312 34	312.26	0.08	673 71	674.23	−0 52	6
undecylbenzene				335.22	335.15	0.07	712.62	713.39	−0.77	6
dodecylbenzene				358.07	358 04	0.03	751 57	752.55	−0.98	6
1-methyl-2-ethylbenzene	1.30	−2.08	3.38							
1-methyl-3-ethylbenzene	−1.80	−3.97	2.17							
1-methyl-4-ethylbenzene	−3.18	−3.34	0.16	151 54	151.01	0 53	398.90	395.22	3.68	18
1,4-diethylbenzene				176 15	176.62	−0.47	434 01	437.81	−3.80	18
1,2,3-triethylbenzene				228.11	237 61	−9.50	507 23	509.66	−2.43	54
1,2,4-triethylbenzene				227.94	231.21	−3 27	518 15	517.93	0.22	27
1,3,5-triethylbenzene				224.18	226.23	−2 05	507.69	505.53	−2.16	162
pentaethylbenzene				339 70	347.50	−7.80	647 89	658 37	−10.48	486
hexaethylbenzene				396 48	408.49	−12.01	697.14	715.33	−18.19	8,748
isopropylbenzene	4.02	−0.87	4.89	151 71	151.71	0.00	388.57	388.55	0.02	18
sec-butylbenzene	−17 36	−19.24	1.88							
isobutylbenzene	−21.51	−18.86	−2.65							
t-butylbenzene	−22 59	−22.59	0.00							
styrene	147 82	147.82	0.00	122 09	122 09	0.00	345.10	345 20	−0.10	2
o-methylstyrene				145.18	150 36	−5.18	383.67	382.73	0.94	3
m-methylstyrene				145 18	144.67	0.51	389.53	385.23	4.30	3
p-methylstyrene				145.18	143 96	1.22	383.67	379.46	4 21	6
1-isopropenylbenzene (α-methylstyrene)	112.97	112.97	0.00	145 18	145.18	0.00	383.67	383.67	0.00	6
***cis*-1-propenylbenzene (*cis*-β-methylstyrene)**				145.18	137.15	8.03	383.67	385.97	−2 30	6
***trans*-1-propenylbenzene (*trans*-β-methylstyrene)**				146.02	145.18	0 84	380.33	380.91	−0.58	6
ethynylbenzene	327.65	327.48	0.17	114 89	114.89	0.00	321.67	321.67	0 00	2
1,1-diphenylethylene	245.64	245.64	0.00							
***cis*-stilbene**	252.34	247.85	4.49							
***trans*-stilbene**	236.14	243.00	−6.86							
diphenylmethane	138.95	138.95	0.00							
1,2-diphenylethane	142.93	142 70	0.23							
biphenyl	181.42	181.42	0.00	162.34	162 34	0.00	392.67	392 67	0 00	8
naphthalene	150.29	150.68	−0.39	132.55	132 54	0.01	335 64	335 63	0 01	4
1-methylnaphthalene	113.51	118 25	−4.74	159.54	159.53	0.01	377 44	377 75	−0 31	3
2-methylnaphthalene	110.54	118.25	−7.71	159.79	159 53	0.26	380 03	377 75	2 28	3
1-ethylnaphthalene				184.18	185.14	−0.96	418 15	420 34	−2 19	3
2-ethylnaphthalene				184 43	185.14	−0 71	420 74	420 34	0 40	3
1-propylnaphthalene				208 11	208 03	0 08	458 36	459 50	−1.14	3
2-propylnaphthalene				208.36	208 03	0 33	460 99	459 50	1 49	3
1-butylnaphthalene				230.87	230 92	−0 05	497 18	498 66	−1.48	3
2-butylnaphthalene				231.12	230 92	0 20	499 82	498 66	1.16	3
1-pentylnaphthalene				253 76	253 81	−0 05	536.64	537 82	−1.18	3
2-pentylnaphthalene				254 01	253 81	0.20	539 28	537 82	1.46	3
1,2-dimethylnaphthalene				184.85	185 58	−0.73	406 81	409.01	−2.20	9
1,3-dimethylnaphthalene				185.10	185.58	−0 48	409.45	409.01	0 44	9
1,4-dimethylnaphthalene				184 85	185 58	−0.73	401 08	403.25	−2.17	18

TABLE 21. Aromatic hydrocarbons in the gas state at 298.15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
1,5-dimethylnaphthalene				184.85	185.58	−0.73	401.08	409.01	−7.93	9
1,6-dimethylnaphthalene				185.10	185.58	−0.48	409.45	409.01	0.44	9
1,7-dimethylnaphthalene				185.10	185.58	−0.48	409.45	409.01	0.44	9
1,8-dimethylnaphthalene	108.66	85.82	22.84							
2,3-dimethylnaphthalene				185.81	185.58	0.23	410.95	403.25	7.70	18
2,6-dimethylnaphthalene				187.07	185.58	1.49	408.69	409.01	−0.32	9
2,7-dimethylnaphthalene				187.07	185.58	1.49	408.69	403.25	5.44	18
2-ethyl-3-methyl-naphthalene				210.46	211.19	−0.73	457.44	451.60	5.84	9
2-ethyl-6-methyl-naphthalene				211.71	211.19	0.52	455.18	451.60	3.58	9
2-ethyl-7-methyl-naphthalene				211.71	211.19	0.52	455.18	451.60	3.58	9
anthracene	230.91	218.50	12.41							
naphthacene	291.42	286.32	5.10							
phenanthrene	207.48	210.30	−2.82							
triphenylene	274.18	269.92	4.26							
chrysene	269.78	269.92	−0.14							
pyrene	225.68	225.68	0.00							
1,2-benzanthracene	294.14	278.12	16.02							

TABLE 22. Aromatic hydrocarbons in the liquid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
benzene	48.95	48.96	−0.01	136.06	136.08	−0.02	173.26	173.22	0.04
toluene	12.38	12.35	0.03	157.23	159.98	−2.75	220.96	208.15	12.81
1,2-dimethylbenzene (o-xylene)	−24.35	−21.00	−3.35	187.82	187.38	0.44	246.02	243.08	2.94
1,3-dimethylbenzene (m-xylene)	−25.36	−24.26	−1.10	183.18	183.88	−0.70	253.80	243.08	10.72
1,4-dimethylbenzene (p-xylene)	−24.35	−24.26	−0.09	183.76	183.88	−0.12	243.51	243.08	0.43
1,2,3-trimethylbenzene	−58.53	−54.35	−4.18	216.44	214.78	1.66	267.94	278.01	−10.07
1,2,4-trimethylbenzene	−61.80	−57.61	−4.19	214.97	211.28	3.69	283.38	278.01	5.37
1,3,5-trimethylbenzene	−63.43	−60.87	−2.56	209.53	207.78	1.75	273.55	278.01	−4.46
1,2,3,4-tetramethyl-benzene	−90.21	−87.70	−2.51	235.98	242.18	−6.20	290.79	312.94	−22.15
1,2,3,5-tetramethyl-benzene	−96.36	−90.96	−5.40	240.16	238.68	1.48	310.03	312.94	−2.91
1,2,4,5-tetramethyl-benzene	−98.99	−90.96	−8.03						
pentamethylbenzene	−122.97	−121.05	−1.92						
hexamethylbenzene	−139.14	−151.14	12.00						
ethylbenzene	−12.34	−12.46	0.12	185.81	182.88	2.93	255.01	255.55	−0.54
propylbenzene	−38.33	−38.19	−0.14	214.72	213.30	1.42	287.78	287.93	−0.15
butylbenzene	−63.18	−63.92	0.74	243.34	243.72	−0.38	321.21	320.31	0.90
1-methyl-2-ethylbenzene	−46.40	−45.81	−0.59						
1-methyl-3-ethylbenzene	−48.70	−49.07	0.37						
1-methyl-4-ethylbenzene	−49.79	−49.07	−0.72						
1-methyl-2-propylbenzene	−72.47	−71.54	−0.93						

TABLE 22. Aromatic hydrocarbons in the liquid state at 298.15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
1-methyl-3-propylbenzene	−76.23	−74.80	−1.43						
1-methyl-4-propylbenzene	−75.06	−74.80	−0.26						
1-methyl-2-isopropylbenzene	−73 30	−78.79	5.49						
1-methyl-3-isopropylbenzene	−78.62	−82.05	3.43						
1-methyl-4-isopropylbenzene	−78.03	−82.05	4.02	236.40	237.86	−1.46	306.69	312.48	−5.79
3-ethyl-1,2-dimethylbenzene	−80.50	−79.16	−1.34						
4-ethyl-1,2-dimethylbenzene	−86.02	−82.42	−3.60						
2-ethyl-1,3-dimethylbenzene	−80.12	−79.16	−0.96						
4-ethyl-1,3-dimethylbenzene	−84.10	−82.42	−1.68						
5-ethyl-1,3-dimethylbenzene	−87.78	−85.68	−2.10						
2-ethyl-1,4-dimethylbenzene	−84.81	−82.42	−2.39						
1,2-diethylbenzene	−68.49	−70.62	2.13						
1,3-diethylbenzene	−73.51	−73.88	0.37						
1,4-diethylbenzene	−72.84	−73.88	1.04						
isopropylbenzene	−41.13	−45.44	4.31	215.40	213.96	1.44	277.57	277.55	0.02
(1-methylpropyl)benzene	−66.40	−68.99	2.59						
(2-methylpropyl)benzene	−69.79	−69.20	−0.59						
t-butylbenzene	−70.71	−70.71	0.00	238.11	238.11	0.00	278.65	278.65	0.00
styrene	103.85	103.85	0.00	182.88	182.90	−0.02	237.57	234.80	2.77
isopropenylbenzene (α-methylstyrene)	70.46	70.46	0.00						
2-propenylbenzene (allylbenzene)	88.03	88.03	0.00						
1-methyl-2-propenylbenzene	56.07	56.07	0.00						
ethynylbenzene	283.47	283.39	0.08						
diphenylmethane	89.66	93.42	−3.76	279.91	279.91	0.00	301.67	301.67	0.00
4-methyldiphenylmethane	61.55	56.81	4.74						
2,5-dimethyldiphenylmethane	24.69	23 46	1.23						
1,1-diphenylethane	48.66	48.66	0.00	294.97	294.98	−0.01			
1,1-diphenyldodecane	593.71	599.18	−5.47	684.92	684.92	0.00			
***cis*-stilbene**	183.30	169.47	13.83						
1,1-diphenylethylene	172.42	172.42	0.00	299.16	299.15	0.01			
biphenyl	116.02	116.02	0.00						
2-methylbiphenyl	108.16	82.67	25.49						
3-methylbiphenyl	85.56	79.41	6.15						
isopropylbiphenyl				338.49	342.32	−3.83			
naphthalene	96.94	96.94	0.00						
1-methylnaphthalene	56.19	60.33	−4.14	224.39	224.3	80.01	254.81	254.81	0.00
2-methylnaphthalene	62.58	60.33	2.25						
1,8-dimethylnaphthalene	41.76	23.72	18.04						
anthracene	158.57	144.92	13.65						
phenanthrene	132.87	136.26	−3.39						
triphenylene	176.52	175.58	0.94						
pyrene	143.13	143.12	0.01						

TABLE 23. Aromatic hydrocarbons in the solid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
benzene	39.08	39.18	−0.10	120.79	120.78	0.01	136.48	136.50	−0.02
toluene	5.73	−0.19	5.92						
1,2-dimethylbenzene (o-xylene)	−37.95	−34.56	−3.39						
1,3-dimethylbenzene (m-xylene)	−36.90	−37.56	0.66						
1,4-dimethylbenzene (p-xylene)	−41.46	−39.56	−1.90						
1,2,3-trimethylbenzene	−68.70	−66.93	−1.77						
1,2,4-trimethylbenzene	−74.98	−71.93	−3.05						
1,3,5-trimethylbenzene	−72.93	−72.93	0.00						
1,2,3,4-tetramethyl benzene	−101.42	−99.30	−2.12						
1,2,3,5-tetramethyl-benzene	−109.29	−104.30	−4.99						
1,2,4,5-tetramethyl-benzene	−119.87	−104.30	−15.57	220.08	217.02	3.06	245.60	250.26	−4.66
pentamethylbenzene	−133.64	−129.67	−3.97	270.29	241.08	29.21	294.14	278.70	15.44
hexamethylbenzene	−161.54	−157.04	−4.50	245.64	265.14	−19.50	306.31	307.14	−0.83
ethylbenzene	−21.51	−22.29	0.78						
propylbenzene	−56.11	−51.70	−4.41						
butylbenzene	−74.39	−81.11	6.72						
1-methyl-4-isopropylbenzene	−87.70	−94.48	6.78						
isopropylbenzene	−48.45	−55.11	6.66						
t-butylbenzene	−79.12	−79.12	0.00						
styrene	92.88	92.88	0.00						
diphenylmethane	71.46	71.66	−0.20	223.84	223.84	0.00	239.32	239.35	−0.03
***trans*-stilbene**	136.94	140.90	−3.96	232.63	232.60	0.03	251.04	251.00	0.04
1,2-diphenylethane	51.55	48.90	2.65	253.55	253.54	0.01	270.29	270.30	−0.01
triphenylmethane				295.81	295.81	0.00	312.13	312.13	0.00
tetraphenylmethane				368.19	368.30	−0.11			
1,1,2-triphenylethane				319.66	325.10	−5.44			
1,1,1-triphenylethane				316.73	339.45	−22.72			
1,1,1,2-tetraphenylethane				395.39	398.77	−3.38			
1,1,2,2-tetraphenylethane				396.64	396.66	−0.02			
pentaphenylethane				473.63	470.33	3.30			
triphenylethylene				309.20	310.10	−0.90			
diphenylacetylene	312.40	312.00	0.40	225.90	225.90	0.00			
biphenyl	99.37	99.36	0.01	197.90	197.86	0.04	205.85	215.50	−9.65
4-methylbiphenyl	55.44	59.99	−4.55						
4,4'-dimethylbiphenyl	14.14	20.62	−6.48						
o-terphenyl				274.34	274.94	−0.60	298.82	294.50	4.32
1,3,5-triphenylbenzene				358.32	352.02	6.30	367.36	373.50	−6.14
naphthalene	77.90	80.44	−2.54	165.69	165.64	0.05	167.40	170.00	−2.60
1-methylnaphthalene	44.27	41.07	3.20						
2-methylnaphthalene	44.85	41.07	3.78	195.98	189.70	6.28	219.99	198.44	21.55
1,8-dimethylnaphthalene	25.94	1.70	24.24	242.80	213.76	29.04	224.72	226.88	−2.16
2,3-dimethylnaphthalene	−0.23	1.70	−1.93						
2,6-dimethylnaphthalene	−5.69	1.70	−7.39	203.55	213.76	−10.21	227.86	226.88	0.98
tetraphenylethylene	311.50	311.48	0.02	387.60	387.60	0.00			
2,7-dimethylnaphthalene	−5.40	1.70	7.10	204.39	213.76	−9.37	228.57	226.88	1.69
anthracene	129.20	121.70	7.50	210.50	210.50	0.00	207.15	203.50	3.65
naphthacene	158.78	162.96	−4.18	236.56	255.36	−18.80	215.39	237.00	−21.61
phenanthrene	116.20	117.50	−1.30	220.62	217.44	3.18	215.06	219.50	−4.44

TABLE 23. Aromatic hydrocarbons in the solid state at 298.15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
triphenylene	151.80	154.56	−2 76	259.20	269.24	−10.04	254.68	269.00	−14.32
fluoranthene	230 25	234.68	−4.43	230.58	236.50	−5.92			
pyrene	125.48	125.58	−0.10	227.65	226.50	1.15	224.89	217.50	7.39
perylene				274.93	285.24	−10.31	264.55	283.00	−18.45
coronene				313.76	303.36	10.40	280.87	279.00	1.87

TABLE 24. Cycloalkane and related hydrocarbons in the gas state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
cyclopropane	53.26	53.26	0.00	55.94	55.94	0.00	237.44	237.44	0.00	6
cyclobutane	28.37	28.37	0.00	72.22	72.22	0.00	265.39	265.39	0.00	8
cyclopentane	−76.40	−76.40	0.00	83.01	83.01	0.00	292.88	292.88	0.00	10
cyclohexane	−123.39	−123.39	0.00	106.27	106.27	0.00	298.24	298.24	0.00	6
cycloheptane	−118.07	−118.07	0.00	123.09	123.09	0.00	342.33	342.33	0.00	2
cyclooctane	−124.39	−124.39	0.00	139.95	139.95	0.00	366.77	366.77	0.00	8
cyclononane	−132.76	−132.76	0.00							
cyclodecane	−162.67	−162.67	0.00							
cycloundecane	−179.37	−179.37	0.00							
cyclododecane	−230.25	−230.25	0.00							
cyclotridecane	−246.35	−246.35	0.00							
cyclotetradecane	−239.24	−239.24	0.00							
cyclopentadecane	−301.42	−301.42	0.00							
cyclohexadecane	−321.67	−321.67	0.00							
cycloheptadecane	−364.30	−364.30	0.00							
cyclopropene	277.06	277.06	0.00							
cyclobutene	156.69	156.69	0.00	67.07	67.07	0.00	263.51	263 51	0.00	2
cyclopentene	34.56	34.56	0.00	75.10	75.10	0.00	289.66	289.66	0.00	2
cyclohexene	−5.02	−5.02	0.00	105.02	105.02	0.00	310.75	310.75	0.00	2
cycloheptene	−9.20	−9.20	0.00							
cyclooctene	−26.99	−26.99	0.00							
1,3-cyclopentadiene	134.35	134.35	0.00							
1,3-cyclohexadiene	106.23	106.23	0.00							
1,3-cycloheptadiene	94.35	94.35	0.00							
1,5-cyclooctadiene	71.34	71.34	0.00							
1,3,5-cyclo-heptatriene	180.87	180.87	0.00	117.78	117.78	0 00	315.64	315.64	0.00	2
cyclooctatetraene	295.85	295.85	0.00	122.01	122.01	0 00	326.77	326.77	0.00	4
spiropentane	185.18	185.18	0.00	88.12	88 12	0 00	282 21	282.21	0.00	4
methylenecyclobutane	121.55	119.46	2.09							
ethylcyclobutane	−26.32	−15.06	11.26							
methylcyclopentane	−106.20	−101.46	−4.74	109 79	109 50	0 29	339.91	339.62	0.29	3
methylenecyclopentane	12.01	14.19	−2.18							
1,1-dimethyl-cyclopentane	−138.24	−130.21	−8.03	133 30	131.68	1.62	359 28	356.15	3.13	18
***trans*-1,2-dimethyl-cyclopentane**	−136.65	−126.52	−10 13	134.47	132.42	2.05	366.81	359.28	7.53	18
***trans*-1,3-dimethyl-cyclopentane**	−133.55	−126.52	−7.03	134.47	132.42	2.05	366.81	359.28	7.53	18

TABLE 24. Cycloalkane and related hydrocarbons in the gas state at 298.15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)			N(tot)
	expt	calc	resd	expt	calc	resd	expt	calc	resd	
ethylcyclopentane	−126.94	−119.83	−7.11	131.75	132.39	−0.64	378.32	378.78	−0.46	3
propylcyclopentane	−147.74	−140.46	−7.28	154.64	155.28	−0.64	417.27	417.94	−0.67	3
butylcyclopentane				177.49	178.17	−0.68	456.22	457.10	−0.88	3
pentylcyclopentane				200.37	201.06	−0.69	495.18	496.26	−1.08	3
hexylcyclopentane				223.22	223.95	−0.73	534.13	535.42	−1.29	3
heptylcyclopentane				246.10	246.84	−0.74	573.04	574.58	−1.54	3
octylcyclopentane				268.99	269.73	−0.74	611.99	613.74	−1.75	3
nonylcyclopentane				291.83	292.62	−0.79	650.95	652.90	−1.95	3
decylcyclopentane	−301.42	−284.87	−16.55	314.72	315.51	−0.79	689.90	692.06	−2.16	3
1-methylcyclopentene	−3.81	0.12	−3.93	100.83	99.22	1.61	326.35	333.07	−6.72	3
3-methylcyclopentene	7.36	9.29	−1.93	100.00	109.72	−9.72	330.54	328.38	2.16	3
4-methylcyclopentene	14.64	9.50	5.14	100.00	100.05	−0.05	328.86	324.20	4.66	3
1-ethylcyclopentene	−19.75	−20.76	1.01							
methylcyclohexane	154.72	−148.47	−6.27	135.02	137.44	−2.42	343.34	344.36	−1.02	3
methylenecyclohexane	−25.23	−32.80	7.57							
1,1-dimethylcyclohexane	−180.87	−177.20	−3.67	154.39	159.62	−5.23	365.01	366.65	−1.64	9
***trans*-1,2-dimethyl-cyclohexane**	−179.87	−173.51	−6.36	158.99	160.36	−1.37	370.91	369.78	1.13	9
***trans*-1,3-dimethyl-cyclohexane**	−176.48	−173.51	−2.97	157.32	160.36	−3.04	376.23	369.78	6.45	9
***trans*-1,4-dimethyl-cyclohexane**	−184.51	−173.51	−11.00	157.74	160.36	−2.62				
ethylcyclohexane	−171.88	−166.82	−5.06	158.82	160.33	−1.51	382.58	383.52	−0.94	3
propylcyclohexane				184.22	183.22	1.00	419.53	422.68	−3.15	3
butylcyclohexane	−213.30	−208.08	−5.22	207.11	206.11	1.00	458.48	461.84	−3.36	3
pentylcyclohexane				229.95	229.00	0.95	497.44	501.00	−3.56	3
dodecylcyclohexane	−378.70	−373.12	−5.58							
1-methylcyclohexene	−43.26	−41.72	−1.54							
1-ethylcyclohexene	−63.43	−60.34	−3.09							
bicyclo[2.2.2]octane	−99.00	−99.00	0.00							
adamantane	−134.60	−134.60	0.00							
bicyclo[3.3.3]undecane	−88.95	−88.95	0.00							

TABLE 25. Cycloalkane and related hydrocarbons in the liquid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
cyclobutane	3.72	3.72	0.00	111.00[a]	111.00	0.00	181.00[a]	181.00	0.00
cyclopentane	−105.06	−105.06	0.00	128.78	128.78	0.00	204.14	204.14	0.00
cyclohexane	−156.44	−156.44	0.00	156.31	156.31	0.00	204.35	204.35	0.00
cycloheptane	−156.61	−156.61	0.00	180.75	180.75	0.00	242.55	242.55	0.00
cyclooctane	−167.74	−167.74	0.00	215.48	215.48	0.00	262.00	262.00	0.00
cyclononane	−181.17	−181.17	0.00						
cyclodecane	−206.69	−206.69	0.00						
cycloundecane	−235.48	−235.48	0.00						
cyclododecane	−306.65	−306.65	0.00						
cyclotridecane	−309.66	−309.66	0.00						
cyclopentene	4.73	4.73	0.00	122.38	122.38	0.00	201.25	201.25	0.00
cyclohexene	−38.49	−38.49	0.00	148.36	148.36	0.00	214.60	214.60	0.00
cyclooctene	−74.02	−74.02	0.00						
1,3-cyclopentadiene	105.98	105.98	0.00						
1,3-cyclohexadiene	73.18	73.18	0.00	144.56	144.56	0.00	197.28	197.28	0.00

TABLE 25. Cycloalkane and related hydrocarbons in the liquid state at 298.15 K — Continued

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
1,4-cyclohexadiene				145.94	145.94	0.00	189.37	189.37	0.00
1,5-cyclooctadiene	30.29	30.29	0.00	208.11	208.11	0.00	264.35	264.35	0.00
1,3,5-cyclo-heptatriene	142.17	142.17	0.00	162.76	162.76	0.00	214.64	214 64	0.00
cyclooctatetraene	254.51	254.51	0.00	185.18	185.18	0.00	220.29	220.29	0.00
spiropentane	157.65	157.65	0.00	134.52	134 52	0.00	193 68	193 68	0.00
methylenecyclobutane	93.85	90.36	3.49	131.13	132.17	−1.04	210.20	204 98	5 22
methylcyclobutane	−44.48	−25.11	−19.37						
ethylcyclobutane	−58.95	−48.66	−10.29						
methylcyclopentane				158.70	155.25	3.45	247.78	245.58	2.20
methylenecyclopentane	−20.08	−18.42	−1 66						
1,1-dimethyl-cyclopentane	−172.05	−165.34	−6.71	187.36	180.59	6.77	265.01	254.12	10 89
***trans*-1,2-dimethyl-cyclopentane**	−171.21	−162.72	−8.49	187.40	183.66	3.74	269.90	272 61	−2 71
***trans*-1,3-dimethyl-cyclopentane**	−168.07	−162.72	−5.35						
ethylcyclopentane	−163.43	−157.44	−5 99	185.31	186.64	−1.33	279.91	277 96	1 95
ethylidenecyclopentane				181 17	182.66	−1.49			
ethenylcyclopentane	−34.81	−31.55	−3.26						
allylcyclopentane				202.92	202.00	.92			
propylcyclopentane	−188.82	−183.17	−5.65	216.27	217.06	−0.79	310.83	310.34	0.49
butylcyclopentane				245.35	247.48	−2.13	343 84	342.72	1 12
decylcyclopentane	−367.31	−363.28	−4.03						
11-cyclopentyl-heneicosane	−648.60	−647.23	−1.37						
bicyclopentyl				238.91	239.48	−0.57			
1-methylcyclopentene	−36.44	−34.77	−1.67	153.10	157.48	−4 38			
3-methylcyclopentene	−17.57	−24.35	6.78						
1-ethylcyclopentene	−58.28	−60.50	2.22	188.28	186.77	1.51			
methylcyclohexane	−190.08	−185.27	−4.81	184.51	183.75	0.76	247 90	246 41	1 49
methylenecyclohexane	−61.30	−69 80	8.50	177.40	175.22	2.18			
1,1-dimethylcyclohexane	−218.74	−216.72	−2.02	209.24	209.09	0.15	267.23	254 95	12.28
1,2-dimethylcyclohexane	−218.24	−214.10	−4.14	212.76	211.19	1.57	273 22	273 44	−0 22
1,3-dimethylcyclohexane	−215.69	−214.10	−1.59	212.84	211.19	1.65	276 27	273 44	2 83
1,4-dimethylcyclohexane	−222.38	−214 10	−8.28	210.25	211.19	−0.94	268 03	273 44	−5 41
ethylcyclohexane	−212.13	−208.82	−3.31	211.79	214.17	−2.38	280 91	278 79	2 12
allylcyclohexane				233 47	229.53	3.94			
ethylidenecyclohexane				203.76	207.93	−4 17			
propylcyclohexane				242.04	244.59	−2.55	311 88	311 17	0 71
butylcyclohexane	−263.09	−260.28	−2.81	271.04	275.01	−3 97	344 97	343 55	1 42
dodecylcyclohexane	−467.56	−466.12	−1.44						
3-cyclohexyleicosane	−666.18	−672.88	6.70						
9-cyclohexyleicosane	−674.13	−672.88	−1.25						
11-cyclohexyl-heneicosane	−689.44	−698.61	9.17						
13-cyclohexyl-pentacosane	−792.66	−801.53	8 87						
1-methylcyclohexene	−81 17	−80.17	−1 00						
1-ethylcyclohexene	−106 69	−103.72	−2 97						
***cis*-hexahydroindan**	−173.10	−173.10	0.00	214 18	214 18	0 00	265.47	265 47	0.00
***trans*-hexahydroindan**	−173.20	−173.20	0.00	209 70	209.70	0 00	258 86	258.86	0 00
***cis*-decalin**	−219.40	−219.40	0.00	232.00	232.00	0.00	265.01	265.01	0 00
***trans*-decalin**	−230.60	−230.60	0.00	228.49	228.49	0.00	264.93	264.93	0.00

[a]Obtained from extrapolation of experimental data of 53RAT/GWI to 298.15 K.

TABLE 26. Cycloalkane and related hydrocarbons in the solid state at 298.15 K

Name	$\Delta_f H°$(kJ/mol)			$C_p°$(J/mol·K)			$S°$(J/mol·K)		
	expt	calc	resd	expt	calc	resd	expt	calc	resd
cyclopentane	−113.05	−113.05	0.00						
cyclohexane	−166.16	−166.16	0.00						
cyclododecane	−306.65	−306.65	0.00						
cyclotetradecane	−374.00	−374.00	0.00						
cyclopentadecane	−376.06	−376.06	0.00						
cyclohexadecane	−403.42	−403.42	0.00						
cycloheptadecane	−430.41	−430.41	0.00						
decylcyclopentane	−401.00	−401.05	−0.05						
dodecylcyclohexane	−514.00	−512.98	−1.02						
2,2-metacyclophane	78.50	78.50	0.00						
2,2-metaparacyclophane	130.90	130.90	0.00	261.50	261.50	0.00			
2,2-paracyclophane	145.10	145.10	0.00	252.34	252.34	0.00	265.68	265.68	0.00
3,3-paracyclophane	26.30	26.30	0.00	324.26	324.26	0.00			
bicyclo[2.2.2]octane	−146.90	−146.90	0.00						
adamantane	194.10	−194.10	0.00						