# Standard Chemical Thermodynamic Properties of Alkane Isomer Groups

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The chemical thermodynamic properties of alkane isomer groups from $C_4H_{10}$ to $C_{10}H_{22}$ have been calculated from 200 to 1500 K from Scott's tables of 1974. The numbers of stereoisomers in each isomer group have been checked and all of them have been included in the calculations. The following properties for alkane isomer groups have been calculated with energy in joules for a standard state pressure of 1 bar: standard heat capacity at constant pressure, standard entropy, standard enthalpy of formation, standard Gibbs energy of formation, standard enthalpy relative to isomer group at 298.15 K, and standard enthalpy relative to the elements at 298.15 K. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 200 to 1500 K. The four basic properties are given for all the individual isomers in joules for a standard state pressure of 1 bar. The properties of individual alkanes from $C_4H_{10}$ to $C_{10}H_{22}$ have also been calculated using the Benson group method and the resulting isomer group properties and equilibrium mole fractions have been calculated.

Key words: alkanes; Benson method; enthalpy of formation; entropy; Gibbs energy of formation; heat capacity; isomer group thermodynamic properties; isomer mole fractions; thermodynamic properties.

## Contents

1. Introduction ..... 1174
2. Standard Thermodynamic Properties of Isomer Groups ..... 1174
   2.1. Theory ..... 1174
   2.2. Stereoisomers ..... 1175
3. Input of Data and Calculations ..... 1176
4. Tables of Standard Thermodynamic Properties of Alkane Isomer Groups ..... 1176
5. Equilibrium Mole Fractions Within Alkane Isomer Groups ..... 1180
6. Estimation of Thermodynamic Properties of Alkane Isomer Groups Using the Benson Group Method ..... 1183
7. Discussion ..... 1188
8. Nomenclature ..... 1188
9. Acknowledgments ..... 1188
10. References ..... 1188

Appendix: Standard Thermodynamic Properties of Individual Alkane Species ..... 1189

### List of Tables

1. Numbers of $N_I$ of isomers in isomer groups .... 1174
2. Numbers of structural formulas, chiral centers, isomers, and lines in tables for alkanes ..... 1176
3. Standard heat capacity at constant pressure for alkane isomer groups in J/K mol ..... 1177
4. Standard entropy for alkane isomer groups in J/K mol ..... 1177
5. Standard enthalpy of formation for alkane isomer groups in kJ/mol ..... 1178
6. Standard Gibbs energy of formation for alkane isomer groups in kJ/mol ..... 1178
7. Standard enthalpy for alkane isomer groups relative to isomer groups at 298.15 K in kJ/mol .. 1179
8. Standard enthalpy for alkane isomer groups relative to the elements at 298.15 K in kJ/mol ..... 1179
9. Equilibrium mole fractions of alkanes within isomer groups ..... 1181
10. Standard heat capacity at constant pressure for alkane isomer groups in J/K mol calculated using Benson group values ..... 1184
11. Standard entropy of alkane isomer groups in J/K mol calculated using Benson group values ... 1184
12. Standard enthalpy of formation of alkane isomer groups in kJ/mol calculated using Benson group values ..... 1185
13. Standard Gibbs energy of formation for alkane isomer groups in kJ/mol calculated using Benson group values ..... 1185
14. Equilibrium mole fractions of alkanes within isomer groups calculated using Benson group values ..... 1186
A1. Standard heat capacity at constant pressure of alkanes in J/K mol ..... 1190
A2. Standard entropy of alkanes in J/K mol ..... 1192
A3. Standard enthalpy of formation of alkanes in kJ/mol ..... 1194
A4. Standard Gibbs energy of formation of alkanes in kJ/mol ..... 1196

## 1. Introduction

When equilibrium calculations are made on organic systems with $C_4$ and larger molecules, the number of isomeric species which have to be included increases very rapidly with the carbon number. The seriousness of this problem is illustrated by Table 1 which shows the numbers of isomers, including stereoisomers, of the alkanes and alkenes, calculated by Read[1] and Nourse.[2] These numbers are so large for the higher hydrocarbons that it becomes impractical to put even all the known data in a calculation, and, of course, we cannot expect that the thermodynamic properties of so many species can be determined in the laboratory, or even be calculated by statistical mechanics. When the standard Gibbs energies of formation are known for all the isomers in a group, B. D. Smith[3] shows that equilibrium calculations for ideal gases can be carried out in two steps: (1) The isomers in a group are treated as a single species and the equilibrium mole fractions of the isomer groups are calculated. (2) The equilibrium mole fraction in an isomer group is distributed between the various individual species in the group. This is possible because the distribution of isomers within a group depends only on the temperature. The first step of this calculation reduces the number of components by the number of independent equilibrium relations between isomers in the group; the isomer group becomes $N_I - (N_I - 1) = 1$ species, where $N_I$ is the number of isomers in the group. This has been done by a number of people[4–9] by using the standard Gibbs energy of formation $\Delta_f G°(I)$ of an isomer group. More recently it has been shown[10] how the corresponding values of $C_P°(I)$, $S°(I)$, and $\Delta_f H°(I)$ can be calculated for the isomer groups (see Sec. 2.1). Tables of these properties for the alkene isomer groups $C_4H_8$, $C_5H_{10}$, and $C_6H_{12}$ have been calculated, and extrapolation formulas for higher carbon numbers, for which data are not available, have been developed.[11]

The existing data on the alkanes is complete through $C_{10}H_{22}$, which has 136 isomers, and on the alkenes through $C_6H_{12}$, which has 18 isomers. Therefore, tables of standard chemical thermodynamic properties of these isomer groups can be prepared. Since the processing of petroleum and the production of synthetic fuels involves alkanes and alkenes of far higher carbon numbers than these, there is also the need to estimate chemical thermodynamic properties of these higher isomer groups. A good deal of work is involved in fully taking advantage of this method, and so this research has been undertaken to make the standard chemical thermodynamic properties of alkane isomer groups readily available. These calculations also indicate the feasibility of extrapolating these isomer group properties to higher carbon numbers.

In 1940 Pitzer[12] correlated existing thermodynamic data on the alkanes and extended them by statistical mechanics. Further work was done by Rossini, Pitzer, Arnett, Braun, and Pimentel[13] who published tables in 1953. Some further small changes were made by Stull, Westrum, and Sinke[14] in publishing their book in 1969. Scott's correlation of 1974[15] incorporates more recent experimental data and considerable theoretical work.[16] Some further changes in Scott's values were made in tables from the Thermodynamics Research Center at Texas A&M.[17] The isomer group properties given in the current paper have been calculated from Scott's tables, with certain corrections which are discussed later.

TABLE 1. Numbers $N_I$ of isomers in isomer groups

| $N_C$ | Alkanes | Alkenes |
|---|---|---|
| 1 | 1 | |
| 2 | 1 | 1 |
| 3 | 1 | 1 |
| 4 | 2 | 4 |
| 5 | 3 | 6 |
| 6 | 5 | 18 |
| 7 | 11 | 42 |
| 8 | 24 | 118 |
| 9 | 55 | 314 |
| 10 | 136 | 895 |
| 11 | 345 | 2 521 |
| 12 | 900 | 7 307 |
| 13 | 2 412 | 21 238 |
| 14 | 6 563 | 62 566 |
| 15 | 18 127 | 185 310 |
| 16 | 50 699 | 553 288 |
| 17 | 143 255 | 1 660 490 |
| 18 | 408 429 | 5 011 299 |
| 19 | 1 173 770 | 15 190 665 |
| 20 | 3 396 844 | 46 244 031 |

## 2. Standard Thermodynamic Properties of Isomer Groups

### 2.1. Theory

When isomers are in equilibrium, it has been known for some time[3–9] that they can be aggregated in calculations of equilibrium mole fractions by use of the standard Gibbs energy of formation $\Delta_f G°(I)$ of the isomer group defined by

$$\Delta_f G°(I) = -RT \ln \left[ \sum_{i=1}^{N_I} \exp(-\Delta_f G_i°/RT) \right], \qquad (1)$$

where $\Delta_f G_i°$ is the standard Gibbs energy of formation of an individual isomer and $N_I$ is the number of isomers in the group, including stereoisomers. The equilibrium mole fractions $r_i$ of various isomers in a group can be calculated using

$$r_i = \frac{y_i}{y_I} = \exp\{[\Delta_f G°(I) - \Delta_f G_i°]/RT\}, \qquad (2)$$

where $y_I$ is the sum of the mole fractions of the individual isomers. These equations can be rearranged to show more clearly the nature of the standard Gibbs energy of formation of an isomer group.

$$\Delta_f G°(I) = \sum_{i=1}^{N_I} r_i \Delta_f G_i° + RT \sum_{i=1}^{N_I} r_i \ln r_i. \qquad (3)$$

The standard Gibbs energy of formation for an isomer group is equal to the weighted average standard Gibbs energy of formation for the isomers in the group plus the Gibbs energy of mixing of the isomer group, assuming ideal gases. Since the Gibbs energy of mixing is necessarily negative, $\Delta_f G°(I)$ is more negative, or less positive, than the weighted average

standard Gibbs energy of formation given by the first term. As can be seen from Eq. (1), $\Delta_f G°(I)$ is more negative than the most negative Gibbs energy of formation in the isomer group. When standard Gibbs energies of formation of isomer groups are used to calculate equilibrium constants for reactions of ideal gases the equilibrium expression is written in terms of equilibrium mole fractions of isomer groups.[10]

Equation (1) provides the key for the calculation of the other thermodynamic properties of an isomer group because the other properties are obtained[10] by the usual differentiations which yield

$$\Delta_f H°(I) = \sum_{i=1}^{N_I} r_i \Delta_f H°_i, \tag{4}$$

$$S°(I) = \sum_{i=1}^{N_I} r_i S°_i + \Delta S°_{mix}, \tag{5}$$

$$C°_p(I) = \sum_{i=1}^{N_I} r_i C°_{Pi} + C°_{P\,LeC}. \tag{6}$$

The entropy of mixing the isomer group is given by

$$\Delta S°_{mix} = -R \sum_{i=1}^{N_I} r_i \ln r_i, \tag{7}$$

and the contribution of the Le Chatelier term to the standard heat capacity at constant pressure is given by

$$C°_{P\,LeC} = \frac{1}{RT^2}\left\{\sum_{i=1}^{N_I} r_i(\Delta_f H°_i)^2 - [\Delta_f H°(I)]^2\right\} = \frac{1}{R}\left(\frac{\sigma_H}{T}\right)^2. \tag{8}$$

This contribution is proportional to the square of the standard deviation $\sigma_H$ of the enthalpy of formation distribution and is, therefore, necessarily positive. If all the isomers had the same enthalpy of formation this contribution would disappear.

For the alkanes, the standard chemical thermodynamic properties for an isomer group are interrelated by

$$\Delta_f G°(I) = \Delta_f H°(I) - T\,[S°(I) - nS°_{graphite} - (n+1)S°_{H_2(g)}], \tag{9}$$

where $n$ is the number of carbon atoms.

### 2.2. Stereoisomers

To calculate the chemical thermodynamic properties for an isomer group, a term must be included for each molecular species, including stereoisomers. In the alkane series, stereoisomerism does not arise until $C_7H_{16}$. As pointed out by Scott,[14] correlations "can provide values of properties for the many compounds that have not been studied experimentally, even ones that have never been synthesized or isolated in the laboratory." In tabulating thermodynamic properties, Scott chose to give the properties for racemic mixtures of enantiomeric molecules by adding $R \ln 2$ to the calculated standard entropy and $-RT \ln 2$ to the standard Gibbs energy of one of the forms at each temperature. This practice has the advantage of avoiding the publication of identical lines for chiral molecules in thermodynamic tables, and so it has been followed here. It can be justified as follows: The Gibbs energy of formation $\Delta_f G°(RS)$ of a racemic mixture is given by

$$\Delta_f G°(RS) = \tfrac{1}{2}\Delta_f G°(R) + \tfrac{1}{2}\Delta_f G°(S) + RT(\tfrac{1}{2}\ln\tfrac{1}{2} + \tfrac{1}{2}\ln\tfrac{1}{2}). \tag{10}$$

Since

$$\Delta_f G°(R) = \Delta_f G°(S),$$

$$\Delta_f G°(RS) = \Delta_f G°(R) - RT \ln 2,$$

so that

$$e^{-\Delta_f G°(RS)/RT} = e^{-\Delta_f G°(R)/RT} e^{\ln 2} = e^{-\Delta_f G°(R)/RT} + e^{-\Delta_f G°(S)/RT}. \tag{11}$$

The mole fraction of the RS pair in the isomer group is twice that of either the R or the S form so that appropriate values of $C°_p(I)$, $S°(I)$, and $\Delta_f H°(I)$ are also obtained using the thermodynamic properties of the racemic mixture.

Compounds are named in tables according to the IUPAC Revised and Collected Recommendations for the Nomenclature of Organic Chemistry, 1978.[18] For example, the two forms of 3-methylhexane are represented by 3R and 3S, and the racemic mixture is represented by 3RS-methylhexane. When there are two identical chiral centers, the *meso*-compound has to be shown on a separate line because it has different thermodynamic properties from the other two forms. For example, the chiral forms of 3,4-dimethylhexane are represented by 3R,4R-dimethylhexane and 3S,4S-dimethylhexane, the racemic mixture is represented by 3RS,4RS-dimethylhexane, and the *meso*-compound is represented by 3R,4S-dimethylhexane. When there are two different chiral centers, there are two different chiral pairs. For example, for 3,4-dimethylheptane there are two racemic mixtures, 3RS,4RS-dimethylheptane and 3RS,4SR-dimethylheptane. The molecule 3,4,5-trimethylheptane has a pseudoasymmetric atom and requires the use of the lower case symbols r and s. The publication on Nomenclature of Organic Chemistry[18] defines a pseudoasymmetric atom as one bonded tetrahedrally to one pair of enantiometric groups (+) – a and (–) – a and also to two atoms or achiral groups b and c that are different from each other. For substances with two chiral centers, Scott also provided tables for equilibrium mixtures of the stereoisomers, but we have not used these tables.

Recently, Nourse[2] has programed a computer to print out the structural formulas of the alkanes and identify the numbers of stereoisomers for each structural formula. The numbers of asymmetric centers and isomers of the alkanes are shown in Table 2. The total number of isomers is equal to the number of structural formulas, plus the number of structures with one chiral center, plus two times the number of structures with two identical chiral centers, plus three times the number of structures with two different chiral centers. The use of Nourse's calculations revealed two errors in Scott's table.

Scott did not identify 3-ethyl-2-methylhexane as having a chiral center, and so $R \ln 2$ has been added to each standard entropy and $-RT \ln 2$ to each standard Gibbs energy of formation. Scott does not provide two tables for 4-ethyl-3-methylheptane; two tables are required since this molecule has two different chiral centers. In calculating thermody-

TABLE 2. Numbers of structural formulas, chiral centers, isomers, and lines in Tables for alkanes

| | Structural formulas | One center | Two centers | | Total isomers | Number of lines |
|---|---|---|---|---|---|---|
| | | | Identical | Different | | |
| $C_4H_{10}$ | 2 | 0 | 0 | 0 | 2 | 2 |
| $C_5H_{12}$ | 3 | 0 | 0 | 0 | 3 | 3 |
| $C_6H_{14}$ | 5 | 0 | 0 | 0 | 5 | 5 |
| $C_7H_{16}$ | 9 | 2 | 0 | 0 | 11 | 9 |
| $C_8H_{18}$ | 18 | 4 | 1 | 0 | 24 | 19 |
| $C_9H_{20}$ | 35 | 12 | 1 | 2 | 55 | 38 |
| $C_{10}H_{22}$ | 75 | 28 | 3 | 9 | 136 | 88[a] |

[a] This number would be 87 except for 3,4,5-trimethylheptane, which has a pseudoasymmetric atom.

namic properties, the assumption has been made that the two diastereomeric pairs of this structure have the same properties. Examination of the other eight diastereomeric pairs showed that the error introduced in this way is not significant.

In tables listing individual isomers, abbreviated names of the type developed by Somayajulu and Zwolinski[19] have been used. Methyl is represented by m, ethyl, by e, *n*-propyl by p, and *iso*-propyl by ip. The last number is the number of carbon atoms in the longest chain.

## 3. Input of Data and Calculations

The calculations in this paper were made using terminals connected to the IBM 370/168 in the MIT Computer Center. Programs were written in APL and tables were printed on a Xerox 8700 printer in the Computer Center. The values of $C_p^\circ$, $S^\circ$, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ in the Scott tables for individual alkane species and racemates were typed in and were checked in the process and later in printouts. In view of the opportunities to introduce errors, two additional types of checks were made: (1) Computer programs were written to calculate first and second differences per 100 K for each species. The second differences provided an especially sensitive method for error detection. (2) A computer program was written to calculate $\Delta_f G^\circ$(I) from $\Delta_f H$(I) and $S^\circ$(I) using Eq. (9). In the final tables no value of $\Delta_f G^\circ$(I) deviates from the value calculated in this way by more than the uncertainty indicated by Scott.

The following corrections have been made to the Scott table.

Table 62 for 3RSe2m6: $R$ ln 2 has been added to each standard entropy and $-RT$ ln 2 to each standard Gibbs energy of formation because of the chiral center.

Table 117 for 4RSe3RSm7: Since the table for the other diastereomeric pair 4RSe3SRm7 has been omitted, Table 117 has been used for both.

The following errors were identified from printouts of first and second differences; the changes make the first and second differences change in a smooth way.

Table 180 for 3e234mmm5: $S^\circ$ at 1100 K was changed from 234.0 to 240.0 cal $K^{-1}$ $mol^{-1}$.

Table 59 for 3R5Smm7: $S^\circ$ at 700 K was changed from 117.9 to 177.9 cal $K^{-1}$ $mol^{-1}$.

Table 6 for *n*-pentane: $\Delta_f G^\circ$ at 1100 K was changed from 94.2 to 96.7 kcal $mol^{-1}$ and $S^\circ$ was changed from 149.3 to 147.0 cal $K^{-1}$ $mol^{-1}$.

## 4. Tables of Standard Thermodynamic Properties of Alkane Isomer Groups

The standard thermodynamic properties of the alkane isomer groups for the ideal gas state from $C_4H_{10}$ to $C_{10}H_{22}$ have been calculated from the tables prepared by Scott[15] after making the corrections described in the preceding section. Since the International Union of Pure and Applied Chemistry has recently recommended that thermodynamic data be given in SI units for a standard state pressure of 1 bar ($10^5$ Pa), this has been done for the tables in this article. The change in standard state pressure from 1 atm to 1 bar does not affect $C_p^\circ$ and $\Delta_f H^\circ$, but the standard entropy of an ideal gas is increased by

$$R \ln(1.013\,25) = 0.109 \text{ J K}^{-1} \text{ mol}^{-1}$$

at any temperature and the standard Gibbs energy of formation is reduced by

$$[RT \ln(1.013\,25)]\delta,$$

where $\delta$ is the net increase in moles of gas in the formation reaction.[20] It is important to emphasize that all calculations in this paper are for ideal gases.

The standard thermodynamic properties $C_p^\circ$(I), $S^\circ$(I), $\Delta_f H^\circ$(I), and $\Delta_f G^\circ$(I) for alkane isomer groups are given in Tables 3–6 along with calculations of the increments in going from one carbon number to the next. These increments provide a basis for the extrapolation of standard thermodynamic properties of alkane isomer groups to higher carbon numbers. In a general way, we would expect these increments to approach constant values as the carbon number increases at constant temperature. The increment in the standard enthalpy of formation at 298.15 K is of special interest because of the variety of homologous series for which it is known. Cox and Pilcher[20] point out that the increment in $\Delta_f H^\circ$(298.15 K) of $-20.62$ kJ $mol^{-1}$ found by Prosen and Rossini[21] for the *n*-alkanes from $C_6H_{14}$ to $C_{12}H_{26}$ has come to be regarded as a "constant of nature" because it satisfactorily fits the experimental data for the higher members of the series of *n*-alk-1-enes, *n*-alkylbenzenes, *n*-alkylcyclopentanes, and *n*-alkylcyclohexanes. However, the increments per carbon atom for the four basic thermodynamic quanti-

Table 3. Standard heat capacity at constant pressure for alkane isomer groups in J/K mol

| T/K | methane | ethane | propane | butanes | pentanes | hexanes | heptanes | octanes | nonanes | decanes |
|---|---|---|---|---|---|---|---|---|---|---|
| 200.00 | 33.51 | 42.26 | 52.89 | 77.57 | 87.07 | 120.41 | 143.08 | 161.69 | 179.37 | 216.25 |
| 273.15 | 34.85 | 49.58 | 67.86 | 103.40 | 152.49 | 167.73 | 193.47 | 206.27 | 262.91 | 348.52 |
| 298.15 | 35.69 | 52.59 | 72.97 | 111.10 | 173.47 | 179.32 | 203.88 | 218.39 | 275.61 | 353.25 |
| 300.00 | 35.77 | 52.84 | 73.39 | 111.51 | 172.39 | 179.98 | 204.64 | 219.15 | 276.40 | 352.61 |
| 400.00 | 40.63 | 66.23 | 93.97 | 136.27 | 203.62 | 208.69 | 234.89 | 261.41 | 304.91 | 345.41 |
| 500.00 | 46.53 | 79.91 | 113.22 | 157.17 | 207.49 | 233.56 | 265.94 | 300.60 | 340.73 | 378.80 |
| 600.00 | 52.3 | 92.9 | 130.5 | 175.6 | 221.8 | 258.9 | 296.7 | 336.4 | 378.5 | 419.7 |
| 700.00 | 58.2 | 104.2 | 145.6 | 192.9 | 239.3 | 281.8 | 324.2 | 368.2 | 412.6 | 457.1 |
| 800.00 | 63.6 | 114.6 | 159.0 | 208.1 | 256.5 | 302.9 | 348.5 | 395.3 | 442.6 | 489.7 |
| 900.00 | 68.2 | 124.3 | 171.1 | 221.8 | 271.9 | 321.2 | 369.9 | 419.0 | 468.5 | 518.0 |
| 1000.00 | 72.8 | 132.6 | 181.6 | 233.8 | 286.1 | 337.3 | 388.2 | 439.4 | 490.9 | 542.5 |
| 1100.00 | 77.0 | 140.2 | 190.8 | 244.7 | 298.3 | 351.3 | 404.4 | 457.4 | 510.5 | 563.7 |
| 1200.00 | 80.3 | 146.9 | 199.2 | 253.9 | 309.2 | 363.9 | 418.6 | 473.1 | 527.8 | 582.5 |
| 1300.00 | 83.7 | 154.8 | 205.0 | 262.2 | 318.9 | 375.4 | 431.8 | 488.1 | 543.7 | 599.7 |
| 1400.00 | 87.9 | 159.0 | 213.4 | 270.4 | 327.2 | 385.2 | 444.4 | 501.0 | 557.7 | 614.2 |
| 1500.00 | 87.9 | 163.2 | 217.6 | 278.5 | 335.4 | 396.4 | 453.6 | 512.8 | 570.9 | 630.1 |

Table 3a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 | C9-C8 | C10-C9 |
|---|---|---|---|---|---|---|---|---|---|
| 200.00 | 8.74 | 10.63 | 24.69 | 9.49 | 33.34 | 22.67 | 18.61 | 17.68 | 36.88 |
| 273.15 | 14.73 | 18.28 | 35.53 | 49.10 | 15.24 | 25.74 | 12.80 | 56.64 | 85.61 |
| 298.15 | 16.90 | 20.38 | 38.13 | 62.37 | 5.85 | 24.55 | 14.52 | 57.22 | 77.63 |
| 300.00 | 17.07 | 20.54 | 38.13 | 60.87 | 7.59 | 24.67 | 14.50 | 57.25 | 76.21 |
| 400.00 | 25.61 | 27.74 | 42.30 | 67.35 | 5.07 | 26.19 | 26.52 | 43.50 | 40.50 |
| 500.00 | 33.39 | 33.30 | 43.95 | 50.32 | 26.06 | 32.38 | 34.66 | 40.13 | 38.07 |
| 600.00 | 40.6 | 37.7 | 45.1 | 46.2 | 37.1 | 37.8 | 39.7 | 42.1 | 41.2 |
| 700.00 | 46.0 | 41.4 | 47.3 | 46.4 | 42.5 | 42.4 | 44.0 | 44.5 | 44.5 |
| 800.00 | 51.0 | 44.4 | 49.1 | 48.4 | 46.4 | 45.6 | 46.8 | 47.3 | 47.2 |
| 900.00 | 56.1 | 46.9 | 50.7 | 50.1 | 49.3 | 48.7 | 49.1 | 49.4 | 49.6 |
| 1000.00 | 59.8 | 49.0 | 52.2 | 52.3 | 51.3 | 50.8 | 51.2 | 51.5 | 51.6 |
| 1100.00 | 63.2 | 50.6 | 53.9 | 53.6 | 53.1 | 53.1 | 52.9 | 53.2 | 53.1 |
| 1200.00 | 66.5 | 52.3 | 54.8 | 55.3 | 54.7 | 54.6 | 54.5 | 54.7 | 54.7 |
| 1300.00 | 71.1 | 50.2 | 57.2 | 56.7 | 56.5 | 56.5 | 56.2 | 55.7 | 56.0 |
| 1400.00 | 71.1 | 54.4 | 57.0 | 56.8 | 58.0 | 59.2 | 56.6 | 56.7 | 56.6 |
| 1500.00 | 75.3 | 54.4 | 61.0 | 56.8 | 61.0 | 57.2 | 59.2 | 58.1 | 59.2 |

Table 4. Standard entropy for alkane isomer groups in J/K mol

| T/K | methane | ethane | propane | butanes | pentanes | hexanes | heptanes | octanes | nonanes | decanes |
|---|---|---|---|---|---|---|---|---|---|---|
| 200.00 | 172.70 | 210.57 | 245.17 | 263.31 | 259.15 | 314.35 | 348.20 | 386.18 | 400.39 | 403.59 |
| 273.15 | 183.29 | 224.79 | 263.83 | 291.41 | 302.11 | 359.19 | 400.97 | 443.56 | 470.10 | 494.05 |
| 298.15 | 186.38 | 229.23 | 270.02 | 300.89 | 317.31 | 374.53 | 418.40 | 462.12 | 493.91 | 524.85 |
| 300.00 | 186.59 | 229.56 | 270.48 | 301.49 | 318.00 | 375.55 | 419.70 | 463.46 | 495.47 | 527.14 |
| 400.00 | 197.51 | 246.59 | 294.41 | 337.13 | 376.44 | 431.68 | 482.76 | 532.45 | 579.02 | 626.47 |
| 500.00 | 207.18 | 262.82 | 317.47 | 369.83 | 422.74 | 480.86 | 538.48 | 594.98 | 650.76 | 706.73 |
| 600.00 | 216.0 | 278.8 | 339.4 | 400.2 | 461.8 | 525.6 | 589.6 | 653.0 | 716.1 | 779.4 |
| 700.00 | 224.8 | 293.8 | 360.8 | 428.6 | 497.6 | 567.2 | 637.6 | 707.3 | 777.2 | 847.0 |
| 800.00 | 232.7 | 309.7 | 381.3 | 455.3 | 530.5 | 606.4 | 682.5 | 758.4 | 834.3 | 910.2 |
| 900.00 | 240.7 | 322.3 | 400.9 | 480.8 | 561.7 | 643.0 | 724.7 | 806.2 | 888.0 | 969.5 |
| 1000.00 | 248.2 | 336.1 | 419.3 | 504.7 | 591.1 | 677.9 | 764.7 | 851.5 | 938.5 | 1025.4 |
| 1100.00 | 255.3 | 349.1 | 436.9 | 527.5 | 618.9 | 710.6 | 802.4 | 894.2 | 986.2 | 1078.1 |
| 1200.00 | 262.0 | 361.6 | 454.1 | 549.2 | 645.2 | 741.8 | 838.3 | 934.7 | 1031.5 | 1128.0 |
| 1300.00 | 268.3 | 373.3 | 470.4 | 569.8 | 670.6 | 771.3 | 872.3 | 973.2 | 1074.4 | 1175.4 |
| 1400.00 | 275.0 | 385.0 | 485.9 | 589.6 | 694.5 | 799.4 | 904.6 | 1009.7 | 1115.1 | 1220.3 |
| 1500.00 | 280.9 | 396.3 | 500.9 | 608.3 | 717.3 | 826.5 | 935.6 | 1044.7 | 1154.1 | 1263.2 |

Table 4a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 | C9-C8 | C10-C9 |
|---|---|---|---|---|---|---|---|---|---|
| 200.00 | 37.87 | 34.60 | 18.14 | -4.16 | 55.20 | 33.84 | 37.99 | 14.20 | 3.20 |
| 273.15 | 41.51 | 39.04 | 27.58 | 10.70 | 57.08 | 41.78 | 42.59 | 26.54 | 23.95 |
| 298.15 | 42.84 | 40.79 | 30.87 | 16.42 | 57.22 | 43.87 | 43.72 | 31.78 | 30.94 |
| 300.00 | 42.97 | 40.92 | 31.01 | 16.51 | 57.55 | 44.15 | 43.76 | 32.01 | 31.67 |
| 400.00 | 49.08 | 47.82 | 42.72 | 39.31 | 55.24 | 51.08 | 49.69 | 46.57 | 47.46 |
| 500.00 | 55.65 | 54.64 | 52.36 | 52.91 | 58.12 | 57.63 | 56.50 | 55.78 | 55.96 |
| 600.00 | 62.8 | 60.7 | 60.8 | 61.6 | 63.9 | 64.0 | 63.4 | 63.1 | 63.3 |
| 700.00 | 69.0 | 66.9 | 67.8 | 69.0 | 69.6 | 70.4 | 69.7 | 69.9 | 69.8 |
| 800.00 | 77.0 | 71.5 | 74.0 | 75.2 | 75.9 | 76.2 | 75.8 | 75.9 | 76.0 |
| 900.00 | 81.6 | 78.7 | 79.9 | 80.9 | 81.3 | 81.7 | 81.5 | 81.7 | 81.6 |
| 1000.00 | 87.9 | 83.3 | 85.4 | 86.3 | 86.8 | 86.8 | 86.8 | 87.0 | 86.9 |
| 1100.00 | 93.7 | 87.9 | 90.6 | 91.4 | 91.7 | 91.8 | 91.7 | 92.1 | 91.9 |
| 1200.00 | 99.6 | 92.5 | 95.1 | 96.0 | 96.6 | 96.4 | 96.5 | 96.7 | 96.5 |
| 1300.00 | 105.0 | 97.1 | 99.4 | 100.8 | 100.7 | 101.0 | 100.9 | 101.1 | 101.0 |
| 1400.00 | 110.0 | 100.8 | 103.8 | 104.9 | 105.0 | 105.2 | 105.0 | 105.4 | 105.2 |
| 1500.00 | 115.5 | 104.6 | 107.4 | 109.1 | 109.1 | 109.1 | 109.0 | 109.4 | 109.2 |

Table 5. Standard enthalpy of formation for alkane isomer groups in kJ/mol

| T/K | methane | ethane | propane | butanes | pentanes | hexanes | heptanes | octanes | nonanes | decanes |
|---|---|---|---|---|---|---|---|---|---|---|
| 200.00 | -71.88 | -78.66 | -97.99 | -125.95 | -160.25 | -171.71 | -190.47 | -208.82 | -235.10 | -263.89 |
| 273.15 | -73.97 | -82.42 | -103.18 | -131.45 | -164.65 | -178.29 | -197.73 | -217.54 | -243.36 | -269.71 |
| 298.15 | -74.73 | -83.68 | -104.89 | -133.14 | -165.52 | -180.13 | -199.88 | -220.26 | -245.51 | -270.79 |
| 300.00 | -74.77 | -83.76 | -105.02 | -133.30 | -165.73 | -180.29 | -200.03 | -220.47 | -245.71 | -270.86 |
| 400.00 | -77.82 | -88.62 | -111.34 | -139.47 | -167.73 | -187.23 | -208.48 | -230.76 | -254.93 | -278.59 |
| 500.00 | -80.67 | -92.72 | -116.69 | -144.75 | -171.09 | -193.62 | -216.19 | -239.66 | -263.96 | -288.07 |
| 600.00 | -83.3 | -96.2 | -120.9 | -149.0 | -175.0 | -198.9 | -222.6 | -246.8 | -271.6 | -296.1 |
| 700.00 | -85.4 | -98.7 | -124.3 | -152.4 | -178.5 | -203.4 | -227.4 | -252.2 | -277.4 | -302.4 |
| 800.00 | -87.0 | -99.2 | -126.4 | -154.9 | -181.1 | -206.2 | -230.8 | -255.9 | -281.4 | -306.7 |
| 900.00 | -88.3 | -101.3 | -128.0 | -156.2 | -182.5 | -207.9 | -233.0 | -258.3 | -283.9 | -309.5 |
| 1000.00 | -89.5 | -101.7 | -128.9 | -157.0 | -183.3 | -208.6 | -233.9 | -259.3 | -284.9 | -310.6 |
| 1100.00 | -90.4 | -101.7 | -128.9 | -157.0 | -183.3 | -208.7 | -234.0 | -259.3 | -285.0 | -310.7 |
| 1200.00 | -90.8 | -100.8 | -128.4 | -156.5 | -182.5 | -207.9 | -233.0 | -258.3 | -283.9 | -309.4 |
| 1300.00 | -91.2 | -100.0 | -127.2 | -155.5 | -181.1 | -206.5 | -231.5 | -256.7 | -282.1 | -307.5 |
| 1400.00 | -91.2 | -98.3 | -125.9 | -153.7 | -179.4 | -204.4 | -229.4 | -254.3 | -279.6 | -304.8 |
| 1500.00 | -91.2 | -96.7 | -124.3 | -152.1 | -177.2 | -202.0 | -226.5 | -251.4 | -276.4 | -301.4 |

Table 5a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 | C9-C8 | C10-C9 |
|---|---|---|---|---|---|---|---|---|---|
| 200.00 | -6.78 | -19.33 | -27.97 | -34.29 | -11.46 | -18.76 | -18.35 | -26.28 | -28.78 |
| 273.15 | -8.45 | -20.75 | -28.27 | -33.20 | -13.64 | -19.44 | -19.81 | -25.82 | -26.35 |
| 298.15 | -8.95 | -21.21 | -28.25 | -32.38 | -14.61 | -19.75 | -20.38 | -25.25 | -25.28 |
| 300.00 | -9.00 | -21.25 | -28.28 | -32.44 | -14.56 | -19.74 | -20.44 | -25.24 | -25.14 |
| 400.00 | -10.79 | -22.72 | -28.13 | -28.26 | -19.49 | -21.25 | -22.28 | -24.17 | -23.66 |
| 500.00 | -12.05 | -23.97 | -28.06 | -26.34 | -22.54 | -22.57 | -23.47 | -24.29 | -24.11 |
| 600.00 | -13.0 | -24.7 | -28.1 | -26.0 | -23.9 | -23.6 | -24.2 | -24.8 | -24.5 |
| 700.00 | -13.4 | -25.5 | -28.1 | -26.1 | -24.9 | -24.0 | -24.8 | -25.2 | -25.1 |
| 800.00 | -12.1 | -27.2 | -28.5 | -26.2 | -25.2 | -24.6 | -25.1 | -25.5 | -25.3 |
| 900.00 | -13.0 | -26.8 | -28.2 | -26.3 | -25.4 | -25.1 | -25.3 | -25.5 | -25.6 |
| 1000.00 | -12.1 | -27.2 | -28.1 | -26.3 | -25.3 | -25.4 | -25.4 | -25.6 | -25.6 |
| 1100.00 | -11.3 | -27.2 | -28.1 | -26.3 | -25.4 | -25.3 | -25.3 | -25.7 | -25.7 |
| 1200.00 | -10.0 | -27.6 | -28.0 | -26.1 | -25.4 | -25.1 | -25.3 | -25.6 | -25.5 |
| 1300.00 | -8.8 | -27.2 | -28.3 | -25.6 | -25.3 | -25.0 | -25.2 | -25.5 | -25.4 |
| 1400.00 | -7.1 | -27.6 | -27.7 | -25.7 | -25.0 | -25.0 | -25.0 | -25.2 | -25.3 |
| 1500.00 | -5.4 | -27.6 | -27.8 | -25.2 | -24.7 | -24.6 | -24.9 | -25.0 | -25.0 |

Table 6. Standard Gibbs energy of formation for alkane isomer groups in kJ/mol

| T/K | methane | ethane | propane | butanes | pentanes | hexanes | heptanes | octanes | nonanes | decanes |
|---|---|---|---|---|---|---|---|---|---|---|
| 200.00 | -58.05 | -47.91 | -49.64 | -56.79 | -65.76 | -63.75 | -64.81 | -66.27 | -70.88 | -75.84 |
| 273.15 | -52.69 | -36.05 | -31.17 | -30.59 | -30.31 | -23.21 | -17.67 | -12.73 | -9.45 | -5.97 |
| 298.15 | -50.68 | -31.73 | -24.46 | -21.22 | -17.86 | -8.87 | -1.05 | 6.19 | 12.13 | 18.28 |
| 300.00 | -50.51 | -31.44 | -23.96 | -20.56 | -17.06 | -7.81 | .20 | 7.60 | 13.72 | 20.09 |
| 400.00 | -41.96 | -13.22 | 4.06 | 17.99 | 33.19 | 50.75 | 68.23 | 85.23 | 101.60 | 118.11 |
| 500.00 | -32.66 | 6.09 | 33.55 | 58.00 | 83.89 | 111.00 | 138.31 | 165.29 | 191.78 | 218.39 |
| 600.00 | -22.9 | 26.1 | 63.8 | 98.9 | 135.2 | 172.5 | 209.9 | 247.0 | 283.6 | 320.5 |
| 700.00 | -12.5 | 46.6 | 95.2 | 140.7 | 187.4 | 234.7 | 282.2 | 329.7 | 376.6 | 423.7 |
| 800.00 | -2.0 | 67.5 | 126.6 | 182.6 | 239.9 | 297.5 | 355.4 | 413.0 | 470.3 | 527.8 |
| 900.00 | 8.5 | 88.9 | 158.4 | 224.9 | 292.4 | 360.5 | 428.7 | 496.8 | 564.5 | 632.3 |
| 1000.00 | 19.4 | 109.8 | 190.3 | 267.2 | 345.3 | 423.9 | 502.4 | 580.8 | 658.8 | 737.0 |
| 1100.00 | 30.2 | 131.2 | 222.1 | 309.7 | 398.1 | 486.9 | 576.0 | 664.8 | 753.2 | 841.8 |
| 1200.00 | 41.1 | 152.1 | 253.9 | 352.0 | 451.0 | 550.2 | 649.5 | 748.8 | 847.5 | 946.4 |
| 1300.00 | 52.4 | 173.1 | 285.8 | 394.4 | 503.8 | 613.2 | 729.1 | 832.7 | 941.7 | 1050.9 |
| 1400.00 | 63.3 | 194.0 | 317.6 | 436.6 | 556.4 | 676.3 | 796.4 | 916.5 | 1035.8 | 1155.5 |
| 1500.00 | 74.2 | 215.0 | 349.0 | 478.8 | 608.8 | 739.1 | 869.6 | 1000.0 | 1129.7 | 1259.6 |

Table 6a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 | C9-C8 | C10-C9 |
|---|---|---|---|---|---|---|---|---|---|
| 200.00 | 10.15 | -1.74 | -7.15 | -8.97 | 2.01 | -1.06 | -1.46 | -4.62 | -4.96 |
| 273.15 | 16.64 | 4.88 | .58 | .28 | 7.10 | 5.54 | 4.94 | 3.27 | 3.48 |
| 298.15 | 18.94 | 7.27 | 3.24 | 3.37 | 8.98 | 7.83 | 7.24 | 5.94 | 6.16 |
| 300.00 | 19.07 | 7.48 | 3.40 | 3.50 | 9.25 | 8.01 | 7.41 | 6.12 | 6.36 |
| 400.00 | 28.75 | 17.28 | 13.92 | 15.20 | 17.57 | 17.47 | 17.00 | 16.37 | 16.51 |
| 500.00 | 38.76 | 27.46 | 24.45 | 25.90 | 27.11 | 27.31 | 26.98 | 26.50 | 26.61 |
| 600.00 | 49.0 | 37.7 | 35.1 | 36.4 | 37.3 | 37.4 | 37.1 | 36.6 | 36.9 |
| 700.00 | 59.1 | 48.6 | 45.5 | 46.6 | 47.4 | 47.5 | 47.5 | 47.0 | 47.1 |
| 800.00 | 69.5 | 59.1 | 55.9 | 57.3 | 57.6 | 57.8 | 57.6 | 57.3 | 57.5 |
| 900.00 | 80.4 | 69.6 | 66.5 | 67.5 | 68.1 | 68.2 | 68.1 | 67.7 | 67.8 |
| 1000.00 | 90.5 | 80.4 | 77.0 | 78.0 | 78.6 | 78.5 | 78.4 | 78.0 | 78.2 |
| 1100.00 | 101.0 | 90.9 | 87.6 | 88.4 | 88.8 | 89.1 | 88.8 | 88.4 | 88.6 |
| 1200.00 | 111.0 | 101.8 | 98.0 | 99.0 | 99.3 | 99.3 | 99.3 | 98.7 | 98.9 |
| 1300.00 | 120.6 | 112.7 | 108.7 | 109.3 | 109.4 | 109.9 | 109.6 | 109.0 | 109.3 |
| 1400.00 | 130.7 | 123.6 | 119.0 | 119.8 | 119.9 | 120.1 | 120.1 | 119.3 | 119.7 |
| 1500.00 | 140.7 | 134.1 | 129.7 | 130.0 | 130.3 | 130.4 | 130.4 | 129.7 | 130.0 |

Table 7. Standard enthalpy for alkane isomer groups relative to isomer group at 298.15 K in kJ/mol

| T/K | methane | ethane | propane | butanes | pentanes | hexanes | heptanes | octanes | nonanes | decanes |
|---|---|---|---|---|---|---|---|---|---|---|
| 200.00 | -3.37 | -4.63 | -6.19 | -9.34 | -14.70 | -14.99 | -17.44 | -18.84 | -23.32 | -30.26 |
| 273.15 | -.90 | -1.34 | -1.82 | -2.78 | -4.54 | -4.51 | -5.14 | -5.51 | -7.01 | -9.02 |
| 298.15 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |
| 300.00 | .08 | .11 | .14 | .18 | .20 | .32 | .40 | .41 | .49 | .70 |
| 400.00 | 3.86 | 6.01 | 8.50 | 12.61 | 20.73 | 19.84 | 22.33 | 24.42 | 29.50 | 35.12 |
| 500.00 | 8.19 | 13.34 | 18.83 | 27.26 | 41.55 | 41.87 | 47.30 | 52.46 | 61.66 | 71.08 |
| 600.00 | 13.0 | 21.8 | 31.0 | 43.9 | 63.1 | 66.5 | 75.4 | 84.3 | 97.5 | 111.0 |
| 700.00 | 18.6 | 31.6 | 44.8 | 62.4 | 86.1 | 93.3 | 106.5 | 119.5 | 137.0 | 154.7 |
| 800.00 | 24.7 | 43.9 | 60.3 | 82.3 | 110.9 | 122.7 | 140.1 | 157.8 | 179.9 | 202.2 |
| 900.00 | 31.5 | 54.8 | 76.6 | 104.0 | 137.4 | 154.0 | 176.0 | 198.4 | 225.5 | 252.5 |
| 1000.00 | 38.3 | 67.6 | 94.1 | 126.7 | 165.3 | 187.1 | 214.0 | 241.4 | 273.5 | 305.7 |
| 1100.00 | 45.8 | 81.1 | 112.9 | 150.7 | 194.5 | 221.4 | 253.5 | 286.3 | 323.6 | 360.9 |
| 1200.00 | 53.8 | 95.7 | 132.4 | 175.6 | 225.0 | 257.3 | 294.9 | 333.1 | 375.7 | 418.5 |
| 1300.00 | 61.9 | 110.5 | 153.0 | 201.4 | 256.6 | 294.3 | 337.5 | 381.2 | 429.4 | 477.8 |
| 1400.00 | 70.6 | 126.4 | 173.9 | 228.4 | 289.0 | 332.6 | 381.3 | 430.7 | 484.7 | 538.7 |
| 1500.00 | 79.4 | 142.4 | 195.6 | 255.6 | 322.3 | 371.7 | 426.5 | 481.5 | 541.4 | 601.2 |

Table 7a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 | C9-C8 | C10-C9 |
|---|---|---|---|---|---|---|---|---|---|
| 200.00 | -1.26 | -1.56 | -3.16 | -5.35 | -.29 | -2.45 | -1.41 | -4.47 | -6.94 |
| 273.15 | -.44 | -.48 | -.96 | -1.75 | .03 | -.63 | -.37 | -1.51 | -2.01 |
| 298.15 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |
| 300.00 | .03 | .03 | .04 | .02 | .12 | .07 | .02 | .08 | .21 |
| 400.00 | 2.16 | 2.49 | 4.11 | 8.11 | -.89 | 2.49 | 2.10 | 5.08 | 5.62 |
| 500.00 | 5.15 | 5.49 | 8.44 | 14.29 | .32 | 5.42 | 5.16 | 9.20 | 9.42 |
| 600.00 | 8.7 | 9.3 | 12.9 | 19.2 | 3.4 | 8.9 | 8.9 | 13.2 | 13.5 |
| 700.00 | 13.0 | 13.2 | 17.6 | 23.8 | 7.2 | 13.2 | 13.0 | 17.5 | 17.7 |
| 800.00 | 19.2 | 16.4 | 22.1 | 28.5 | 11.8 | 17.5 | 17.7 | 22.1 | 22.3 |
| 900.00 | 23.3 | 21.8 | 27.4 | 33.4 | 16.6 | 22.0 | 22.4 | 27.1 | 27.0 |
| 1000.00 | 29.3 | 26.5 | 32.6 | 38.6 | 21.8 | 26.9 | 27.5 | 32.1 | 32.1 |
| 1100.00 | 35.4 | 31.7 | 37.8 | 43.8 | 26.9 | 32.2 | 32.8 | 37.3 | 37.3 |
| 1200.00 | 41.9 | 36.6 | 43.3 | 49.4 | 32.3 | 37.7 | 38.1 | 42.7 | 42.8 |
| 1300.00 | 48.6 | 42.5 | 48.4 | 55.2 | 37.8 | 43.2 | 43.7 | 48.2 | 48.4 |
| 1400.00 | 55.8 | 47.6 | 54.5 | 60.6 | 43.6 | 48.7 | 49.4 | 54.0 | 54.0 |
| 1500.00 | 63.1 | 53.1 | 60.0 | 66.7 | 49.4 | 54.7 | 55.1 | 59.8 | 59.8 |

Table 8. Standard enthalpy for alkane isomer groups relative to the elements at 298.15 K in kJ/mol

| T/K | methane | ethane | propane | butanes | pentanes | hexanes | heptanes | octanes | nonanes | decanes |
|---|---|---|---|---|---|---|---|---|---|---|
| 200.00 | -78.09 | -88.31 | -111.08 | -142.48 | -180.22 | -195.12 | -217.31 | -239.10 | -268.83 | -301.05 |
| 273.15 | -75.63 | -85.02 | -106.71 | -135.92 | -170.06 | -184.64 | -205.02 | -225.76 | -252.52 | -279.81 |
| 298.15 | -74.73 | -83.68 | -104.89 | -133.14 | -165.52 | -180.13 | -199.88 | -220.26 | -245.51 | -270.79 |
| 300.00 | -74.64 | -83.57 | -104.75 | -132.96 | -165.32 | -179.81 | -199.48 | -219.85 | -245.02 | -270.09 |
| 400.00 | -70.87 | -77.67 | -96.39 | -120.53 | -144.79 | -160.29 | -177.55 | -195.84 | -216.01 | -235.67 |
| 500.00 | -66.54 | -70.34 | -86.07 | -105.88 | -123.97 | -138.26 | -152.58 | -167.80 | -183.85 | -199.71 |
| 600.00 | -61.7 | -61.9 | -73.8 | -89.2 | -102.4 | -113.6 | -124.5 | -136.0 | -148.0 | -159.8 |
| 700.00 | -56.1 | -52.1 | -60.1 | -70.8 | -79.4 | -86.8 | -93.4 | -100.8 | -108.5 | -116.1 |
| 800.00 | -50.0 | -39.8 | -44.6 | -50.8 | -54.7 | -57.5 | -59.7 | -62.4 | -65.6 | -68.6 |
| 900.00 | -43.3 | -28.9 | -28.3 | -29.2 | -28.1 | -26.1 | -23.9 | -21.9 | -20.0 | -18.3 |
| 1000.00 | -36.4 | -16.0 | -10.8 | -6.4 | -.2 | 7.0 | 14.1 | 21.2 | 28.0 | 34.9 |
| 1100.00 | -28.9 | -2.5 | 8.0 | 17.6 | 28.9 | 41.2 | 53.7 | 66.0 | 78.1 | 90.1 |
| 1200.00 | -21.0 | 12.0 | 27.5 | 42.5 | 59.5 | 77.1 | 95.0 | 112.8 | 130.2 | 147.7 |
| 1300.00 | -12.8 | 26.8 | 48.1 | 68.2 | 91.1 | 114.2 | 137.6 | 160.9 | 183.9 | 207.0 |
| 1400.00 | -4.2 | 42.7 | 69.0 | 95.2 | 123.5 | 152.5 | 181.5 | 210.4 | 239.2 | 267.9 |
| 1500.00 | 4.6 | 58.7 | 90.7 | 122.4 | 156.8 | 191.6 | 226.6 | 261.3 | 295.9 | 330.4 |

Table 8a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 | C9-C8 | C10-C9 |
|---|---|---|---|---|---|---|---|---|---|
| 200.00 | -10.22 | -22.77 | -31.40 | -37.73 | -14.90 | -22.19 | -21.79 | -29.72 | -32.22 |
| 273.15 | -9.39 | -21.69 | -29.21 | -34.14 | -14.58 | -20.38 | -20.75 | -26.76 | -27.29 |
| 298.15 | -8.95 | -21.21 | -28.25 | -32.38 | -14.61 | -19.75 | -20.38 | -25.25 | -25.28 |
| 300.00 | -8.92 | -21.18 | -28.21 | -32.37 | -14.49 | -19.67 | -20.37 | -25.17 | -25.07 |
| 400.00 | -6.80 | -18.72 | -24.14 | -24.27 | -15.50 | -17.26 | -18.29 | -20.17 | -19.66 |
| 500.00 | -3.80 | -15.73 | -19.81 | -18.09 | -14.29 | -14.32 | -15.23 | -16.05 | -15.86 |
| 600.00 | -.2 | -11.9 | -15.3 | -13.2 | -11.2 | -10.9 | -11.5 | -12.1 | -11.8 |
| 700.00 | 4.1 | -8.1 | -10.7 | -8.6 | -7.4 | -6.6 | -7.4 | -7.7 | -7.6 |
| 800.00 | 10.2 | -4.9 | -6.2 | -3.8 | -2.8 | -2.3 | -2.7 | -3.2 | -3.0 |
| 900.00 | 14.4 | .6 | -.9 | 1.1 | 2.0 | 2.2 | 2.0 | 1.8 | 1.8 |
| 1000.00 | 20.3 | 5.3 | 4.3 | 6.2 | 7.2 | 7.1 | 7.1 | 6.9 | 6.9 |
| 1100.00 | 26.4 | 10.5 | 9.6 | 11.4 | 12.3 | 12.4 | 12.4 | 12.0 | 12.0 |
| 1200.00 | 33.0 | 15.4 | 15.0 | 17.0 | 17.7 | 17.9 | 17.7 | 17.4 | 17.5 |
| 1300.00 | 39.7 | 21.3 | 20.1 | 22.8 | 23.1 | 23.4 | 23.3 | 23.0 | 23.1 |
| 1400.00 | 46.8 | 26.3 | 26.2 | 28.2 | 29.0 | 29.0 | 29.0 | 28.7 | 28.7 |
| 1500.00 | 54.1 | 31.9 | 31.8 | 34.4 | 34.8 | 35.0 | 34.7 | 34.6 | 34.5 |

ties for isomer groups are not constant, except at the higher temperatures. As shown in Table 5, the increments in $\Delta_f H°(\mathrm{I})$ per carbon vary from $-14.60$ to $-32.38$ kJ mol$^{-1}$ at 298.15 K.However, at about 600 K and above the increments per carbon atom are quite constant. The reason for this, which will be discussed later, is that particular isomers in each isomer group may tend to dominate at lower temperatures because they have lower enthalpies of formation. At higher temperatures, where the mole fractions of isomers in the isomer group are determined primarily by the entropy of formation, the increments per carbon atom vary much less with carbon number. The tables of increments per carbon atom give a good indication of the extent to which standard thermodynamic properties of isomer groups may be extrapolated above $C_{10}H_{22}$ for each temperature.

Table 7 gives

$$H°(\mathrm{I},T) - H°(\mathrm{I},298.15\ \mathrm{K}),$$

the standard enthalpy for an isomer group relative to the isomer group at 298.15 K. Scott[15] had given values for $H° - H°(0\ \mathrm{K})$, but for isomer groups 298.15 K is a better reference temperature since at 0 K a single isomer or racemate is present at equilibrium.

With regard to the uncertainties in the statistical mechanical correlations, Scott has rounded to the number of decimal digits appropriate to the accuracy. However, he points out that as a matter of practical convenience a uniform pattern of rounding and subscripting was used throughout the tables. This means that the rounding may be overly conservative for the lower alkanes and may attribute undue accuracy to the values for the most highly branched decanes, for which no calorimetric data exist. We have followed Scott's indicated accuracy as closely as possible.

Table 8 gives values for

$$H°(\mathrm{I},T) - H°(\mathrm{I},298.15\ \mathrm{K}) + \Delta_f H°(\mathrm{I},298.15\ \mathrm{K}),$$

the standard enthalpy for the isomer group relative to the elements at 298.15 K. This quantity allows the direct calculation of heat effects when the reactants and products are at different temperatures. The values in Table 8 were not calculated directly from Scott's tables since they can be calculated from $\Delta_f H°(\mathrm{I})$ and values of $H° - H°(298.15\ \mathrm{K})$ for graphite and hydrogen gas.

## 5. Equilibrium Mole Fractions Within Alkane Isomer Groups

The equilibrium mole fractions within isomer groups calculated from Scott's standard Gibbs energies of formation are given in Table 9. Since the uncertainties in $\Delta_f G°(\mathrm{I})$ and $\Delta_f G_i^\circ$ are about the same, the uncertainty in the difference is nearly independent of the relative values of the two parameters, but the uncertainty in the difference does increase with temperature. Since the nearly constant uncertainty is in the exponent in the calculation, the equilibrium mole fractions of the isomers at a given temperature are uncertain by the same factor, whether they are large or small. The usual equation for the propagation of variance indicates that the equilibrium mole fractions are uncertain by about 15% at the lower temperatures and 10% at the higher temperatures. This makes it difficult to indicate the uncertainties in the table.It could be done by using exponential notation, but this makes it difficult to compare the mole fractions of various isomers.

Table 9 shows that in general the more highly branched isomers have very low equilibrium mole fractions at any temperature. The isomers with more methyl groups and more opportunities for steric hindrance have more positive standard Gibbs energies of formation. At higher temperatures, these differences are not so pronounced, reflecting the fact that the statistical mechanical entropies are more similar than the enthalpies of formation. However, 22mm3, 22mm4, 22mm5, 22mm6, 225mmm6, and 2255mmmm6 present striking exceptions to these generalizations. Since the calculated equilibrium mole fraction of the decane 2255mmmm6 is 0.86 at 200 K, we made some additional calculations using the properties of 224RS5mmmm6 (with the entropy of mixing and Gibbs energy of mixing removed) replacing Scott's values for 2255mmmm6. With these new values, 2255mmmm6 had an equilibrium mole fraction of 0.012 at 200 K and 0.0006 at 1500 K, and 226mmm7 ($y_i = 0.52$) and 225RSmmm7 ($y_i = 0.26$) became the most abundant species at 200 K. However, as Professor Kenneth S. Pitzer pointed out to me, 2255mmmm6 is di-neopentyl which does not have much strain because the neopentyl groups are so far apart. In general, multiple branching introduces strained structures, but in this case the strain is modeled accurately by neohexane (22mm4) which is quite stable relative to the other hexanes at low temperatures. The stability of di-neopentyl and of other species referred to earlier in this paragraph at low temperatures is confirmed by calculations using the Benson group method, which are described in the next section. The values in Tables 3 to 9 have all been calculated using Scott's values.[16] Since the heat of combustion has not been determined for 2255mmmm6, it certainly would be desirable to obtain experimental data on this species to determine how low its standard enthalpy of formation is.

Table 9. Equilibrium mole fractions within alkane isomer groups

| T/K | 200 | 273 | 298 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| butanes | | | | | | | | | | | | | | | | |
| 4 | .0324 | .1203 | .1606 | .1619 | .3170 | .4424 | .5418 | .5889 | .6232 | .6617 | .6911 | .6950 | .7156 | .7169 | .7252 | .7323 |
| 2m3 | .9676 | .8797 | .8394 | .8381 | .6830 | .5576 | .4582 | .4111 | .3768 | .3383 | .3089 | .3050 | .2844 | .2831 | .2748 | .2677 |
| pentanes | | | | | | | | | | | | | | | | |
| 5 | .0003 | .0098 | .0214 | .0212 | .1177 | .2245 | .2951 | .3623 | .3967 | .4242 | .4449 | .4616 | .4749 | .4861 | .4868 | .4952 |
| 2m4 | .0068 | .0946 | .1571 | .1563 | .4411 | .5554 | .5773 | .5577 | .5433 | .5305 | .5174 | .5059 | .4953 | .4861 | .4868 | .4789 |
| 22mm3 | .9929 | .8956 | .8214 | .8225 | .4411 | .2200 | .1276 | .0801 | .0601 | .0453 | .0378 | .0325 | .0298 | .0277 | .0265 | .0259 |
| hexanes | | | | | | | | | | | | | | | | |
| 6 | .0015 | .0168 | .0281 | .0289 | .0913 | .1542 | .2091 | .2354 | .2646 | .2941 | .3077 | .3188 | .3256 | .3330 | .3305 | .3326 |
| 2m5 | .0345 | .1345 | .1736 | .1738 | .2797 | .3150 | .3180 | .3138 | .3196 | .3110 | .3077 | .3046 | .2994 | .2965 | .2968 | .3007 |
| 3m5 | .0091 | .0545 | .0772 | .0790 | .1629 | .2106 | .2273 | .2530 | .2485 | .2487 | .2516 | .2536 | .2532 | .2539 | .2570 | .2543 |
| 22mm4 | .9324 | .7322 | .6477 | .6432 | .3736 | .2306 | .1625 | .1233 | .0967 | .0813 | .0715 | .0643 | .0634 | .0583 | .0589 | .0581 |
| 23mm4 | .0225 | .0620 | .0734 | .0751 | .0925 | .0895 | .0831 | .0745 | .0706 | .0650 | .0615 | .0587 | .0583 | .0583 | .0568 | .0543 |
| heptanes | | | | | | | | | | | | | | | | |
| 7 | .0013 | .0141 | .0226 | .0234 | .0680 | .1110 | .1402 | .1693 | .1932 | .1972 | .2100 | .2179 | .2234 | .2280 | .2285 | .2252 |
| 2m6 | .0330 | .1174 | .1450 | .1484 | .2164 | .2337 | .2318 | .2258 | .2192 | .2205 | .2100 | .2082 | .2054 | .2030 | .1979 | .1969 |
| 3RSm6 | .0147 | .0797 | .1088 | .1116 | .2032 | .2558 | .2742 | .3010 | .3002 | .3084 | .3140 | .3142 | .3124 | .3107 | .3157 | .3150 |
| 3e5 | .0006 | .0045 | .0067 | .0069 | .0166 | .0243 | .0310 | .0324 | .0354 | .0368 | .0399 | .0401 | .0417 | .0415 | .0422 | .0421 |
| 22mm5 | .6582 | .4262 | .3606 | .3550 | .1838 | .1098 | .0779 | .0576 | .0484 | .0412 | .0379 | .0350 | .0338 | .0329 | .0328 | .0322 |
| 23RSmm5 | .0120 | .0494 | .0623 | .0631 | .0943 | .1024 | .1090 | .1024 | .1030 | .1008 | .0987 | .0956 | .0966 | .0973 | .0964 | .1007 |
| 24mm5 | .1418 | .1576 | .1499 | .1484 | .1111 | .0837 | .0717 | .0576 | .0516 | .0487 | .0464 | .0460 | .0435 | .0432 | .0422 | .0421 |
| 33mm5 | .0435 | .0714 | .0738 | .0734 | .0663 | .0543 | .0471 | .0402 | .0377 | .0368 | .0343 | .0350 | .0353 | .0356 | .0365 | .0381 |
| 223mmm4 | .0948 | .0797 | .0702 | .0698 | .0401 | .0250 | .0172 | .0137 | .0114 | .0096 | .0088 | .0081 | .0078 | .0079 | .0078 | .0079 |
| octanes | | | | | | | | | | | | | | | | |
| 8 | .0010 | .0093 | .0146 | .0152 | .0440 | .0730 | .0964 | .1119 | .1288 | .1370 | .1488 | .1507 | .1527 | .1528 | .1574 | .1524 |
| 2m7 | .0236 | .0761 | .0937 | .0947 | .1381 | .1538 | .1595 | .1603 | .1555 | .1448 | .1488 | .1439 | .1404 | .1414 | .1364 | .1378 |
| 3RSm7 | .0111 | .0546 | .0728 | .0736 | .1381 | .1736 | .1886 | .1989 | .2130 | .2142 | .2116 | .2075 | .2136 | .2082 | .2099 | .2061 |
| 4m7 | .0048 | .0225 | .0297 | .0303 | .0558 | .0709 | .0815 | .0839 | .0883 | .0926 | .0899 | .0953 | .0963 | .0960 | .0952 | .0953 |
| 3e6 | .0012 | .0077 | .0112 | .0114 | .0273 | .0407 | .0493 | .0586 | .0605 | .0662 | .0699 | .0725 | .0718 | .0732 | .0740 | .0753 |
| 22mm6 | .5077 | .2973 | .2494 | .2464 | .1281 | .0776 | .0536 | .0409 | .0323 | .0286 | .0256 | .0242 | .0222 | .0221 | .0210 | .0211 |
| 23RSmm6 | .0080 | .0281 | .0346 | .0352 | .0518 | .0579 | .0583 | .0586 | .0569 | .0592 | .0572 | .0576 | .0582 | .0580 | .0575 | .0576 |
| 24RSmm6 | .0989 | .1449 | .1478 | .1490 | .1399 | .1233 | .1140 | .1041 | .0940 | .0926 | .0899 | .0870 | .0849 | .0855 | .0855 | .0862 |
| 25mm6 | .1678 | .1876 | .1810 | .1791 | .1330 | .0988 | .0750 | .0630 | .0534 | .0473 | .0423 | .0400 | .0367 | .0351 | .0336 | .0326 |
| 33mm6 | .0477 | .0644 | .0636 | .0644 | .0558 | .0474 | .0417 | .0381 | .0366 | .0358 | .0346 | .0365 | .0367 | .0379 | .0388 | .0412 |
| 3RS4RSmm6 | .0006 | .0038 | .0052 | .0063 | .0105 | .0136 | .0152 | .0173 | .0172 | .0183 | .0180 | .0192 | .0196 | .0204 | .0203 | .0211 |
| 3R4Smm6 | .0006 | .0036 | .0050 | .0051 | .0101 | .0133 | .0152 | .0161 | .0172 | .0183 | .0180 | .0192 | .0196 | .0204 | .0203 | .0211 |
| 3e2m5 | .0007 | .0033 | .0045 | .0045 | .0091 | .0123 | .0152 | .0161 | .0172 | .0173 | .0180 | .0192 | .0196 | .0204 | .0203 | .0211 |
| 3e3m5 | .0002 | .0009 | .0011 | .0011 | .0018 | .0021 | .0022 | .0023 | .0024 | .0026 | .0027 | .0028 | .0030 | .0031 | .0034 | .0036 |
| 223RSmmm5 | .0100 | .0135 | .0132 | .0133 | .0109 | .0086 | .0072 | .0063 | .0055 | .0053 | .0051 | .0051 | .0051 | .0051 | .0054 | .0055 |
| 224mmm5 | .1094 | .0720 | .0615 | .0602 | .0333 | .0210 | .0152 | .0121 | .0098 | .0084 | .0080 | .0074 | .0075 | .0075 | .0074 | .0077 |
| 233mmm5 | .0025 | .0054 | .0060 | .0059 | .0067 | .0063 | .0061 | .0059 | .0055 | .0057 | .0056 | .0059 | .0060 | .0064 | .0069 | .0074 |
| 234mm5 | .0012 | .0031 | .0037 | .0037 | .0049 | .0053 | .0056 | .0055 | .0055 | .0057 | .0059 | .0059 | .0060 | .0064 | .0067 | .0070 |
| 2233mmmm4 | .0029 | .0017 | .0014 | .0014 | .0007 | .0004 | .0003 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 |
| nonanes | | | | | | | | | | | | | | | | |
| 9 | .0001 | .0029 | .0056 | .0059 | .0238 | .0437 | .0599 | .0729 | .0818 | .0904 | .0952 | .0994 | .0989 | .1003 | .1015 | .1003 |
| 2m8 | .0026 | .0241 | .0359 | .0367 | .0748 | .0921 | .0991 | .0972 | .0988 | .0956 | .0952 | .0949 | .0909 | .0893 | .0879 | .0877 |
| 3RSm8 | .0012 | .0167 | .0274 | .0280 | .0729 | .1028 | .1172 | .1296 | .1353 | .1338 | .1424 | .1369 | .1383 | .1367 | .1353 | .1356 |
| 4RSm8 | .0010 | .0144 | .0231 | .0237 | .0604 | .0849 | .0991 | .1044 | .1120 | .1196 | .1164 | .1193 | .1219 | .1217 | .1215 | .1186 |
| 3e7 | .0001 | .0025 | .0044 | .0046 | .0151 | .0249 | .0306 | .0382 | .0410 | .0437 | .0447 | .0457 | .0465 | .0462 | .0477 | .0464 |
| 4e7 | .0001 | .0021 | .0037 | .0038 | .0124 | .0203 | .0259 | .0308 | .0339 | .0370 | .0385 | .0398 | .0410 | .0412 | .0413 | .0419 |
| 22mm7 | .0543 | .0941 | .0956 | .0938 | .0685 | .0455 | .0333 | .0266 | .0218 | .0189 | .0164 | .0159 | .0150 | .0139 | .0141 | .0139 |
| 23RSmm7 | .0009 | .0096 | .0144 | .0148 | .0310 | .0376 | .0394 | .0410 | .0410 | .0391 | .0385 | .0398 | .0393 | .0396 | .0385 | .0392 |
| 24RSmm7 | .0091 | .0368 | .0462 | .0464 | .0604 | .0585 | .0551 | .0509 | .0495 | .0489 | .0495 | .0478 | .0485 | .0481 | .0477 | .0479 |
| 25RSmm7 | .0184 | .0891 | .1131 | .1147 | .1494 | .1391 | .1275 | .1122 | .0988 | .0904 | .0861 | .0828 | .0769 | .0765 | .0734 | .0717 |
| 26mm7 | .0189 | .0605 | .0705 | .0705 | .0729 | .0597 | .0507 | .0410 | .0361 | .0331 | .0299 | .0276 | .0269 | .0259 | .0250 | .0237 |
| 33mm7 | .0056 | .0220 | .0269 | .0271 | .0330 | .0307 | .0282 | .0266 | .0248 | .0236 | .0233 | .0230 | .0238 | .0239 | .0250 | .0253 |
| 3RS4SRmm7 | .0001 | .0020 | .0033 | .0034 | .0093 | .0135 | .0157 | .0173 | .0193 | .0200 | .0210 | .0210 | .0218 | .0222 | .0232 | .0237 |
| 3RS4RSmm7 | .0001 | .0021 | .0035 | .0036 | .0096 | .0139 | .0157 | .0186 | .0193 | .0200 | .0210 | .0210 | .0218 | .0222 | .0224 | .0237 |
| 3RS5RSmm7 | .0015 | .0098 | .0133 | .0134 | .0218 | .0239 | .0238 | .0231 | .0232 | .0223 | .0221 | .0220 | .0218 | .0222 | .0216 | .0222 |
| 3R5Smm7 | .0013 | .0081 | .0110 | .0111 | .0185 | .0208 | .0201 | .0215 | .0205 | .0211 | .0200 | .0200 | .0201 | .0205 | .0201 | .0200 |
| 44mm7 | .0020 | .0069 | .0083 | .0084 | .0099 | .0092 | .0087 | .0084 | .0085 | .0082 | .0085 | .0088 | .0091 | .0095 | .0102 | .0106 |
| 3RSe2m6 | .0003 | .0035 | .0058 | .0059 | .0161 | .0241 | .0289 | .0324 | .0361 | .0378 | .0381 | .0402 | .0420 | .0426 | .0433 | .0444 |
| 4e2m6 | .0012 | .0075 | .0091 | .0093 | .0155 | .0177 | .0185 | .0186 | .0181 | .0189 | .0181 | .0183 | .0185 | .0190 | .0187 | .0187 |
| 3e3m6 | .0001 | .0006 | .0009 | .0009 | .0019 | .0024 | .0027 | .0031 | .0033 | .0035 | .0036 | .0040 | .0043 | .0045 | .0048 | .0052 |
| 3e4RSm6 | .0000 | .0005 | .0009 | .0010 | .0034 | .0060 | .0080 | .0097 | .0109 | .0121 | .0134 | .0139 | .0144 | .0150 | .0157 | .0164 |
| 223RSmmm6 | .0010 | .0038 | .0045 | .0046 | .0051 | .0045 | .0038 | .0033 | .0031 | .0028 | .0028 | .0028 | .0028 | .0027 | .0029 | .0030 |
| 224RSmmm6 | .0055 | .0155 | .0174 | .0175 | .0169 | .0133 | .0103 | .0091 | .0080 | .0073 | .0066 | .0064 | .0065 | .0064 | .0066 | .0068 |
| 225mmm6 | .8649 | .5318 | .4149 | .4105 | .1494 | .0654 | .0362 | .0231 | .0159 | .0121 | .0099 | .0088 | .0080 | .0072 | .0068 | .0066 |
| 233mmm6 | .0002 | .0012 | .0015 | .0015 | .0023 | .0024 | .0025 | .0025 | .0024 | .0025 | .0027 | .0028 | .0029 | .0031 | .0033 | .0036 |
| 23RS4SRmmm6 | .0000 | .0004 | .0007 | .0007 | .0017 | .0025 | .0029 | .0033 | .0035 | .0039 | .0040 | .0042 | .0044 | .0049 | .0050 | .0052 |
| 23RS4RSmmm6 | .0000 | .0005 | .0008 | .0008 | .0019 | .0026 | .0029 | .0033 | .0035 | .0039 | .0040 | .0042 | .0044 | .0047 | .0050 | .0052 |
| 23RS5mmm6 | .0080 | .0254 | .0298 | .0300 | .0314 | .0267 | .0219 | .0200 | .0181 | .0169 | .0156 | .0152 | .0150 | .0150 | .0151 | .0148 |
| 244mmm6 | .0012 | .0050 | .0063 | .0064 | .0083 | .0079 | .0074 | .0068 | .0066 | .0069 | .0066 | .0070 | .0073 | .0075 | .0079 | .0084 |
| 334RSmmm6 | .0000 | .0004 | .0007 | .0007 | .0015 | .0019 | .0023 | .0025 | .0026 | .0028 | .0031 | .0034 | .0036 | .0039 | .0043 | .0046 |
| 33ee5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 |
| 3e22mm5 | .0000 | .0000 | .0001 | .0001 | .0002 | .0003 | .0004 | .0004 | .0005 | .0005 | .0005 | .0006 | .0006 | .0007 | .0007 | .0007 |
| 3e23mm5 | .0000 | .0000 | .0000 | .0000 | .0001 | .0002 | .0003 | .0003 | .0003 | .0004 | .0004 | .0005 | .0005 | .0006 | .0007 | .0007 |
| 3e24mm5 | .0000 | .0000 | .0000 | .0000 | .0002 | .0004 | .0006 | .0008 | .0009 | .0011 | .0012 | .0013 | .0015 | .0017 | .0017 | .0019 |
| 2233mmmm5 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 |
| 223RS4mmmm5 | .0000 | .0001 | .0001 | .0001 | .0002 | .0003 | .0003 | .0003 | .0003 | .0003 | .0004 | .0004 | .0004 | .0004 | .0005 | .0005 |
| 2244mmmm5 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 |
| 2334mmmm5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 |

Table 9 continued

| T/K | 200 | 273 | 298 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| decanes | | | | | | | | | | | | | | | | |
| 10 | .0000 | .0010 | .0023 | .0025 | .0133 | .0266 | .0393 | .0487 | .0532 | .0606 | .0627 | .0643 | .0652 | .0675 | .0674 | .0654 |
| 2m9 | .0002 | .0083 | .0150 | .0154 | .0423 | .0560 | .0598 | .0649 | .0643 | .0641 | .0627 | .0614 | .0625 | .0601 | .0584 | .0572 |
| 3RSm9 | .0001 | .0058 | .0113 | .0118 | .0407 | .0619 | .0770 | .0805 | .0880 | .0896 | .0892 | .0927 | .0912 | .0920 | .0899 | .0885 |
| 4RSm9 | .0001 | .0050 | .0097 | .0101 | .0341 | .0522 | .0651 | .0697 | .0729 | .0758 | .0806 | .0808 | .0804 | .0819 | .0807 | .0800 |
| 5m9 | .0000 | .0025 | .0049 | .0051 | .0175 | .0263 | .0333 | .0340 | .0365 | .0387 | .0399 | .0407 | .0394 | .0393 | .0393 | .0396 |
| 3e8 | .0000 | .0009 | .0019 | .0020 | .0086 | .0151 | .0201 | .0237 | .0266 | .0293 | .0295 | .0309 | .0307 | .0311 | .0317 | .0313 |
| 4RSe8 | .0000 | .0015 | .0032 | .0033 | .0143 | .0255 | .0333 | .0392 | .0469 | .0484 | .0513 | .0536 | .0551 | .0556 | .0563 | .0572 |
| 22mm8 | .0050 | .0326 | .0400 | .0408 | .0387 | .0280 | .0219 | .0166 | .0142 | .0120 | .0113 | .0103 | .0099 | .0094 | .0093 | .0090 |
| 23RSmm8 | .0001 | .0033 | .0059 | .0062 | .0171 | .0229 | .0259 | .0255 | .0266 | .0262 | .0266 | .0258 | .0259 | .0257 | .0256 | .0256 |
| 24RSmm8 | .0008 | .0132 | .0197 | .0202 | .0350 | .0367 | .0362 | .0340 | .0343 | .0328 | .0326 | .0324 | .0320 | .0311 | .0306 | .0313 |
| 25RSmm8 | .0014 | .0262 | .0400 | .0415 | .0708 | .0713 | .0550 | .0604 | .0567 | .0512 | .0487 | .0467 | .0466 | .0441 | .0438 | .0423 |
| 26RSmm8 | .0016 | .0292 | .0450 | .0466 | .0803 | .0813 | .0770 | .0697 | .0643 | .0606 | .0567 | .0561 | .0529 | .0515 | .0506 | .0500 |
| 27mm8 | .0017 | .0296 | .0290 | .0296 | .0407 | .0363 | .0306 | .0274 | .0235 | .0221 | .0197 | .0187 | .0178 | .0174 | .0166 | .0160 |
| 33mm8 | .0005 | .0075 | .0111 | .0114 | .0184 | .0185 | .0170 | .0166 | .0161 | .0158 | .0161 | .0156 | .0163 | .0161 | .0166 | .0171 |
| 3RS4SRmm8 | .0000 | .0007 | .0015 | .0016 | .0057 | .0091 | .0112 | .0124 | .0133 | .0142 | .0146 | .0149 | .0150 | .0155 | .0154 | .0160 |
| 3RS4RSmm8 | .0000 | .0008 | .0016 | .0017 | .0059 | .0092 | .0112 | .0124 | .0133 | .0142 | .0146 | .0149 | .0150 | .0155 | .0154 | .0160 |
| 3RS5RSmm8 | .0002 | .0055 | .0089 | .0092 | .0196 | .0231 | .0238 | .0255 | .0250 | .0248 | .0253 | .0246 | .0249 | .0247 | .0256 | .0256 |
| 3RS5SRmm8 | .0002 | .0045 | .0074 | .0076 | .0167 | .0203 | .0219 | .0221 | .0221 | .0221 | .0229 | .0225 | .0229 | .0228 | .0238 | .0239 |
| 3RS6RSmm8 | .0002 | .0054 | .0090 | .0093 | .0206 | .0238 | .0238 | .0237 | .0221 | .0209 | .0207 | .0196 | .0193 | .0188 | .0185 | .0183 |
| 3R6Smm8 | .0002 | .0054 | .0090 | .0093 | .0206 | .0238 | .0238 | .0237 | .0221 | .0209 | .0207 | .0196 | .0193 | .0188 | .0185 | .0183 |
| 44mm8 | .0004 | .0052 | .0075 | .0077 | .0122 | .0123 | .0122 | .0116 | .0110 | .0113 | .0113 | .0118 | .0122 | .0123 | .0129 | .0135 |
| 4RS5RSmm8 | .0000 | .0003 | .0006 | .0006 | .0023 | .0036 | .0044 | .0049 | .0055 | .0058 | .0059 | .0062 | .0062 | .0064 | .0065 | .0067 |
| 4R5Smm8 | .0000 | .0003 | .0006 | .0006 | .0023 | .0035 | .0044 | .0049 | .0055 | .0058 | .0059 | .0062 | .0065 | .0066 | .0068 | .0067 |
| 4p7 | .0000 | .0002 | .0004 | .0005 | .0019 | .0034 | .0048 | .0056 | .0063 | .0072 | .0076 | .0078 | .0084 | .0083 | .0087 | .0087 |
| 4ip7 | .0000 | .0003 | .0005 | .0005 | .0019 | .0031 | .0038 | .0045 | .0049 | .0052 | .0053 | .0054 | .0057 | .0057 | .0059 | .0060 |
| 3RSe2m7 | .0000 | .0006 | .0012 | .0013 | .0047 | .0076 | .0095 | .0108 | .0118 | .0127 | .0125 | .0130 | .0132 | .0138 | .0139 | .0140 |
| 4RSe2m7 | .0002 | .0038 | .0062 | .0063 | .0140 | .0172 | .0185 | .0191 | .0194 | .0209 | .0207 | .0205 | .0210 | .0211 | .0214 | .0216 |
| 5e2m7 | .0002 | .0045 | .0075 | .0077 | .0173 | .0205 | .0219 | .0205 | .0194 | .0187 | .0187 | .0179 | .0178 | .0174 | .0166 | .0165 |
| 3e3m7 | .0000 | .0002 | .0004 | .0004 | .0012 | .0016 | .0019 | .0021 | .0023 | .0024 | .0025 | .0027 | .0028 | .0029 | .0032 | .0033 |
| 4RSe3RSm7 | .0000 | .0002 | .0003 | .0003 | .0016 | .0030 | .0041 | .0052 | .0059 | .0065 | .0072 | .0075 | .0080 | .0083 | .0084 | .0087 |
| 4RSe3SRm7 | .0000 | .0002 | .0003 | .0003 | .0016 | .0030 | .0041 | .0052 | .0059 | .0065 | .0072 | .0075 | .0080 | .0083 | .0084 | .0087 |
| 3e5RSm7 | .0001 | .0018 | .0033 | .0034 | .0095 | .0131 | .0156 | .0166 | .0171 | .0177 | .0178 | .0187 | .0185 | .0188 | .0192 | .0196 |
| 3e4RSm7 | .0000 | .0002 | .0003 | .0003 | .0016 | .0031 | .0044 | .0052 | .0063 | .0068 | .0076 | .0078 | .0084 | .0087 | .0090 | .0093 |
| 4e4m7 | .0000 | .0001 | .0002 | .0002 | .0007 | .0010 | .0012 | .0013 | .0015 | .0016 | .0018 | .0019 | .0021 | .0022 | .0024 | .0026 |
| 223RSmmm7 | .0001 | .0013 | .0019 | .0020 | .0029 | .0027 | .0025 | .0022 | .0020 | .0019 | .0019 | .0018 | .0018 | .0018 | .0019 | .0019 |
| 224RSmmm7 | .0004 | .0045 | .0060 | .0061 | .0078 | .0067 | .0057 | .0049 | .0046 | .0041 | .0039 | .0039 | .0039 | .0040 | .0041 | .0042 |
| 225RSmmm7 | .0353 | .1276 | .1325 | .1319 | .0813 | .0440 | .0281 | .0191 | .0142 | .0113 | .0097 | .0086 | .0077 | .0072 | .0070 | .0067 |
| 226mmm7 | .0715 | .1621 | .1542 | .1534 | .0745 | .0360 | .0219 | .0143 | .0104 | .0086 | .0072 | .0062 | .0057 | .0055 | .0053 | .0051 |
| 233mmm7 | .0000 | .0004 | .0007 | .0007 | .0014 | .0016 | .0016 | .0017 | .0017 | .0017 | .0018 | .0018 | .0019 | .0020 | .0021 | .0023 |
| 23RS4SRmmm7 | .0000 | .0001 | .0003 | .0003 | .0008 | .0013 | .0016 | .0018 | .0020 | .0022 | .0024 | .0025 | .0026 | .0028 | .0030 | .0031 |
| 23RS4RSmmm7 | .0000 | .0001 | .0003 | .0003 | .0009 | .0013 | .0016 | .0018 | .0020 | .0022 | .0023 | .0025 | .0026 | .0027 | .0029 | .0030 |
| 23RS5RSmmm7 | .0002 | .0034 | .0053 | .0054 | .0093 | .0096 | .0095 | .0087 | .0081 | .0077 | .0076 | .0075 | .0074 | .0074 | .0075 | .0074 |
| 23RS5SRmmm7 | .0002 | .0031 | .0048 | .0050 | .0088 | .0092 | .0087 | .0087 | .0081 | .0077 | .0076 | .0075 | .0074 | .0074 | .0075 | .0076 |
| 23RS6mmm7 | .0012 | .0165 | .0237 | .0238 | .0333 | .0291 | .0238 | .0205 | .0183 | .0167 | .0153 | .0142 | .0138 | .0133 | .0129 | .0126 |
| 244mmm7 | .0001 | .0012 | .0018 | .0018 | .0030 | .0031 | .0032 | .0032 | .0031 | .0031 | .0034 | .0034 | .0038 | .0038 | .0042 | .0045 |
| 24RS5SRmmm7 | .0001 | .0019 | .0030 | .0031 | .0057 | .0062 | .0062 | .0061 | .0059 | .0058 | .0059 | .0057 | .0057 | .0059 | .0061 | .0060 |
| 24RS5RSmmm7 | .0001 | .0021 | .0032 | .0033 | .0060 | .0064 | .0062 | .0061 | .0059 | .0061 | .0059 | .0060 | .0060 | .0061 | .0061 | .0062 |
| 246mmm7 | .0040 | .0191 | .0221 | .0223 | .0191 | .0141 | .0112 | .0093 | .0086 | .0077 | .0076 | .0072 | .0071 | .0072 | .0070 | .0071 |
| 255mmm7 | .0089 | .0481 | .0551 | .0561 | .0456 | .0303 | .0219 | .0166 | .0133 | .0120 | .0102 | .0099 | .0095 | .0090 | .0090 | .0090 |
| 334RSmmm7 | .0000 | .0001 | .0002 | .0003 | .0007 | .0010 | .0013 | .0013 | .0015 | .0016 | .0018 | .0019 | .0020 | .0021 | .0024 | .0026 |
| 335RSmmm7 | .0000 | .0013 | .0020 | .0021 | .0046 | .0054 | .0057 | .0056 | .0059 | .0058 | .0062 | .0062 | .0068 | .0069 | .0075 | .0079 |
| 3RS44mmm7 | .0000 | .0001 | .0002 | .0002 | .0005 | .0008 | .0009 | .0011 | .0012 | .0014 | .0014 | .0016 | .0018 | .0019 | .0021 | .0024 |
| 3RS45RSmmm7 | .0000 | .0000 | .0001 | .0001 | .0003 | .0006 | .0008 | .0010 | .0011 | .0013 | .0014 | .0015 | .0016 | .0018 | .0019 | .0020 |
| s3R45Smmm7 | .0000 | .0000 | .0000 | .0000 | .0002 | .0003 | .0004 | .0005 | .0006 | .0007 | .0007 | .0008 | .0008 | .0009 | .0010 | .0010 |
| r3R45Smmm7 | .0000 | .0000 | .0000 | .0000 | .0002 | .0003 | .0004 | .0005 | .0006 | .0007 | .0007 | .0008 | .0008 | .0009 | .0009 | .0010 |
| 3ip2m6 | .0000 | .0000 | .0000 | .0000 | .0001 | .0002 | .0003 | .0004 | .0005 | .0006 | .0006 | .0007 | .0008 | .0009 | .0009 | .0010 |
| 33ee6 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 |
| 34ee6 | .0000 | .0000 | .0000 | .0000 | .0001 | .0003 | .0005 | .0008 | .0009 | .0011 | .0012 | .0013 | .0014 | .0015 | .0015 | .0016 |
| 3RSe22mm6 | .0000 | .0000 | .0000 | .0000 | .0002 | .0003 | .0004 | .0005 | .0005 | .0005 | .0006 | .0006 | .0006 | .0007 | .0007 | .0008 |
| 4e22mm6 | .0000 | .0007 | .0010 | .0011 | .0017 | .0017 | .0016 | .0014 | .0014 | .0013 | .0012 | .0013 | .0013 | .0013 | .0013 | .0013 |
| 3RSe23mm6 | .0000 | .0000 | .0000 | .0000 | .0001 | .0002 | .0002 | .0003 | .0003 | .0004 | .0004 | .0005 | .0005 | .0006 | .0006 | .0007 |
| 4e23RSmm6 | .0000 | .0000 | .0001 | .0001 | .0003 | .0005 | .0007 | .0009 | .0010 | .0011 | .0013 | .0014 | .0015 | .0016 | .0017 | .0019 |
| 3RSe24SRmm6 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0002 | .0003 | .0004 | .0006 | .0006 | .0007 | .0008 | .0009 | .0010 | .0011 |
| 3RSe24RSmm6 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0002 | .0003 | .0004 | .0006 | .0006 | .0007 | .0008 | .0009 | .0010 | .0011 |
| 4e24mm6 | .0000 | .0000 | .0001 | .0001 | .0003 | .0004 | .0005 | .0005 | .0006 | .0006 | .0007 | .0007 | .0008 | .0009 | .0009 | .0010 |
| 3e25mm6 | .0001 | .0016 | .0024 | .0025 | .0046 | .0051 | .0053 | .0049 | .0049 | .0046 | .0046 | .0045 | .0045 | .0045 | .0046 | .0046 |
| 4e33mm6 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0002 | .0002 | .0003 | .0003 | .0004 | .0004 | .0005 | .0005 | .0006 |
| 3e34RSmm6 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 | .0003 | .0003 | .0003 | .0004 | .0004 |
| 2233mmmm6 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 |
| 223RS4RSmmmm6 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 |
| 223RS4SRmmmm6 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 |
| 223RS5mmmm6 | .0008 | .0039 | .0043 | .0043 | .0032 | .0021 | .0015 | .0012 | .0009 | .0008 | .0007 | .0007 | .0007 | .0007 | .0007 | .0007 |
| 2244mmmm6 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 | .0002 | .0003 |
| 224RS5mmmm6 | .0003 | .0029 | .0037 | .0038 | .0038 | .0028 | .0021 | .0017 | .0014 | .0013 | .0012 | .0011 | .0011 | .0011 | .0011 | .0011 |
| 2255mmmm6 | .8633 | .3998 | .2646 | .2538 | .0439 | .0111 | .0041 | .0019 | .0011 | .0008 | .0006 | .0004 | .0004 | .0003 | .0003 | .0003 |
| 2334RSmmmm6 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 | .0003 |
| 2335mmmm6 | .0000 | .0001 | .0002 | .0002 | .0004 | .0004 | .0004 | .0005 | .0004 | .0005 | .0005 | .0005 | .0006 | .0006 | .0007 | .0008 |
| 23RS44mmmm6 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 | .0003 | .0003 | .0004 | .0004 |
| 23RS4RS5mmmm6 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0003 | .0003 | .0003 | .0003 |
| 23R4S5mmmm6 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 | .0002 | .0002 | .0003 | .0003 | .0003 | .0003 |
| 3344mmmm6 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 |
| 3ip24mm5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 |
| 33ee2m5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 |
| 3e223mmm5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 |
| 3RSe224mmm5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 |
| 3e234mmm5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 |
| 22334mmmmm5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 |
| 22344mmmmm5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 |

## 6. Estimation of Thermodynamic Properties of Alkane Isomer Groups Using the Benson Group Method

Group additivity methods have been quite useful for estimating chemical thermodynamic properties, and Benson and co-workers have calculated group values involving many elements and have extended the method to include non-next-nearest neighbor corrections.[23,24] It is therefore of interest to calculate the thermodynamic properties of alkane isomer groups using the Benson method for comparison with the values calculated from the Scott tables. Since Benson gives values for the contributions to the heat capacity from 300 to 1500 K, his method has been used to calculate standard thermodynamic properties for the temperature range used by Scott even though the values may not be as reliable at 200 K.

In order to make these calculations, the structure of each alkane species must be examined to divide it into C–$(H)_3(C)$, C – $(H)_2(C)_2$, C–(H)$(C)_3$, and C–$(C)_4$ groups and to determine the total symmetry number, number of optical isomers, number of alkane *gauche* corrections, and 1,5H repulsions. The group assignments were checked by matrix multiplication to be sure they accounted for the correct numbers of carbon and hydrogen atoms. The symmetry numbers get to be as high as 19 683 (for 2,2,3,4,4-pentamethylpentane). In calculating symmetry numbers, we have been assisted by a report by Davies, Syverud, and Steiner.[25]

The numbers of *gauche* corrections to be applied to the various alkane isomers were obtained as follows: The usual zig–zag formulas were written for the backbone structure and the branches were added. Each bond not connected to a carbon in a methyl group was examined to see the nature of the bonding of the carbon atoms at each end of the bond. If the carbons at each end are each bonded to just one more carbon atom, the number of *gauche* corrections for that bond is zero. Thus there are no *gauche* corrections for *n*-alkanes. If the carbon atom at one end of the bond is bonded to two other carbon atoms and the carbon atom at the other end of the bond was bonded to one other, the number of *gauche* corrections is one. An example is 2-methylbutane. If the carbon atoms at both ends of the bond are bonded to two additional carbon atoms, the number of *gauche* corrections is 2. An example is 2,3-dimethylbutane. If the carbon atom at one end of the bond is bonded to three other carbon atoms and the carbon atom at the other end of the bond is bonded to one other, the number of *gauche* corrections is 2. An example is 2,2-dimethylbutane. If the carbon atom at one end of the bond is bonded to three other carbon atoms and the one at the other end of the bond is bonded to two, the *gauche* correction is 4. An example is 2,2,3-trimethylbutane. If the carbons at both ends of the bond are bonded to three other carbons, the *gauche* correction is 6. An example is 2,2,3,3-tetramethylbutane. The *gauche* correction for a molecule is the sum of these numbers for the molecule. All the assignments of groups and corrections were made by two people independently.

The matrix of numbers of contributions is then matrix multiplied by a matrix of the Benson values to obtain for each isomer the sum of the contributions to $\Delta_f H^\circ_{298}$, $S^\circ_{\text{int}\,298}$, $C^\circ_{P300}$, $C^\circ_{P400}$, $C^\circ_{P500}$, $C^\circ_{P600}$, $C^\circ_{P800}$, $C_{P1000}$, and $C^\circ_{P1500}$. This matrix is the input to the following four programs:

1. CAPACITY. This program fits the heat capacities by least squares for each isomer to the equation

$$C^\circ_P = \alpha + \beta T + \gamma T^2, \tag{12}$$

and then uses these parameters to calculate $C^\circ_P$ for each isomer at the desired temperatures.

2. ENTROPY. This program uses the $\alpha$, $\beta$, and $\gamma$ parameters calculated in CAPACITY to calculate the standard entropy at the desired temperature using

$$S^\circ = S^\circ_0 + \alpha \ln T + \beta T + (\gamma/2)T^2 - R\ln(\text{TSN/OPT}), \tag{13}$$

where TSN is the total symmetry number and OPT is the number of optical isomers (1 or 2). The quantity $S^\circ_0$ is simply a parameter in this equation and is not to be interpreted literally.

3. ENTHALPY. This program uses the parameters calculated in CAPACITY in the equation

$$\Delta_f H^\circ = \Delta_f H^\circ_0 + \alpha T + (\beta/2)T^2 + (\gamma/3)T^3 - n(H^\circ - H^\circ_{298})_{\text{graph}} - (n+1)(H^\circ - H^\circ_{298})_{H_2}, \tag{14}$$

to calculate $\Delta_f H^\circ$ for each isomer at the desired temperatures. The quantity $\Delta_f H^\circ_0$ is simply a parameter in this equation and is not to be interpreted literally.

4. GIBBS. This program uses the results of the preceding two progams plus values of $S^\circ$ for graphite and hydrogen at the various temperatures to calculate $\Delta_f G^\circ$ for the various isomers at these temperatures using Eq. (9).

The outputs of these four programs are combined in the computer to obtain tables for $C^\circ_P$, $S^\circ$, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ for each isomer with rows for 200, 273.15, 298.15, 300, 400, 500, 600, 700, 800, 900, 1000, 1100, 1200, 1300, 1400, and 1500 K.

The standard thermodynamic properties of the alkane isomer groups calculated using the Benson parameters are given in Tables 10 to 13 along with increments per carbon atom. These values are in quite good agreement with the values calculated from Scott's tables. The values for $CH_4$ are from the Scott table since the properties of $CH_4$ cannot be calculated from Benson groups.

In addition the mole fractions $r_i$ of the individual species within isomer groups were calculated using the Benson parameters, and the results are given in Table 14. This method also indicates that 2255mmmm6 is quite stable at low temperatures.

The isomer group values calculated using the Benson method have been rounded in the same way as the values calculated from Scott's tables. Benson[24] states that the values of $C^\circ_p$ and $S^\circ$ estimated using his group values are on the average within $\pm$ 1.2 J K$^{-1}$ mol$^{-1}$ of the measured values, and $\Delta_f H^\circ$ and $\Delta_f G^\circ$ are within $\pm$ 2 kJ mol$^{-1}$. However, he points out larger errors may be encountered for heavily substituted species.

Table 10. Standard heat capacity at constant pressure for alkane isomer groups in J/K mol calculated using Benson group values

| T/K | methane | ethane | propane | butanes | pentanes | hexanes | heptanes | octanes | nonanes | decanes |
|---|---|---|---|---|---|---|---|---|---|---|
| 200.00 | 33.51 | 38.26 | 55.94 | 77.63 | 99.38 | 131.67 | 164.57 | 197.38 | 292.18 | 337.50 |
| 273.15 | 34.85 | 48.77 | 70.80 | 103.07 | 160.44 | 163.91 | 191.31 | 208.78 | 287.84 | 295.89 |
| 298.15 | 35.69 | 52.24 | 75.71 | 110.75 | 181.15 | 172.10 | 198.31 | 217.38 | 279.20 | 290.05 |
| 300.00 | 35.77 | 52.49 | 76.07 | 111.30 | 182.48 | 172.67 | 198.82 | 218.04 | 278.84 | 289.98 |
| 400.00 | 40.63 | 65.74 | 94.77 | 136.30 | 207.22 | 199.59 | 227.63 | 254.80 | 292.84 | 317.48 |
| 500.00 | 46.53 | 78.02 | 112.04 | 156.17 | 206.81 | 225.41 | 258.63 | 292.03 | 329.34 | 361.77 |
| 600.00 | 52.3 | 89.3 | 127.9 | 174.0 | 218.5 | 251.2 | 289.4 | 327.9 | 368.1 | 406.1 |
| 700.00 | 58.2 | 99.6 | 142.3 | 190.6 | 235.4 | 275.8 | 318.4 | 361.2 | 404.9 | 447.5 |
| 800.00 | 63.6 | 109.0 | 155.3 | 205.9 | 253.0 | 298.5 | 344.9 | 391.5 | 438.7 | 485.1 |
| 900.00 | 68.2 | 117.3 | 166.9 | 219.7 | 269.6 | 318.8 | 368.6 | 418.5 | 468.7 | 518.5 |
| 1000.00 | 72.8 | 124.7 | 177.0 | 231.9 | 284.4 | 336.7 | 389.3 | 442.0 | 494.9 | 547.6 |
| 1100.00 | 77.0 | 131.1 | 185.7 | 242.5 | 297.2 | 352.0 | 406.9 | 461.9 | 517.1 | 572.2 |
| 1200.00 | 80.3 | 136.5 | 193.0 | 251.2 | 307.8 | 364.5 | 421.4 | 478.2 | 535.3 | 592.2 |
| 1300.00 | 83.7 | 140.9 | 198.8 | 258.2 | 316.2 | 374.4 | 432.6 | 490.9 | 549.3 | 607.6 |
| 1400.00 | 87.9 | 144.4 | 203.3 | 263.4 | 322.3 | 381.4 | 440.6 | 499.9 | 559.2 | 618.4 |
| 1500.00 | 87.9 | 146.8 | 206.3 | 266.7 | 326.1 | 385.8 | 445.4 | 505.1 | 564.9 | 624.6 |

Table 10a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 | C9-C8 | C10-C9 |
|---|---|---|---|---|---|---|---|---|---|
| 200.00 | 4.74 | 17.68 | 21.69 | 21.75 | 32.28 | 32.91 | 32.80 | 94.80 | 45.32 |
| 273.15 | 13.91 | 22.04 | 32.27 | 57.37 | 3.48 | 27.39 | 17.47 | 79.06 | 8.05 |
| 298.15 | 16.55 | 23.47 | 35.05 | 70.40 | -9.05 | 26.21 | 19.07 | 61.82 | 10.85 |
| 300.00 | 16.72 | 23.58 | 35.23 | 71.19 | -9.81 | 26.15 | 19.22 | 60.80 | 11.14 |
| 400.00 | 25.12 | 29.02 | 41.54 | 70.92 | -7.64 | 28.05 | 27.17 | 38.04 | 24.64 |
| 500.00 | 31.49 | 34.03 | 44.13 | 50.64 | 18.60 | 33.22 | 33.41 | 37.30 | 32.44 |
| 600.00 | 37.0 | 38.6 | 46.1 | 44.4 | 32.7 | 38.2 | 38.5 | 40.2 | 38.0 |
| 700.00 | 41.5 | 42.7 | 48.3 | 44.8 | 40.4 | 42.6 | 42.8 | 43.7 | 42.6 |
| 800.00 | 45.4 | 46.3 | 50.6 | 47.1 | 45.4 | 46.5 | 46.6 | 47.1 | 46.5 |
| 900.00 | 49.1 | 49.6 | 52.9 | 49.8 | 49.3 | 49.8 | 49.9 | 50.2 | 49.8 |
| 1000.00 | 51.9 | 52.3 | 55.0 | 52.4 | 52.3 | 52.6 | 52.7 | 52.9 | 52.6 |
| 1100.00 | 54.1 | 54.6 | 56.8 | 54.7 | 54.8 | 55.0 | 55.0 | 55.2 | 55.0 |
| 1200.00 | 56.1 | 56.5 | 58.3 | 56.5 | 56.7 | 56.8 | 56.9 | 57.0 | 56.9 |
| 1300.00 | 57.2 | 57.9 | 59.4 | 58.0 | 58.2 | 58.3 | 58.3 | 58.4 | 58.3 |
| 1400.00 | 56.5 | 58.9 | 60.1 | 58.9 | 59.1 | 59.2 | 59.2 | 59.3 | 59.3 |
| 1500.00 | 59.0 | 59.4 | 60.5 | 59.4 | 59.6 | 59.7 | 59.7 | 59.8 | 59.7 |

Table 11. Standard entropy for alkane isomer groups in J/K mol calculated using Benson group values

| T/K | methane | ethane | propane | butanes | pentanes | hexanes | heptanes | octanes | nonanes | decanes |
|---|---|---|---|---|---|---|---|---|---|---|
| 200.00 | 172.70 | 212.64 | 243.90 | 262.07 | 262.94 | 319.23 | 350.32 | 386.29 | 383.30 | 422.28 |
| 273.15 | 183.29 | 226.13 | 263.55 | 290.11 | 302.34 | 365.38 | 405.98 | 448.45 | 477.72 | 523.44 |
| 298.15 | 186.38 | 230.55 | 269.96 | 299.47 | 317.32 | 380.10 | 423.04 | 467.10 | 502.50 | 549.02 |
| 300.00 | 186.59 | 230.87 | 270.43 | 300.16 | 318.44 | 381.16 | 424.26 | 468.45 | 504.23 | 550.82 |
| 400.00 | 197.51 | 247.81 | 294.91 | 335.79 | 376.21 | 434.63 | 485.34 | 536.17 | 585.21 | 637.02 |
| 500.00 | 207.18 | 263.82 | 317.94 | 368.39 | 422.19 | 481.93 | 539.44 | 597.03 | 654.35 | 712.56 |
| 600.00 | 216.0 | 279.1 | 339.8 | 398.5 | 460.8 | 525.3 | 589.3 | 653.5 | 717.8 | 782.5 |
| 700.00 | 224.8 | 293.6 | 360.6 | 426.6 | 495.7 | 565.9 | 636.2 | 706.6 | 777.4 | 848.2 |
| 800.00 | 232.7 | 307.5 | 380.5 | 453.0 | 528.3 | 604.2 | 680.4 | 756.8 | 833.7 | 910.5 |
| 900.00 | 240.7 | 320.9 | 399.4 | 478.1 | 559.1 | 640.6 | 722.5 | 804.5 | 887.1 | 969.6 |
| 1000.00 | 248.2 | 333.6 | 417.6 | 501.9 | 588.3 | 675.1 | 762.4 | 849.9 | 937.9 | 1025.8 |
| 1100.00 | 255.3 | 345.8 | 434.9 | 524.5 | 616.0 | 708.0 | 800.3 | 892.9 | 986.1 | 1079.1 |
| 1200.00 | 262.0 | 357.4 | 451.3 | 546.0 | 642.3 | 739.1 | 836.4 | 933.9 | 1032.0 | 1129.8 |
| 1300.00 | 268.3 | 368.5 | 467.0 | 566.4 | 667.3 | 768.7 | 870.6 | 972.7 | 1075.4 | 1177.9 |
| 1400.00 | 275.0 | 379.1 | 481.9 | 585.7 | 691.0 | 796.7 | 903.0 | 1009.4 | 1116.5 | 1223.3 |
| 1500.00 | 280.9 | 389.2 | 496.1 | 604.0 | 713.3 | 823.2 | 933.5 | 1044.1 | 1155.3 | 1266.2 |

Table 11a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 | C9-C8 | C10-C9 |
|---|---|---|---|---|---|---|---|---|---|
| 200.00 | 39.94 | 31.26 | 18.17 | .87 | 56.29 | 31.09 | 35.97 | -2.99 | 38.98 |
| 273.15 | 42.84 | 37.42 | 26.56 | 12.23 | 63.04 | 40.60 | 42.47 | 29.27 | 45.71 |
| 298.15 | 44.17 | 39.41 | 29.51 | 17.84 | 62.78 | 42.94 | 44.07 | 35.40 | 46.52 |
| 300.00 | 44.28 | 39.56 | 29.73 | 18.28 | 62.72 | 43.10 | 44.18 | 35.78 | 46.59 |
| 400.00 | 50.30 | 47.10 | 40.88 | 40.42 | 58.42 | 50.71 | 50.83 | 49.04 | 51.81 |
| 500.00 | 56.64 | 54.12 | 50.45 | 53.80 | 59.74 | 57.51 | 57.59 | 57.31 | 58.21 |
| 600.00 | 63.1 | 60.7 | 58.7 | 62.3 | 64.5 | 64.0 | 64.1 | 64.4 | 64.6 |
| 700.00 | 68.8 | 67.0 | 66.0 | 69.2 | 70.2 | 70.2 | 70.4 | 70.8 | 70.9 |
| 800.00 | 74.8 | 72.9 | 72.6 | 75.3 | 75.9 | 76.2 | 76.4 | 76.9 | 76.8 |
| 900.00 | 80.2 | 78.6 | 78.6 | 81.0 | 81.5 | 81.9 | 82.1 | 82.6 | 82.5 |
| 1000.00 | 85.4 | 84.0 | 84.3 | 86.4 | 86.9 | 87.3 | 87.5 | 88.0 | 87.9 |
| 1100.00 | 90.5 | 89.1 | 89.6 | 91.5 | 92.0 | 92.4 | 92.6 | 93.2 | 93.0 |
| 1200.00 | 95.4 | 93.9 | 94.7 | 96.3 | 96.8 | 97.3 | 97.5 | 98.1 | 97.9 |
| 1300.00 | 100.2 | 98.5 | 99.4 | 100.9 | 101.4 | 101.9 | 102.1 | 102.7 | 102.5 |
| 1400.00 | 104.1 | 102.8 | 103.8 | 105.2 | 105.8 | 106.2 | 106.4 | 107.1 | 106.8 |
| 1500.00 | 108.3 | 106.9 | 108.0 | 109.3 | 109.9 | 110.3 | 110.5 | 111.2 | 110.9 |

Table 12. Standard enthalpy of formation for alkane isomer groups in kJ/mol calculated using Benson group values

| T/K | methane | ethane | propane | butanes | pentanes | hexanes | heptanes | octanes | nonanes | decanes |
|---|---|---|---|---|---|---|---|---|---|---|
| 200.00 | -71.88 | -80.15 | -99.36 | -127.66 | -159.15 | -169.92 | -190.26 | -209.31 | -239.33 | -257.21 |
| 273.15 | -73.97 | -84.02 | -104.28 | -125.11 | -154.71 | -164.81 | -183.78 | -216.77 | -225.53 | -260.65 |
| 298.15 | -74.73 | -85.35 | -105.98 | -134.89 | -165.47 | -178.24 | -199.13 | -219.66 | -243.85 | -263.44 |
| 300.00 | -74.77 | -85.45 | -106.11 | -135.02 | -165.55 | -178.40 | -199.31 | -219.88 | -244.03 | -263.67 |
| 400.00 | -77.82 | -90.29 | -112.23 | -141.18 | -167.94 | -186.20 | -208.39 | -230.56 | -254.07 | -275.78 |
| 500.00 | -80.67 | -94.52 | -117.56 | -146.46 | -171.51 | -193.39 | -216.77 | -240.14 | -264.20 | -287.28 |
| 600.00 | -83.3 | -98.1 | -122.0 | -150.9 | -175.8 | -199.5 | -223.8 | -248.1 | -272.8 | -296.9 |
| 700.00 | -85.4 | -101.0 | -125.5 | -154.4 | -179.6 | -204.4 | -229.3 | -254.3 | -279.5 | -304.2 |
| 800.00 | -87.0 | -103.3 | -128.2 | -157.0 | -182.5 | -207.8 | -233.2 | -258.5 | -284.1 | -309.2 |
| 900.00 | -88.3 | -104.9 | -130.1 | -158.8 | -184.4 | -210.0 | -235.6 | -261.1 | -286.8 | -312.1 |
| 1000.00 | -89.5 | -106.1 | -131.3 | -159.7 | -185.3 | -211.0 | -236.5 | -262.0 | -287.7 | -313.0 |
| 1100.00 | -90.4 | -106.8 | -131.9 | -159.9 | -185.4 | -210.9 | -236.3 | -261.7 | -287.2 | -312.3 |
| 1200.00 | -90.8 | -107.1 | -132.0 | -159.6 | -184.9 | -210.1 | -235.3 | -260.4 | -285.6 | -310.5 |
| 1300.00 | -91.2 | -107.2 | -131.8 | -158.9 | -183.9 | -208.8 | -233.7 | -258.4 | -283.2 | -307.8 |
| 1400.00 | -91.2 | -107.1 | -131.3 | -158.0 | -182.6 | -207.2 | -231.6 | -256.0 | -280.4 | -304.6 |
| 1500.00 | -91.2 | -106.9 | -130.8 | -157.0 | -181.3 | -205.5 | -229.6 | -253.6 | -277.7 | -301.5 |

Table 12a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 | C9-C8 | C10-C9 |
|---|---|---|---|---|---|---|---|---|---|
| 200.00 | -8.27 | -19.21 | -28.30 | -31.49 | -10.78 | -20.34 | -19.05 | -30.02 | -17.88 |
| 273.15 | -10.05 | -20.26 | -20.83 | -29.60 | -10.10 | -18.97 | -32.99 | -8.75 | -35.12 |
| 298.15 | -10.63 | -20.63 | -28.91 | -30.59 | -12.76 | -20.89 | -20.54 | -24.19 | -19.58 |
| 300.00 | -10.69 | -20.65 | -28.91 | -30.53 | -12.85 | -20.91 | -20.57 | -24.15 | -19.63 |
| 400.00 | -12.46 | -21.95 | -28.95 | -26.76 | -18.26 | -22.19 | -22.17 | -23.52 | -21.71 |
| 500.00 | -13.85 | -23.04 | -28.90 | -25.05 | -21.88 | -23.38 | -23.38 | -24.06 | -23.08 |
| 600.00 | -14.8 | -23.9 | -28.9 | -24.9 | -23.7 | -24.3 | -24.3 | -24.7 | -24.1 |
| 700.00 | -15.6 | -24.6 | -28.9 | -25.2 | -24.8 | -25.0 | -24.9 | -25.2 | -24.7 |
| 800.00 | -16.2 | -25.0 | -28.8 | -25.5 | -25.3 | -25.4 | -25.3 | -25.5 | -25.1 |
| 900.00 | -16.7 | -25.2 | -28.7 | -25.6 | -25.6 | -25.6 | -25.5 | -25.7 | -25.3 |
| 1000.00 | -16.5 | -25.2 | -28.4 | -25.6 | -25.6 | -25.6 | -25.5 | -25.7 | -25.3 |
| 1100.00 | -16.4 | -25.1 | -28.0 | -25.5 | -25.5 | -25.4 | -25.3 | -25.5 | -25.2 |
| 1200.00 | -16.3 | -24.9 | -27.6 | -25.3 | -25.3 | -25.2 | -25.1 | -25.2 | -24.9 |
| 1300.00 | -16.0 | -24.6 | -27.1 | -25.0 | -24.9 | -24.8 | -24.7 | -24.8 | -24.6 |
| 1400.00 | -15.9 | -24.2 | -26.7 | -24.6 | -24.6 | -24.5 | -24.4 | -24.4 | -24.2 |
| 1500.00 | -15.7 | -23.9 | -26.2 | -24.3 | -24.2 | -24.1 | -24.0 | -24.1 | -23.8 |

Table 13. Standard Gibbs energy of formation for alkane isomer groups in kJ/mol calculated using Benson group values

| T/K | methane | ethane | propane | butanes | pentanes | hexanes | heptanes | octanes | nonanes | decanes |
|---|---|---|---|---|---|---|---|---|---|---|
| 200.00 | -58.05 | -49.80 | -50.76 | -58.19 | -65.36 | -62.89 | -64.95 | -66.70 | -71.62 | -72.79 |
| 273.15 | -52.69 | -38.05 | -32.16 | -23.87 | -20.45 | -11.99 | -5.08 | -13.31 | 6.31 | -4.93 |
| 298.15 | -50.68 | -33.78 | -25.49 | -22.52 | -17.75 | -8.56 | -1.58 | 5.42 | 11.35 | 18.57 |
| 300.00 | -50.51 | -33.46 | -24.99 | -21.83 | -16.84 | -7.52 | -.36 | 6.81 | 12.92 | 20.31 |
| 400.00 | -41.96 | -15.38 | 3.01 | 16.88 | 33.12 | 50.66 | 67.36 | 84.04 | 100.08 | 116.81 |
| 500.00 | -32.66 | 3.84 | 32.44 | 57.01 | 83.76 | 110.71 | 137.27 | 163.80 | 189.78 | 216.30 |
| 600.00 | -22.9 | 23.9 | 62.9 | 98.1 | 135.2 | 172.1 | 208.8 | 245.4 | 281.4 | 318.0 |
| 700.00 | -12.5 | 44.4 | 94.0 | 139.9 | 187.4 | 234.5 | 281.3 | 328.1 | 374.3 | 421.0 |
| 800.00 | -2.0 | 65.4 | 125.5 | 182.2 | 240.0 | 297.4 | 354.6 | 411.7 | 468.1 | 525.0 |
| 900.00 | 8.5 | 86.5 | 157.4 | 224.7 | 292.9 | 360.7 | 428.2 | 495.6 | 562.3 | 629.4 |
| 1000.00 | 19.4 | 107.9 | 189.4 | 267.3 | 346.0 | 424.1 | 502.0 | 579.7 | 656.6 | 734.1 |
| 1100.00 | 30.2 | 129.3 | 221.5 | 310.1 | 399.1 | 487.7 | 575.8 | 663.9 | 751.1 | 838.8 |
| 1200.00 | 41.1 | 150.8 | 253.6 | 352.8 | 452.3 | 551.2 | 649.7 | 748.0 | 845.5 | 943.5 |
| 1300.00 | 52.4 | 172.3 | 285.7 | 395.5 | 505.3 | 614.6 | 723.3 | 831.9 | 939.6 | 1047.8 |
| 1400.00 | 63.3 | 193.8 | 317.8 | 438.1 | 558.3 | 677.8 | 796.9 | 915.7 | 1033.5 | 1152.0 |
| 1500.00 | 74.2 | 215.3 | 349.9 | 480.6 | 611.2 | 741.0 | 870.3 | 999.3 | 1127.3 | 1255.9 |

Table 13a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 | C9-C8 | C10-C9 |
|---|---|---|---|---|---|---|---|---|---|
| 200.00 | 8.26 | -.96 | -7.43 | -7.16 | 2.46 | -2.06 | -1.75 | -4.92 | -1.17 |
| 273.15 | 14.64 | 5.89 | 8.29 | 3.43 | 9.05 | 6.31 | -8.23 | 19.62 | -11.24 |
| 298.15 | 16.90 | 8.30 | 2.97 | 4.77 | 9.19 | 6.98 | 7.00 | 5.93 | 7.22 |
| 300.00 | 17.05 | 8.47 | 3.16 | 4.98 | 9.33 | 7.15 | 7.17 | 6.11 | 7.39 |
| 400.00 | 26.58 | 18.39 | 13.87 | 16.24 | 17.54 | 16.70 | 16.67 | 16.04 | 16.74 |
| 500.00 | 36.51 | 28.60 | 24.57 | 26.75 | 26.95 | 26.56 | 26.53 | 25.98 | 26.51 |
| 600.00 | 46.8 | 39.0 | 35.3 | 37.1 | 36.9 | 36.6 | 36.6 | 36.1 | 36.5 |
| 700.00 | 56.9 | 49.6 | 46.0 | 47.4 | 47.1 | 46.9 | 46.8 | 46.2 | 46.7 |
| 800.00 | 67.4 | 60.2 | 56.6 | 57.8 | 57.4 | 57.2 | 57.1 | 56.5 | 56.9 |
| 900.00 | 78.1 | 70.8 | 67.3 | 68.2 | 67.8 | 67.5 | 67.4 | 66.7 | 67.2 |
| 1000.00 | 88.5 | 81.5 | 78.0 | 78.7 | 78.2 | 77.8 | 77.7 | 77.0 | 77.5 |
| 1100.00 | 99.1 | 92.2 | 88.6 | 89.1 | 88.5 | 88.2 | 88.0 | 87.2 | 87.7 |
| 1200.00 | 109.7 | 102.8 | 99.2 | 99.5 | 98.9 | 98.5 | 98.3 | 97.5 | 98.0 |
| 1300.00 | 119.9 | 113.4 | 109.7 | 109.9 | 109.2 | 108.8 | 108.6 | 107.7 | 108.2 |
| 1400.00 | 130.5 | 124.1 | 120.2 | 120.2 | 119.5 | 119.0 | 118.8 | 117.8 | 118.4 |
| 1500.00 | 141.1 | 134.6 | 130.7 | 130.6 | 129.8 | 129.3 | 129.0 | 128.0 | 128.6 |

Table 14. Equilibrium mole fractions within alkane isomer groups calculated using Benson group values

| T/K | 200 | 273 | 298 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| butanes | | | | | | | | | | | | | | | | |
| 4 | .0204 | .0854 | .1166 | .1190 | .2574 | .3795 | .4717 | .5390 | .5884 | .6253 | .6536 | .6758 | .6934 | .7078 | .7196 | .7295 |
| 2m3 | .9796 | .9146 | .8834 | .8810 | .7426 | .6205 | .5283 | .4610 | .4116 | .3747 | .3464 | .3242 | .3066 | .2922 | .2804 | .2705 |
| pentanes | | | | | | | | | | | | | | | | |
| 5 | .0005 | .0140 | .0281 | .0294 | .1351 | .2430 | .3200 | .3739 | .4129 | .4422 | .4648 | .4827 | .4971 | .5090 | .5188 | .5271 |
| 2m4 | .0094 | .1026 | .1654 | .1705 | .4275 | .5329 | .5497 | .5398 | .5240 | .5082 | .4940 | .4819 | .4715 | .4626 | .4550 | .4485 |
| 22mm3 | .9901 | .8834 | .8065 | .8001 | .4374 | .2241 | .1303 | .0863 | .0631 | .0497 | .0411 | .0354 | .0314 | .0284 | .0262 | .0244 |
| hexanes | | | | | | | | | | | | | | | | |
| 6 | .0039 | .0271 | .0403 | .0414 | .1047 | .1636 | .2101 | .2457 | .2731 | .2943 | .3111 | .3246 | .3355 | .3445 | .3520 | .3584 |
| 2m5 | .0742 | .1996 | .2374 | .2400 | .3312 | .3588 | .3609 | .3548 | .3465 | .3382 | .3307 | .3240 | .3182 | .3131 | .3087 | .3049 |
| 3m5 | .0099 | .0457 | .0615 | .0627 | .1211 | .1604 | .1845 | .1996 | .2095 | .2162 | .2211 | .2247 | .2275 | .2297 | .2316 | .2331 |
| 22mm4 | .5555 | .3605 | .3110 | .3077 | .1811 | .1206 | .0894 | .0718 | .0611 | .0540 | .0492 | .0458 | .0433 | .0414 | .0400 | .0388 |
| 23mm4 | .3566 | .3670 | .3497 | .3482 | .2619 | .1967 | .1550 | .1281 | .1099 | .0972 | .0879 | .0809 | .0754 | .0711 | .0677 | .0648 |
| heptanes | | | | | | | | | | | | | | | | |
| 7 | .0020 | .0158 | .0237 | .0244 | .0631 | .1003 | .1307 | .1547 | .1734 | .1882 | .2000 | .2094 | .2171 | .2234 | .2287 | .2331 |
| 2m6 | .0385 | .1162 | .1398 | .1414 | .1996 | .2199 | .2246 | .2233 | .2201 | .2163 | .2125 | .2091 | .2059 | .2031 | .2006 | .1983 |
| 3RSm6 | .0103 | .0532 | .0725 | .0739 | .1459 | .1966 | .2296 | .2513 | .2661 | .2766 | .2842 | .2900 | .2944 | .2980 | .3009 | .3033 |
| 3e5 | .0002 | .0020 | .0031 | .0032 | .0089 | .0146 | .0196 | .0236 | .0268 | .0295 | .0317 | .0335 | .0351 | .0364 | .0376 | .0386 |
| 22mm5 | .2879 | .2099 | .1832 | .1813 | .1091 | .0739 | .0556 | .0452 | .0388 | .0346 | .0317 | .0296 | .0280 | .0269 | .0260 | .0252 |
| 23RSmm5 | .0988 | .1958 | .2135 | .2145 | .2307 | .2156 | .1972 | .1814 | .1688 | .1589 | .1510 | .1447 | .1396 | .1354 | .1319 | .1290 |
| 24mm5 | .1848 | .2137 | .2059 | .2052 | .1578 | .1206 | .0964 | .0806 | .0698 | .0621 | .0565 | .0522 | .0488 | .0461 | .0440 | .0422 |
| 33mm5 | .0077 | .0165 | .0185 | .0186 | .0219 | .0222 | .0218 | .0215 | .0213 | .0212 | .0212 | .0213 | .0215 | .0217 | .0219 | .0221 |
| 223mmm4 | .3698 | .1768 | .1398 | .1375 | .0631 | .0362 | .0244 | .0184 | .0149 | .0127 | .0112 | .0102 | .0095 | .0090 | .0085 | .0082 |
| octanes | | | | | | | | | | | | | | | | |
| 8 | .0012 | .0094 | .0141 | .0144 | .0377 | .0609 | .0806 | .0964 | .1089 | .1188 | .1267 | .1331 | .1383 | .1425 | .1460 | .1489 |
| 2m7 | .0240 | .0693 | .0829 | .0839 | .1192 | .1337 | .1384 | .1391 | .1382 | .1365 | .1347 | .1329 | .1312 | .1295 | .1281 | .1267 |
| 3RSm7 | .0064 | .0317 | .0430 | .0438 | .0872 | .1195 | .1415 | .1566 | .1671 | .1746 | .1801 | .1843 | .1875 | .1901 | .1921 | .1938 |
| 4m7 | .0032 | .0159 | .0215 | .0219 | .0436 | .0597 | .0708 | .0783 | .0835 | .0873 | .0901 | .0922 | .0938 | .0950 | .0961 | .0969 |
| 3e6 | .0004 | .0036 | .0056 | .0057 | .0159 | .0267 | .0362 | .0440 | .0505 | .0558 | .0602 | .0639 | .0670 | .0697 | .0721 | .0741 |
| 22mm6 | .1799 | .1252 | .1086 | .1075 | .0652 | .0449 | .0343 | .0282 | .0243 | .0218 | .0201 | .0188 | .0179 | .0171 | .0166 | .0161 |
| 23RSmm6 | .0617 | .1168 | .1266 | .1272 | .1378 | .1310 | .1216 | .1130 | .1060 | .1003 | .0957 | .0920 | .0889 | .0864 | .0842 | .0824 |
| 24RSmm6 | .0617 | .1168 | .1266 | .1272 | .1378 | .1310 | .1216 | .1130 | .1060 | .1003 | .0957 | .0920 | .0889 | .0864 | .0842 | .0824 |
| 25mm6 | .1155 | .1274 | .1221 | .1217 | .0943 | .0733 | .0594 | .0502 | .0438 | .0392 | .0358 | .0332 | .0311 | .0294 | .0281 | .0270 |
| 33mm6 | .0096 | .0197 | .0219 | .0220 | .0261 | .0269 | .0269 | .0268 | .0267 | .0268 | .0269 | .0271 | .0274 | .0277 | .0280 | .0282 |
| 3RS4RSmm6 | .0041 | .0134 | .0164 | .0166 | .0252 | .0293 | .0311 | .0318 | .0320 | .0321 | .0320 | .0319 | .0318 | .0317 | .0316 | .0315 |
| 3R4Smm6 | .0021 | .0067 | .0082 | .0083 | .0126 | .0146 | .0155 | .0159 | .0160 | .0160 | .0160 | .0160 | .0159 | .0158 | .0158 | .0158 |
| 3e2m5 | .0041 | .0134 | .0164 | .0166 | .0252 | .0293 | .0311 | .0318 | .0320 | .0321 | .0320 | .0319 | .0318 | .0317 | .0316 | .0315 |
| 3e3m5 | .0001 | .0003 | .0005 | .0005 | .0012 | .0018 | .0023 | .0028 | .0033 | .0036 | .0040 | .0043 | .0047 | .0050 | .0052 | .0055 |
| 223RSmmm5 | .0617 | .0483 | .0430 | .0426 | .0275 | .0197 | .0154 | .0129 | .0113 | .0102 | .0095 | .0090 | .0087 | .0084 | .0082 | .0080 |
| 224mmm5 | .0397 | .0290 | .0254 | .0252 | .0156 | .0109 | .0084 | .0069 | .0060 | .0054 | .0050 | .0047 | .0045 | .0044 | .0042 | .0041 |
| 233mmm5 | .0124 | .0166 | .0167 | .0167 | .0151 | .0132 | .0118 | .0109 | .0102 | .0098 | .0096 | .0094 | .0093 | .0092 | .0092 | .0092 |
| 234mmm5 | .2966 | .2147 | .1864 | .1845 | .1090 | .0718 | .0522 | .0408 | .0336 | .0288 | .0254 | .0230 | .0211 | .0196 | .0185 | .0175 |
| 2233mmmm4 | .1155 | .0218 | .0141 | .0137 | .0038 | .0017 | .0010 | .0007 | .0005 | .0004 | .0004 | .0003 | .0003 | .0003 | .0003 | .0003 |
| nonanes | | | | | | | | | | | | | | | | |
| 9 | .0001 | .0031 | .0054 | .0056 | .0186 | .0325 | .0445 | .0543 | .0622 | .0685 | .0735 | .0776 | .0808 | .0835 | .0857 | .0875 |
| 2m8 | .0022 | .0229 | .0319 | .0325 | .0588 | .0712 | .0765 | .0785 | .0789 | .0787 | .0781 | .0774 | .0767 | .0759 | .0751 | .0744 |
| 3RSm8 | .0006 | .0105 | .0165 | .0170 | .0430 | .0637 | .0782 | .0883 | .0955 | .1006 | .1045 | .1074 | .1096 | .1114 | .1127 | .1138 |
| 4RSm8 | .0006 | .0105 | .0165 | .0170 | .0430 | .0637 | .0782 | .0883 | .0955 | .1006 | .1045 | .1074 | .1096 | .1114 | .1127 | .1138 |
| 3e7 | .0000 | .0012 | .0021 | .0022 | .0079 | .0142 | .0200 | .0248 | .0289 | .0322 | .0349 | .0372 | .0392 | .0409 | .0423 | .0435 |
| 4e7 | .0000 | .0012 | .0021 | .0022 | .0079 | .0142 | .0200 | .0248 | .0289 | .0322 | .0349 | .0372 | .0392 | .0409 | .0423 | .0435 |
| 22mm7 | .0166 | .0413 | .0418 | .0417 | .0322 | .0239 | .0189 | .0159 | .0139 | .0126 | .0116 | .0110 | .0104 | .0100 | .0097 | .0095 |
| 23RSmm7 | .0057 | .0386 | .0487 | .0494 | .0680 | .0698 | .0671 | .0637 | .0606 | .0578 | .0555 | .0536 | .0520 | .0506 | .0494 | .0484 |
| 24RSmm7 | .0057 | .0386 | .0487 | .0494 | .0680 | .0698 | .0671 | .0637 | .0606 | .0578 | .0555 | .0536 | .0520 | .0506 | .0494 | .0484 |
| 25RSmm7 | .0057 | .0386 | .0487 | .0494 | .0680 | .0698 | .0671 | .0637 | .0606 | .0578 | .0555 | .0536 | .0520 | .0506 | .0494 | .0484 |
| 26mm7 | .0107 | .0421 | .0470 | .0472 | .0465 | .0390 | .0328 | .0283 | .0250 | .0226 | .0208 | .0193 | .0182 | .0172 | .0165 | .0158 |
| 33mm7 | .0009 | .0065 | .0084 | .0085 | .0129 | .0143 | .0149 | .0151 | .0153 | .0154 | .0156 | .0158 | .0160 | .0162 | .0164 | .0166 |
| 3RS4SRmm7 | .0008 | .0088 | .0126 | .0129 | .0249 | .0312 | .0343 | .0359 | .0366 | .0370 | .0371 | .0372 | .0372 | .0371 | .0371 | .0370 |
| 3RS4RSmm7 | .0008 | .0088 | .0126 | .0129 | .0249 | .0312 | .0343 | .0359 | .0366 | .0370 | .0371 | .0372 | .0372 | .0371 | .0371 | .0370 |
| 3RS5RSmm7 | .0008 | .0088 | .0126 | .0129 | .0249 | .0312 | .0343 | .0359 | .0366 | .0370 | .0371 | .0372 | .0372 | .0371 | .0371 | .0370 |
| 3R5Smm7 | .0004 | .0044 | .0063 | .0064 | .0124 | .0156 | .0172 | .0179 | .0183 | .0185 | .0186 | .0186 | .0186 | .0186 | .0185 | .0185 |
| 44mm7 | .0004 | .0033 | .0042 | .0043 | .0064 | .0072 | .0074 | .0075 | .0076 | .0077 | .0078 | .0079 | .0080 | .0081 | .0082 | .0083 |
| 3RSe2m6 | .0008 | .0088 | .0126 | .0129 | .0249 | .0312 | .0343 | .0359 | .0366 | .0370 | .0371 | .0372 | .0372 | .0371 | .0371 | .0370 |
| 4e2m6 | .0004 | .0044 | .0063 | .0064 | .0124 | .0156 | .0172 | .0179 | .0183 | .0185 | .0186 | .0186 | .0186 | .0186 | .0185 | .0185 |
| 3e3m6 | .0000 | .0003 | .0006 | .0006 | .0017 | .0029 | .0039 | .0048 | .0056 | .0063 | .0070 | .0076 | .0082 | .0087 | .0092 | .0097 |
| 3e4RSm6 | .0001 | .0020 | .0033 | .0034 | .0091 | .0139 | .0175 | .0202 | .0221 | .0236 | .0248 | .0258 | .0266 | .0272 | .0278 | .0283 |
| 223RSmmm6 | .0057 | .0160 | .0165 | .0165 | .0136 | .0105 | .0085 | .0073 | .0065 | .0059 | .0055 | .0053 | .0051 | .0049 | .0048 | .0047 |
| 224RSmmm6 | .0427 | .0696 | .0638 | .0633 | .0372 | .0235 | .0166 | .0129 | .0107 | .0092 | .0083 | .0076 | .0071 | .0067 | .0064 | .0062 |
| 225mmm6 | .1598 | .1520 | .1231 | .1211 | .0509 | .0262 | .0163 | .0115 | .0088 | .0072 | .0062 | .0055 | .0050 | .0046 | .0043 | .0040 |
| 233mmm6 | .0011 | .0055 | .0064 | .0065 | .0075 | .0070 | .0065 | .0061 | .0059 | .0057 | .0055 | .0055 | .0054 | .0054 | .0054 | .0054 |
| 23RS4SRmmm6 | .0073 | .0325 | .0372 | .0374 | .0393 | .0342 | .0295 | .0259 | .0232 | .0212 | .0197 | .0186 | .0176 | .0169 | .0163 | .0158 |
| 23RS4RSmmm6 | .0073 | .0325 | .0372 | .0374 | .0393 | .0342 | .0295 | .0259 | .0232 | .0212 | .0197 | .0186 | .0176 | .0169 | .0163 | .0158 |
| 23RS5mmm6 | .0548 | .1418 | .1434 | .1432 | .1076 | .0765 | .0577 | .0460 | .0384 | .0332 | .0295 | .0268 | .0246 | .0230 | .0217 | .0206 |
| 244mmm6 | .0086 | .0239 | .0248 | .0248 | .0204 | .0157 | .0128 | .0109 | .0097 | .0089 | .0083 | .0079 | .0076 | .0074 | .0072 | .0071 |
| 334RSmmm6 | .0003 | .0025 | .0033 | .0034 | .0055 | .0063 | .0067 | .0069 | .0071 | .0072 | .0074 | .0076 | .0078 | .0079 | .0081 | .0083 |
| 33ee5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0002 | .0002 | .0003 | .0003 | .0003 | .0004 | .0004 | .0005 |
| 3e22mm5 | .0004 | .0018 | .0021 | .0022 | .0025 | .0023 | .0022 | .0020 | .0020 | .0019 | .0018 | .0018 | .0018 | .0018 | .0018 | .0018 |
| 3e23mm5 | .0000 | .0003 | .0004 | .0004 | .0010 | .0014 | .0017 | .0019 | .0021 | .0023 | .0025 | .0026 | .0028 | .0029 | .0030 | .0032 |
| 3e24mm5 | .0037 | .0162 | .0186 | .0187 | .0197 | .0171 | .0147 | .0129 | .0116 | .0106 | .0099 | .0093 | .0088 | .0084 | .0081 | .0079 |
| 2233mmmm5 | .0011 | .0023 | .0022 | .0022 | .0015 | .0011 | .0008 | .0007 | .0006 | .0006 | .0006 | .0005 | .0005 | .0005 | .0005 | .0005 |
| 223RS4mmmm5 | .0548 | .0587 | .0487 | .0480 | .0215 | .0115 | .0073 | .0052 | .0041 | .0034 | .0029 | .0026 | .0024 | .0022 | .0021 | .0020 |
| 2244mmmm5 | .5982 | .1373 | .0806 | .0776 | .0139 | .0044 | .0020 | .0012 | .0008 | .0006 | .0005 | .0004 | .0003 | .0003 | .0003 | .0003 |
| 2334mmmm5 | .0007 | .0023 | .0025 | .0025 | .0022 | .0017 | .0014 | .0012 | .0011 | .0010 | .0010 | .0009 | .0009 | .0009 | .0009 | .0009 |

Table 14 continued

| T/K | 200 | 273 | 298 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| decanes | | | | | | | | | | | | | | | | |
| 10 | .0001 | .0021 | .0035 | .0036 | .0113 | .0197 | .0271 | .0332 | .0381 | .0421 | .0453 | .0478 | .0499 | .0515 | .0529 | .0540 |
| 2m9 | .0020 | .0155 | .0207 | .0210 | .0358 | .0431 | .0465 | .0479 | .0484 | .0484 | .0481 | .0477 | .0473 | .0468 | .0464 | .0459 |
| 3RSm9 | .0005 | .0071 | .0107 | .0110 | .0262 | .0386 | .0475 | .0539 | .0585 | .0619 | .0643 | .0662 | .0676 | .0687 | .0695 | .0702 |
| 4RSm9 | .0005 | .0071 | .0107 | .0110 | .0262 | .0386 | .0475 | .0539 | .0585 | .0619 | .0643 | .0662 | .0676 | .0687 | .0695 | .0702 |
| 5m9 | .0003 | .0036 | .0054 | .0055 | .0131 | .0193 | .0238 | .0270 | .0293 | .0309 | .0322 | .0331 | .0338 | .0344 | .0348 | .0351 |
| 3e8 | .0000 | .0008 | .0014 | .0014 | .0048 | .0086 | .0121 | .0152 | .0177 | .0198 | .0215 | .0230 | .0242 | .0252 | .0261 | .0268 |
| 4RSe8 | .0001 | .0016 | .0028 | .0029 | .0096 | .0172 | .0243 | .0303 | .0354 | .0396 | .0430 | .0459 | .0483 | .0504 | .0522 | .0537 |
| 22mm8 | .0147 | .0280 | .0271 | .0270 | .0196 | .0145 | .0115 | .0097 | .0085 | .0077 | .0072 | .0068 | .0064 | .0062 | .0060 | .0058 |
| 23RSmm8 | .0050 | .0261 | .0316 | .0319 | .0414 | .0423 | .0408 | .0389 | .0371 | .0355 | .0342 | .0330 | .0321 | .0312 | .0305 | .0299 |
| 24RSmm8 | .0050 | .0261 | .0316 | .0319 | .0414 | .0423 | .0408 | .0389 | .0371 | .0355 | .0342 | .0330 | .0321 | .0312 | .0305 | .0299 |
| 25RSmm8 | .0050 | .0261 | .0316 | .0319 | .0414 | .0423 | .0408 | .0389 | .0371 | .0355 | .0342 | .0330 | .0321 | .0312 | .0305 | .0299 |
| 26RSmm8 | .0050 | .0261 | .0316 | .0319 | .0414 | .0423 | .0408 | .0389 | .0371 | .0355 | .0342 | .0330 | .0321 | .0312 | .0305 | .0299 |
| 27mm8 | .0094 | .0285 | .0305 | .0305 | .0283 | .0236 | .0200 | .0173 | .0154 | .0139 | .0128 | .0119 | .0112 | .0106 | .0102 | .0098 |
| 33mm8 | .0008 | .0044 | .0055 | .0055 | .0079 | .0087 | .0090 | .0092 | .0094 | .0095 | .0096 | .0097 | .0099 | .0100 | .0101 | .0102 |
| 3RS4SRmm8 | .0007 | .0060 | .0082 | .0083 | .0151 | .0189 | .0209 | .0219 | .0224 | .0227 | .0229 | .0229 | .0229 | .0229 | .0229 | .0228 |
| 3RS4RSmm8 | .0007 | .0060 | .0082 | .0083 | .0151 | .0189 | .0209 | .0219 | .0224 | .0227 | .0229 | .0229 | .0229 | .0229 | .0229 | .0228 |
| 3RS5RSmm8 | .0007 | .0060 | .0082 | .0083 | .0151 | .0189 | .0209 | .0219 | .0224 | .0227 | .0229 | .0229 | .0229 | .0229 | .0229 | .0228 |
| 3RS5SRmm8 | .0007 | .0060 | .0082 | .0083 | .0151 | .0189 | .0209 | .0219 | .0224 | .0227 | .0229 | .0229 | .0229 | .0229 | .0229 | .0228 |
| 3RS6RSmm8 | .0003 | .0030 | .0041 | .0042 | .0076 | .0095 | .0104 | .0110 | .0112 | .0114 | .0114 | .0115 | .0115 | .0115 | .0114 | .0114 |
| 3RS6SRmm8 | .0002 | .0015 | .0020 | .0021 | .0038 | .0047 | .0052 | .0055 | .0056 | .0057 | .0057 | .0057 | .0057 | .0057 | .0057 | .0057 |
| 44mm8 | .0008 | .0044 | .0055 | .0055 | .0079 | .0087 | .0090 | .0092 | .0094 | .0095 | .0096 | .0097 | .0099 | .0100 | .0101 | .0102 |
| 4RS5RSmm8 | .0003 | .0030 | .0041 | .0042 | .0076 | .0095 | .0104 | .0110 | .0112 | .0114 | .0114 | .0115 | .0115 | .0115 | .0114 | .0114 |
| 4R5Smm8 | .0003 | .0030 | .0041 | .0042 | .0076 | .0095 | .0104 | .0110 | .0112 | .0114 | .0114 | .0115 | .0115 | .0115 | .0114 | .0114 |
| 4p7 | .0000 | .0003 | .0005 | .0005 | .0016 | .0029 | .0040 | .0051 | .0059 | .0066 | .0072 | .0077 | .0081 | .0084 | .0087 | .0089 |
| 4ip7 | .0003 | .0030 | .0041 | .0042 | .0076 | .0095 | .0104 | .0110 | .0112 | .0114 | .0114 | .0115 | .0115 | .0115 | .0114 | .0114 |
| 3RSe2m7 | .0007 | .0060 | .0082 | .0083 | .0151 | .0189 | .0209 | .0219 | .0224 | .0227 | .0229 | .0229 | .0229 | .0229 | .0229 | .0228 |
| 4RSe2m7 | .0007 | .0060 | .0082 | .0083 | .0151 | .0189 | .0209 | .0219 | .0224 | .0227 | .0229 | .0229 | .0229 | .0229 | .0229 | .0228 |
| 5e2m7 | .0003 | .0030 | .0041 | .0042 | .0076 | .0095 | .0104 | .0110 | .0112 | .0114 | .0114 | .0115 | .0115 | .0115 | .0114 | .0114 |
| 3e3m7 | .0000 | .0002 | .0004 | .0004 | .0010 | .0017 | .0024 | .0029 | .0034 | .0039 | .0043 | .0047 | .0050 | .0054 | .0057 | .0060 |
| 4RSe3RSm7 | .0001 | .0014 | .0021 | .0022 | .0055 | .0084 | .0107 | .0123 | .0136 | .0145 | .0153 | .0159 | .0164 | .0168 | .0172 | .0175 |
| 4RSe3SRm7 | .0001 | .0014 | .0021 | .0022 | .0055 | .0084 | .0107 | .0123 | .0136 | .0145 | .0153 | .0159 | .0164 | .0168 | .0172 | .0175 |
| 3e5RSm7 | .0001 | .0014 | .0021 | .0022 | .0055 | .0084 | .0107 | .0123 | .0136 | .0145 | .0153 | .0159 | .0164 | .0168 | .0172 | .0175 |
| 3e4RSm7 | .0001 | .0014 | .0021 | .0022 | .0055 | .0084 | .0107 | .0123 | .0136 | .0145 | .0153 | .0159 | .0164 | .0168 | .0172 | .0175 |
| 4e4m7 | .0000 | .0002 | .0004 | .0004 | .0010 | .0017 | .0024 | .0029 | .0034 | .0039 | .0043 | .0047 | .0050 | .0054 | .0057 | .0060 |
| 223RSmmm7 | .0050 | .0108 | .0107 | .0107 | .0083 | .0064 | .0052 | .0044 | .0040 | .0036 | .0034 | .0032 | .0031 | .0030 | .0030 | .0029 |
| 224RSmmm7 | .0009 | .0030 | .0033 | .0033 | .0034 | .0031 | .0029 | .0027 | .0025 | .0025 | .0024 | .0024 | .0023 | .0023 | .0023 | .0023 |
| 225RSmmm7 | .0009 | .0030 | .0033 | .0033 | .0034 | .0031 | .0029 | .0027 | .0025 | .0025 | .0024 | .0024 | .0023 | .0023 | .0023 | .0023 |
| 226mmm7 | .1409 | .1031 | .0798 | .0783 | .0310 | .0159 | .0099 | .0070 | .0054 | .0044 | .0038 | .0034 | .0031 | .0028 | .0026 | .0025 |
| 233mmm7 | .0010 | .0037 | .0042 | .0042 | .0045 | .0043 | .0040 | .0037 | .0036 | .0035 | .0034 | .0034 | .0033 | .0033 | .0033 | .0033 |
| 23RS4SRmmm7 | .0065 | .0220 | .0241 | .0242 | .0239 | .0207 | .0179 | .0158 | .0142 | .0131 | .0122 | .0114 | .0109 | .0104 | .0100 | .0097 |
| 23RS4RSmmm7 | .0065 | .0220 | .0241 | .0242 | .0239 | .0207 | .0179 | .0158 | .0142 | .0131 | .0122 | .0114 | .0109 | .0104 | .0100 | .0097 |
| 23RS5RSmmm7 | .0065 | .0220 | .0241 | .0242 | .0239 | .0207 | .0179 | .0158 | .0142 | .0131 | .0122 | .0114 | .0109 | .0104 | .0100 | .0097 |
| 23RS5SRmmm7 | .0065 | .0220 | .0241 | .0242 | .0239 | .0207 | .0179 | .0158 | .0142 | .0131 | .0122 | .0114 | .0109 | .0104 | .0100 | .0097 |
| 23RS6mmm7 | .0483 | .0961 | .0930 | .0926 | .0655 | .0464 | .0351 | .0281 | .0236 | .0204 | .0182 | .0165 | .0152 | .0142 | .0134 | .0127 |
| 244mmm7 | .0002 | .0010 | .0013 | .0013 | .0019 | .0021 | .0022 | .0023 | .0023 | .0024 | .0024 | .0024 | .0025 | .0025 | .0026 | .0026 |
| 24RS5SRmmm7 | .0065 | .0220 | .0241 | .0242 | .0239 | .0207 | .0179 | .0158 | .0142 | .0131 | .0122 | .0114 | .0109 | .0104 | .0100 | .0097 |
| 24RS5RSmmm7 | .0065 | .0220 | .0241 | .0242 | .0239 | .0207 | .0179 | .0158 | .0142 | .0131 | .0122 | .0114 | .0109 | .0104 | .0100 | .0097 |
| 246mmm7 | .0242 | .0481 | .0465 | .0463 | .0328 | .0232 | .0175 | .0141 | .0118 | .0102 | .0091 | .0082 | .0076 | .0071 | .0067 | .0064 |
| 255mmm7 | .0075 | .0162 | .0161 | .0160 | .0124 | .0095 | .0078 | .0067 | .0059 | .0054 | .0051 | .0049 | .0047 | .0045 | .0044 | .0044 |
| 334RSmmm7 | .0003 | .0017 | .0022 | .0022 | .0033 | .0038 | .0041 | .0042 | .0043 | .0045 | .0046 | .0047 | .0048 | .0049 | .0050 | .0051 |
| 335RSmmm7 | .0000 | .0005 | .0007 | .0007 | .0014 | .0019 | .0023 | .0025 | .0028 | .0030 | .0032 | .0034 | .0036 | .0037 | .0039 | .0040 |
| 3RS44mmm7 | .0003 | .0017 | .0022 | .0022 | .0033 | .0038 | .0041 | .0042 | .0043 | .0045 | .0046 | .0047 | .0048 | .0049 | .0050 | .0051 |
| 3RS45RSmmm7 | .0009 | .0050 | .0062 | .0063 | .0088 | .0093 | .0092 | .0089 | .0086 | .0083 | .0081 | .0079 | .0078 | .0076 | .0075 | .0074 |
| s3R45Smmm7 | .0004 | .0025 | .0031 | .0032 | .0044 | .0046 | .0046 | .0044 | .0043 | .0042 | .0041 | .0040 | .0039 | .0038 | .0038 | .0037 |
| r3R45Smmm7 | .0004 | .0025 | .0031 | .0032 | .0044 | .0046 | .0046 | .0044 | .0043 | .0042 | .0041 | .0040 | .0039 | .0038 | .0038 | .0037 |
| 3ip2m6 | .0032 | .0110 | .0120 | .0121 | .0120 | .0104 | .0090 | .0079 | .0071 | .0065 | .0061 | .0057 | .0054 | .0052 | .0050 | .0049 |
| 33ee6 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0002 | .0003 | .0004 | .0005 | .0006 | .0008 | .0009 | .0010 | .0011 | .0012 |
| 34ee6 | .0000 | .0001 | .0001 | .0001 | .0005 | .0009 | .0014 | .0017 | .0021 | .0023 | .0026 | .0028 | .0029 | .0031 | .0032 | .0033 |
| 3RSe22mm6 | .0007 | .0025 | .0028 | .0028 | .0030 | .0028 | .0026 | .0025 | .0024 | .0023 | .0023 | .0022 | .0022 | .0022 | .0022 | .0022 |
| 4e22mm6 | .0025 | .0054 | .0054 | .0053 | .0041 | .0032 | .0026 | .0022 | .0020 | .0018 | .0017 | .0016 | .0016 | .0015 | .0015 | .0015 |
| 3RSe23mm6 | .0000 | .0004 | .0006 | .0006 | .0012 | .0017 | .0021 | .0024 | .0026 | .0028 | .0031 | .0032 | .0034 | .0036 | .0037 | .0039 |
| 4e23RSmm6 | .0009 | .0050 | .0062 | .0063 | .0088 | .0093 | .0092 | .0089 | .0086 | .0083 | .0081 | .0079 | .0078 | .0076 | .0075 | .0074 |
| 3RSe24SRmm6 | .0009 | .0050 | .0062 | .0063 | .0088 | .0093 | .0092 | .0089 | .0086 | .0083 | .0081 | .0079 | .0078 | .0076 | .0075 | .0074 |
| 3RSe24RSmm6 | .0009 | .0050 | .0062 | .0063 | .0088 | .0093 | .0092 | .0089 | .0086 | .0083 | .0081 | .0079 | .0078 | .0076 | .0075 | .0074 |
| 4e24mm6 | .0001 | .0009 | .0011 | .0011 | .0017 | .0019 | .0020 | .0021 | .0022 | .0022 | .0023 | .0023 | .0024 | .0024 | .0025 | .0025 |
| 3e25mm6 | .0065 | .0220 | .0241 | .0242 | .0239 | .0207 | .0179 | .0158 | .0142 | .0131 | .0122 | .0114 | .0109 | .0104 | .0100 | .0097 |
| 4e33mm6 | .0000 | .0002 | .0003 | .0003 | .0006 | .0009 | .0010 | .0012 | .0013 | .0014 | .0015 | .0016 | .0017 | .0018 | .0019 | .0019 |
| 3e34RSmm6 | .0000 | .0001 | .0001 | .0001 | .0004 | .0008 | .0011 | .0013 | .0016 | .0018 | .0020 | .0023 | .0024 | .0026 | .0028 | .0030 |
| 2233mmmm6 | .0010 | .0015 | .0014 | .0014 | .0009 | .0006 | .0005 | .0004 | .0004 | .0004 | .0003 | .0003 | .0003 | .0003 | .0003 | .0003 |
| 223RS4RSmmmm6 | .0001 | .0006 | .0007 | .0007 | .0007 | .0007 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 |
| 223RS4SRmmmm6 | .0001 | .0006 | .0007 | .0007 | .0007 | .0007 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 |
| 223RS5mmmm6 | .0484 | .0398 | .0316 | .0310 | .0131 | .0070 | .0044 | .0032 | .0025 | .0021 | .0018 | .0016 | .0015 | .0014 | .0013 | .0012 |
| 2244mmmm6 | .0000 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 |
| 224RS5mmmm6 | .0083 | .0110 | .0097 | .0096 | .0054 | .0034 | .0025 | .0019 | .0016 | .0014 | .0013 | .0012 | .0011 | .0011 | .0010 | .0010 |
| 2255mmmm6 | .5275 | .0931 | .0523 | .0502 | .0085 | .0027 | .0012 | .0007 | .0005 | .0004 | .0003 | .0002 | .0002 | .0002 | .0002 | .0002 |
| 2334RSmmmm6 | .0003 | .0014 | .0016 | .0017 | .0019 | .0019 | .0018 | .0017 | .0017 | .0016 | .0016 | .0016 | .0016 | .0016 | .0016 | .0017 |
| 2335mmmm6 | .0002 | .0009 | .0010 | .0010 | .0011 | .0010 | .0010 | .0009 | .0009 | .0009 | .0009 | .0008 | .0008 | .0008 | .0009 | .0009 |
| 23RS44mmmm6 | .0001 | .0004 | .0005 | .0005 | .0008 | .0009 | .0010 | .0010 | .0011 | .0011 | .0011 | .0012 | .0012 | .0012 | .0013 | .0013 |
| 23RS4RS5mmmm6 | .0310 | .0405 | .0355 | .0351 | .0189 | .0114 | .0077 | .0057 | .0045 | .0038 | .0032 | .0029 | .0026 | .0024 | .0022 | .0021 |
| 23R4S5mmmm6 | .0310 | .0405 | .0355 | .0351 | .0189 | .0114 | .0077 | .0057 | .0045 | .0038 | .0032 | .0029 | .0026 | .0024 | .0022 | .0021 |
| 3344mmmm6 | .0000 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 | .0003 | .0003 | .0003 | .0003 |
| 3ip24mm5 | .0103 | .0135 | .0118 | .0117 | .0063 | .0038 | .0026 | .0019 | .0015 | .0013 | .0011 | .0010 | .0009 | .0008 | .0007 | .0007 |
| 33ee2m5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 | .0003 | .0003 | .0003 | .0004 | .0004 |
| 3e223mmm5 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0002 | .0002 | .0002 | .0002 | .0002 | .0002 |
| 3RSe224mmm5 | .0001 | .0006 | .0007 | .0007 | .0007 | .0007 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 | .0006 |
| 3e234mmm5 | .0000 | .0002 | .0002 | .0002 | .0004 | .0004 | .0005 | .0005 | .0005 | .0005 | .0005 | .0006 | .0006 | .0006 | .0006 | .0006 |
| 22334mmmmm5 | .0000 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 | .0001 |
| 22344mmmmm5 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 | .0000 |

## 7. Discussion

The values of standard thermodynamic properties of isomer groups calculated here may be used in predicting equilibrium compositions of organic systems at temperature and catalyst conditions where isomers in an isomer group are in equilibrium. If a certain catalyst does not equilibrate all isomers in a group, then the isomer group thermodynamic properties to be used should be calculated by using the properties of only those isomers which are equilibrated. However, the exclusion of highly branched isomers (which in general have very low equilibrium mole fractions) will not have much effect on the calculated isomer group properties, especially at higher temperatures.

The fact that the increments per carbon atom in the various standard thermodynamic properties for isomer groups approach constant values at higher carbon numbers indicates that extrapolations can be made to higher carbon numbers, but these extrapolations must be tempered by the experimental uncertainties. As the carbon number increases, the equilibrium mole fractions of individual molecular species become of less interest because there are so many of them and because gas chromatographic analytical methods yield mole fractions of isomer groups, rather than individual isomers, at higher carbon numbers.

More experimental data is needed on certain highly branched alkanes such as 2255mmmm6 to provide a sounder basis for statistical mechanical correlations of thermodynamic properties and for improvements in Benson group values and non-next-nearest neighbor corrections. In view of the geometric increase in the number of isomers with carbon number, it will also be important to seek opportunities to obtain chemical thermodynamic properties of isomer groups at higher carbon numbers directly from chemical equilibrium data.

## 8. Nomenclature

$C^\circ_{Pi}$ = standard heat capacity at constant pressure of isomer $i$, J K$^{-1}$ mol$^{-1}$

$C^\circ_P$(I) = standard heat capacity at constant pressure of isomer group I, J K$^{-1}$ mol$^{-1}$

$\Delta_f G^\circ_i$ = standard Gibbs energy of formation of isomer $i$, kJ mol$^{-1}$

$\Delta_f G^\circ$(I) = standard Gibbs energy of formation of isomer group I, kJ mol$^{-1}$

$H^\circ(\mathrm{I},T) - H^\circ(\mathrm{I},298.15\ \mathrm{K})$ = standard enthalpy for an isomer group relative to the isomer group at 298.15 K, kJ mol$^{-1}$

$\Delta_f H^\circ_i$ = standard enthalpy of formation of isomer $i$, kJ mol$^{-1}$

$\Delta_f H^\circ$(I) = standard enthalpy of formation of isomer group I, kJ mol$^{-1}$

$N_\mathrm{I}$ = number of isomers in an isomer group

$r_i$ = equilibrium mole fraction of species $i$ in an isomer group

$S^\circ_i$ = standard entropy of isomer $i$, J K$^{-1}$ mol$^{-1}$

$S^\circ$(I) = standard entropy of isomer group I, J K$^{-1}$ mol$^{-1}$

$y_i$ = mole fraction of isomer $i$

$y_\mathrm{I}$ = mole fraction of isomer group I

$\sigma_H$ = standard deviation of the enthalpies of formation, kJ mol$^{-1}$

## 9. Acknowledgments

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## Appendix: Standard Thermodynamic Properties of Individual Alkane Species

Since tables of standard thermodynamic properties in joules for a standard state pressure of 1 bar have been used to calculate the isomer group properties, the four basic properties from the Scott tables, as corrected, are given in Tables A1–A4. The standard heat capacities at constant pressure are all zero at 0 K. The standard entropies at 0 K are zero for single species, but are equal to 5.77 J $K^{-1}$ $mol^{-1}$ for racemates. The standard enthalpies of formation at 0 K are not the $\Delta_f H_0^\circ$ parameters from Eq. (14), but are the ideal gas values calculated by Scott.

Table A1. Standard heat capacity at constant pressure of alkanes in J/K mol

| T/K | 0 | 200 | 298.15 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| methane | .00 | 33.51 | 35.69 | 35.77 | 40.63 | 46.53 | 52.30 | 58.16 | 63.60 | 68.20 | 72.80 | 77.0 | 80.3 | 83.7 | 87.9 | 87.9 |
| ethane | .00 | 42.26 | 52.59 | 52.84 | 66.23 | 79.91 | 92.88 | 104.18 | 114.64 | 124.26 | 132.63 | 140.2 | 146.9 | 154.8 | 159.0 | 163.2 |
| propane | .00 | 52.89 | 72.97 | 73.39 | 93.97 | 113.22 | 130.54 | 145.60 | 158.99 | 171.13 | 181.59 | 190.8 | 199.2 | 205.0 | 213.4 | 217.6 |
| butanes | | | | | | | | | | | | | | | | |
| 4 | .00 | 76.82 | 97.49 | 97.91 | 123.22 | 147.49 | 169.03 | 187.86 | 204.18 | 218.40 | 230.96 | 241.8 | 251.5 | 259.4 | 267.8 | 276.1 |
| 2m3 | .00 | 70.50 | 96.78 | 97.28 | 123.93 | 148.57 | 170.71 | 189.95 | 207.11 | 222.17 | 235.98 | 247.7 | 258.2 | 267.8 | 276.1 | 284.5 |
| pentanes | | | | | | | | | | | | | | | | |
| 5 | .00 | 93.55 | 120.04 | 120.62 | 152.55 | 182.59 | 208.78 | 231.38 | 250.62 | 266.94 | 281.58 | 293.7 | 304.6 | 313.8 | 322.2 | 330.5 |
| 2m4 | .00 | 84.94 | 118.87 | 119.50 | 152.88 | 183.26 | 210.04 | 233.05 | 253.13 | 270.70 | 286.19 | 299.6 | 311.3 | 322.2 | 330.5 | 338.9 |
| 22mm3 | .00 | 80.54 | 120.83 | 121.55 | 155.98 | 186.98 | 214.64 | 238.91 | 261.08 | 280.33 | 297.90 | 313.4 | 327.2 | 338.9 | 351.5 | 359.8 |
| hexanes | | | | | | | | | | | | | | | | |
| 6 | .00 | 110.58 | 142.59 | 143.26 | 181.54 | 217.28 | 248.11 | 274.05 | 296.23 | 315.06 | 331.37 | 345.2 | 357.3 | 368.2 | 376.6 | 389.1 |
| 2m5 | .00 | 101.34 | 142.21 | 143.01 | 183.51 | 219.83 | 251.04 | 277.40 | 300.41 | 320.08 | 337.23 | 351.9 | 364.8 | 376.6 | 389.1 | 397.5 |
| 3m5 | .00 | 98.91 | 140.12 | 140.88 | 181.17 | 217.48 | 248.95 | 275.73 | 298.74 | 318.82 | 335.98 | 351.0 | 364.0 | 376.6 | 384.9 | 397.5 |
| 22mm4 | .00 | 101.46 | 141.46 | 142.26 | 183.13 | 220.33 | 253.13 | 281.58 | 306.69 | 328.44 | 348.11 | 365.3 | 380.3 | 393.3 | 405.8 | 418.4 |
| 23mm4 | .00 | 93.14 | 139.41 | 140.21 | 181.71 | 218.36 | 250.20 | 277.40 | 301.67 | 322.59 | 340.58 | 356.9 | 370.7 | 384.9 | 393.3 | 405.8 |
| heptanes | | | | | | | | | | | | | | | | |
| 7 | .00 | 127.65 | 165.18 | 165.98 | 210.66 | 252.09 | 287.44 | 317.15 | 342.25 | 363.59 | 381.58 | 397.1 | 410.5 | 422.6 | 435.1 | 443.5 |
| 2m6 | .00 | 118.57 | 164.51 | 165.35 | 211.96 | 253.80 | 289.53 | 319.66 | 345.60 | 367.77 | 386.60 | 403.3 | 417.6 | 431.0 | 443.5 | 451.9 |
| 3RSm6 | .00 | 115.39 | 163.59 | 164.47 | 211.71 | 253.76 | 289.53 | 319.66 | 345.60 | 367.77 | 386.60 | 403.3 | 417.6 | 431.0 | 443.5 | 451.9 |
| 3e5 | .00 | 125.35 | 165.98 | 166.82 | 211.54 | 252.63 | 288.28 | 318.40 | 343.92 | 366.10 | 385.35 | 402.1 | 416.3 | 431.0 | 439.3 | 451.9 |
| 22mm5 | .00 | 116.86 | 166.69 | 167.65 | 216.77 | 259.78 | 296.65 | 328.03 | 355.22 | 379.07 | 399.99 | 418.4 | 434.7 | 447.7 | 464.4 | 477.0 |
| 23RSmm5 | .00 | 104.98 | 160.83 | 161.84 | 211.04 | 253.72 | 289.95 | 321.33 | 347.69 | 371.12 | 391.20 | 408.4 | 423.8 | 439.3 | 451.9 | 460.2 |
| 24mm5 | .00 | 115.44 | 170.75 | 171.71 | 220.08 | 261.37 | 296.23 | 326.35 | 352.29 | 374.47 | 394.13 | 411.3 | 426.3 | 439.3 | 451.9 | 464.4 |
| 33mm5 | .00 | 113.72 | 165.77 | 166.69 | 215.35 | 258.45 | 295.81 | 327.61 | 355.22 | 379.49 | 400.41 | 419.2 | 435.6 | 451.9 | 464.4 | 477.0 |
| 223mmm4 | .00 | 111.46 | 163.26 | 164.22 | 212.84 | 256.06 | 293.72 | 326.35 | 355.22 | 380.74 | 402.92 | 422.6 | 440.2 | 456.1 | 468.6 | 481.2 |
| octanes | | | | | | | | | | | | | | | | |
| 8 | .00 | 144.77 | 187.78 | 188.70 | 239.74 | 286.81 | 326.77 | 360.24 | 388.28 | 411.71 | 431.37 | 448.5 | 463.2 | 477.0 | 489.5 | 497.9 |
| 2m7 | .00 | 135.65 | 187.23 | 188.20 | 241.25 | 288.78 | 329.28 | 363.17 | 391.62 | 416.31 | 436.81 | 454.8 | 470.7 | 485.3 | 497.9 | 510.4 |
| 3RSm7 | .00 | 132.67 | 185.81 | 186.82 | 240.16 | 287.82 | 328.03 | 362.33 | 391.20 | 415.47 | 436.39 | 454.4 | 470.3 | 485.3 | 497.9 | 510.4 |
| 4m7 | .00 | 131.88 | 187.02 | 188.03 | 242.34 | 290.16 | 330.54 | 364.43 | 392.88 | 417.14 | 437.65 | 455.6 | 471.1 | 485.3 | 497.9 | 510.4 |
| 3e6 | .00 | 142.05 | 189.62 | 190.58 | 241.96 | 288.53 | 328.44 | 361.92 | 390.79 | 415.05 | 435.97 | 454.0 | 469.4 | 485.3 | 497.9 | 506.3 |
| 22mm6 | .00 | 134.72 | 188.28 | 189.33 | 243.84 | 292.42 | 333.88 | 369.45 | 399.99 | 426.35 | 449.36 | 469.4 | 487.0 | 502.1 | 518.8 | 531.4 |
| 23RSmm6 | .00 | 121.80 | 184.10 | 185.18 | 240.91 | 289.24 | 330.12 | 364.84 | 394.13 | 419.66 | 441.41 | 460.2 | 477.0 | 493.7 | 506.3 | 518.8 |
| 24RSmm6 | .00 | 129.91 | 192.30 | 193.38 | 247.94 | 294.76 | 334.30 | 368.19 | 397.06 | 421.75 | 443.50 | 462.3 | 478.6 | 493.7 | 506.3 | 518.8 |
| 25mm6 | .00 | 126.02 | 185.48 | 186.52 | 241.25 | 289.24 | 330.12 | 364.84 | 394.13 | 419.66 | 441.41 | 460.7 | 477.0 | 493.7 | 506.3 | 518.8 |
| 33mm6 | .00 | 129.12 | 190.87 | 191.96 | 248.70 | 297.48 | 338.90 | 373.63 | 403.76 | 429.70 | 452.29 | 472.0 | 489.5 | 506.3 | 518.8 | 531.4 |
| 3RS4RSmm6 | .00 | 116.15 | 181.59 | 182.72 | 239.74 | 288.53 | 329.70 | 364.43 | 393.71 | 419.24 | 441.41 | 460.2 | 477.0 | 493.7 | 506.3 | 518.8 |
| 3R4Smm6 | .00 | 117.49 | 183.18 | 184.26 | 240.71 | 288.95 | 329.70 | 364.01 | 393.71 | 419.24 | 440.99 | 459.8 | 476.6 | 489.5 | 506.3 | 518.8 |
| 3e2m5 | .00 | 134.10 | 192.05 | 193.05 | 244.68 | 290.33 | 329.70 | 363.59 | 392.88 | 418.40 | 440.16 | 459.4 | 475.7 | 489.5 | 506.3 | 514.6 |
| 3e3m5 | .00 | 127.99 | 187.99 | 189.07 | 244.60 | 293.21 | 334.72 | 370.28 | 400.83 | 427.19 | 450.20 | 470.3 | 487.9 | 502.1 | 518.8 | 531.4 |
| 223RSmmm5 | .00 | 121.96 | 185.64 | 186.77 | 243.80 | 292.92 | 334.72 | 370.70 | 402.08 | 429.70 | 453.55 | 474.5 | 493.3 | 510.4 | 527.2 | 539.7 |
| 224mmm5 | .00 | 130.58 | 188.41 | 189.45 | 244.60 | 293.42 | 335.56 | 371.96 | 403.34 | 430.53 | 454.80 | 475.7 | 494.5 | 510.4 | 527.2 | 539.7 |
| 233mmm5 | .00 | 121.25 | 187.02 | 188.20 | 245.18 | 294.34 | 336.39 | 372.79 | 404.17 | 431.37 | 455.22 | 476.6 | 495.0 | 510.4 | 527.2 | 539.7 |
| 234mmm5 | .00 | 123.68 | 191.59 | 192.72 | 247.69 | 294.43 | 334.30 | 369.03 | 398.74 | 424.68 | 447.27 | 467.4 | 484.5 | 502.1 | 514.6 | 527.2 |
| 2233mmmm4 | .00 | 129.87 | 187.19 | 188.28 | 244.01 | 293.76 | 337.23 | 375.30 | 409.20 | 438.90 | 465.26 | 488.7 | 509.6 | 527.2 | 543.9 | 560.7 |
| nonanes | | | | | | | | | | | | | | | | |
| 9 | .00 | 161.92 | 210.41 | 211.42 | 268.82 | 321.54 | 366.10 | 403.34 | 433.88 | 459.82 | 481.58 | 500.0 | 516.3 | 531.4 | 543.9 | 556.5 |
| 2m8 | .00 | 152.80 | 209.83 | 210.92 | 270.33 | 323.51 | 368.61 | 405.85 | 437.65 | 464.42 | 487.02 | 506.7 | 523.4 | 539.7 | 552.3 | 564.8 |
| 3RSm8 | .00 | 149.75 | 208.57 | 209.66 | 269.45 | 322.80 | 367.77 | 405.43 | 437.23 | 464.01 | 486.60 | 506.3 | 523.0 | 539.7 | 552.3 | 564.8 |
| 4RSm8 | .00 | 149.12 | 209.28 | 210.41 | 270.75 | 324.13 | 369.03 | 406.68 | 438.06 | 464.42 | 487.44 | 506.7 | 523.8 | 539.7 | 552.3 | 564.8 |
| 3e7 | .00 | 159.28 | 211.88 | 212.97 | 270.37 | 322.50 | 366.94 | 404.17 | 435.97 | 462.75 | 485.34 | 505.0 | 522.2 | 535.6 | 552.3 | 564.8 |
| 4e7 | .00 | 158.70 | 213.30 | 214.35 | 272.34 | 324.43 | 368.61 | 405.85 | 437.23 | 463.59 | 486.18 | 505.8 | 522.6 | 539.7 | 552.3 | 564.8 |
| 22mm7 | .00 | 151.75 | 211.25 | 212.38 | 273.47 | 327.73 | 374.05 | 412.96 | 446.01 | 474.88 | 499.57 | 521.3 | 540.2 | 556.5 | 573.2 | 585.8 |
| 23RSmm7 | .00 | 139.87 | 206.44 | 207.65 | 269.07 | 322.80 | 368.19 | 406.68 | 439.32 | 466.93 | 490.78 | 511.3 | 529.7 | 543.9 | 560.7 | 573.2 |
| 24RSmm7 | .00 | 146.31 | 215.85 | 217.07 | 278.82 | 331.41 | 375.72 | 412.54 | 444.34 | 471.12 | 494.55 | 514.6 | 532.2 | 548.1 | 560.7 | 577.4 |
| 25RSmm7 | .00 | 140.25 | 206.98 | 208.15 | 269.66 | 323.38 | 369.03 | 407.10 | 439.74 | 467.35 | 491.20 | 511.7 | 529.7 | 543.9 | 560.7 | 573.2 |
| 26mm7 | .00 | 143.43 | 209.24 | 210.41 | 271.96 | 325.68 | 371.12 | 409.20 | 441.41 | 468.61 | 492.46 | 513.0 | 530.9 | 548.1 | 560.7 | 573.2 |
| 33mm7 | .00 | 147.15 | 212.84 | 214.01 | 276.10 | 330.28 | 376.14 | 415.05 | 448.11 | 476.56 | 501.24 | 522.6 | 541.8 | 560.7 | 573.2 | 589.9 |
| 3RS4SRmm7 | .00 | 134.39 | 206.44 | 207.65 | 270.66 | 324.55 | 369.87 | 407.94 | 440.16 | 467.77 | 491.62 | 512.1 | 529.7 | 543.9 | 560.7 | 573.2 |
| 3RS4RSmm7 | .00 | 133.01 | 204.76 | 206.02 | 269.62 | 324.13 | 369.87 | 407.94 | 440.16 | 467.77 | 491.62 | 512.1 | 530.1 | 548.1 | 560.7 | 573.2 |
| 3RS5RSmm7 | .00 | 140.39 | 212.51 | 213.68 | 274.68 | 327.36 | 371.96 | 409.61 | 441.41 | 469.03 | 492.46 | 513.0 | 530.9 | 548.1 | 560.7 | 573.2 |
| 3R5Smm7 | .00 | 145.52 | 214.39 | 215.56 | 275.81 | 327.86 | 371.96 | 409.61 | 441.41 | 469.03 | 492.46 | 513.0 | 530.9 | 548.1 | 560.7 | 573.2 |
| 44mm7 | .00 | 144.52 | 215.98 | 217.23 | 282.09 | 336.60 | 382.00 | 420.07 | 452.29 | 479.90 | 504.17 | 525.1 | 543.9 | 560.7 | 577.4 | 589.9 |
| 3RSe2m6 | .00 | 150.75 | 215.06 | 216.15 | 274.22 | 325.43 | 369.45 | 407.10 | 439.32 | 466.52 | 490.36 | 510.9 | 528.9 | 543.9 | 560.7 | 573.2 |
| 4e2m6 | .00 | 157.95 | 218.61 | 219.74 | 277.73 | 329.11 | 372.79 | 410.03 | 441.83 | 469.03 | 492.88 | 513.0 | 530.5 | 548.1 | 560.7 | 573.2 |
| 3e3m6 | .00 | 143.39 | 212.88 | 214.14 | 277.48 | 331.75 | 377.40 | 415.89 | 448.94 | 476.98 | 501.66 | 523.0 | 541.8 | 560.7 | 573.2 | 589.9 |
| 3e4RSm6 | .00 | 145.90 | 214.05 | 215.18 | 273.76 | 324.97 | 369.03 | 406.27 | 438.48 | 466.10 | 489.95 | 510.4 | 528.4 | 543.9 | 560.7 | 573.2 |
| 223RSmmm6 | .00 | 139.20 | 208.66 | 209.87 | 272.88 | 327.48 | 374.05 | 413.80 | 448.11 | 477.81 | 503.75 | 526.3 | 546.4 | 564.8 | 581.6 | 594.1 |
| 224RSmmm6 | .00 | 144.60 | 209.45 | 210.66 | 272.29 | 326.77 | 373.63 | 413.38 | 448.11 | 477.81 | 503.75 | 526.3 | 546.8 | 564.8 | 581.6 | 594.1 |
| 225mmm6 | .00 | 141.80 | 207.86 | 209.07 | 271.37 | 326.18 | 373.21 | 412.96 | 447.69 | 477.39 | 503.34 | 526.3 | 546.4 | 564.8 | 581.6 | 594.1 |
| 233mmm6 | .00 | 136.65 | 212.05 | 213.34 | 278.15 | 332.88 | 379.07 | 418.40 | 451.87 | 481.16 | 506.68 | 529.3 | 548.9 | 564.8 | 581.6 | 598.3 |
| 23RS4SRmmm6 | .00 | 138.24 | 214.35 | 215.56 | 276.60 | 328.70 | 373.21 | 411.29 | 443.92 | 472.37 | 497.06 | 518.4 | 537.2 | 552.3 | 569.0 | 581.6 |
| 23RS4RSmmm6 | .00 | 134.72 | 211.29 | 212.55 | 275.22 | 328.36 | 373.21 | 411.71 | 444.34 | 472.79 | 497.48 | 518.8 | 537.6 | 552.3 | 569.0 | 581.6 |
| 23RS5mmm6 | .00 | 135.73 | 211.25 | 212.55 | 275.77 | 329.16 | 374.05 | 412.54 | 445.18 | 473.63 | 497.90 | 519.2 | 538.1 | 556.5 | 569.0 | 585.8 |
| 244mmm6 | .00 | 142.63 | 212.30 | 213.51 | 276.27 | 330.91 | 377.40 | 417.14 | 451.45 | 481.16 | 506.68 | 529.3 | 549.4 | 569.0 | 581.6 | 598.3 |
| 334RSmmm6 | .00 | 131.75 | 209.20 | 210.50 | 275.68 | 330.70 | 376.98 | 416.73 | 450.62 | 479.90 | 505.43 | 528.0 | 548.1 | 564.8 | 581.6 | 598.3 |
| 33ee5 | 00 | 153.89 | 216.73 | 217.86 | 276.31 | 328.49 | 373.63 | 412.54 | 445.60 | 474.47 | 499.15 | 520.9 | 539.7 | 556.5 | 573.2 | 585.8 |
| 3e22mm5 | 00 | 140.62 | 203.80 | 205.02 | 266.98 | 322.08 | 369.45 | 410.03 | 444.76 | 474.88 | 501.24 | 523.8 | 544.3 | 560.7 | 577.4 | 594.1 |
| 3e23mm5 | 00 | 136.65 | 212.17 | 213.43 | 275.68 | 329.20 | 375.30 | 414.63 | 448.52 | 478.23 | 504.17 | 526.8 | 546.8 | 564.8 | 581.6 | 598.3 |
| 3e24mm5 | 00 | 139.70 | 207.78 | 208.99 | 270.37 | 323.88 | 369.45 | 408.36 | 441.83 | 470.28 | 495.39 | 517.1 | 536.0 | 552.3 | 569.0 | 581.6 |
| 2233mmmm5 | 00 | 138.49 | 212.05 | 213.34 | 277.44 | 332.71 | 380.33 | 421.75 | 457.73 | 489.11 | 517.14 | 541.8 | 564.0 | 585.8 | 602.5 | 619.2 |
| 223RS4mmmm5 | 00 | 135.31 | 207.28 | 208.53 | 272.00 | 327.06 | 374.47 | 415.05 | 450.20 | 481.16 | 508.36 | 532.2 | 553.1 | 573.2 | 589.9 | 602.5 |
| 2244mmmm5 | 00 | 153.72 | 214.60 | 215.77 | 276.56 | 331.21 | 379.07 | 420.49 | 456.47 | 488.69 | 516.72 | 541.4 | 563.6 | 581.6 | 602.5 | 619.2 |
| 2334mmmm5 | 00 | 153.13 | 218.28 | 219.53 | 282.34 | 335.64 | 381.16 | 420.91 | 455.22 | 485.34 | 512.12 | 535.6 | 556.5 | 573.2 | 589.9 | 606.7 |

Table A1 continued

| T/K | 0 | 200 | 298.15 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| decanes | | | | | | | | | | | | | | | | |
| 10 | .00 | 179.08 | 233.05 | 234.18 | 297.98 | 356.43 | 405.85 | 446.43 | 479.90 | 508.36 | 531.79 | 551.9 | 569.4 | 585.8 | 598.3 | 610.9 |
| 2m9 | .00 | 169.95 | 232.46 | 233.68 | 299.49 | 358.40 | 407.94 | 449.36 | 483.67 | 512.54 | 537.23 | 558.1 | 576.6 | 594.1 | 606.7 | 623.4 |
| 3RSm9 | .00 | 166.86 | 231.17 | 232.38 | 298.53 | 357.52 | 407.10 | 448.52 | 482.83 | 512.12 | 536.81 | 557.7 | 576.1 | 594.1 | 606.7 | 623.4 |
| 4RSm9 | .00 | 166.19 | 232.00 | 233.26 | 300.03 | 359.11 | 408.78 | 449.78 | 484.09 | 512.96 | 537.64 | 558.6 | 576.6 | 594.1 | 606.7 | 623.4 |
| 5m9 | .00 | 166.31 | 231.46 | 232.67 | 299.24 | 358.36 | 407.94 | 449.36 | 483.67 | 512.54 | 537.23 | 558.1 | 576.6 | 594.1 | 606.7 | 623.4 |
| 3e8 | .00 | 176.36 | 234.64 | 235.81 | 299.66 | 357.52 | 406.68 | 447.69 | 482.00 | 510.87 | 535.55 | 556.9 | 575.3 | 589.9 | 606.7 | 619.2 |
| 4RSe8 | .00 | 175.81 | 235.35 | 236.52 | 300.96 | 358.86 | 407.94 | 448.52 | 482.83 | 511.70 | 536.39 | 557.3 | 575.7 | 589.9 | 606.7 | 619.2 |
| 22mm8 | .00 | 168.95 | 233.89 | 235.14 | 302.50 | 362.38 | 412.96 | 455.64 | 492.04 | 523.00 | 549.78 | 572.8 | 592.9 | 610.9 | 627.6 | 644.3 |
| 23RSmm8 | .00 | 156.90 | 229.20 | 230.50 | 298.36 | 357.82 | 407.94 | 449.78 | 485.34 | 515.47 | 540.99 | 563.2 | 582.4 | 598.3 | 615.0 | 631.8 |
| 24RSmm8 | .00 | 163.59 | 238.11 | 239.41 | 307.27 | 365.47 | 414.22 | 455.22 | 489.53 | 518.82 | 544.34 | 565.7 | 584.9 | 602.5 | 619.2 | 631.8 |
| 25RSmm8 | .00 | 156.73 | 230.41 | 231.75 | 300.24 | 359.82 | 409.61 | 451.45 | 486.60 | 516.72 | 542.25 | 564.0 | 583.2 | 602.5 | 615.0 | 631.8 |
| 26RSmm8 | .00 | 157.53 | 230.58 | 231.88 | 300.16 | 359.70 | 409.61 | 451.45 | 486.60 | 516.72 | 542.25 | 564.0 | 583.2 | 602.5 | 615.0 | 631.8 |
| 27mm8 | .00 | 160.58 | 231.88 | 233.17 | 301.12 | 360.58 | 410.45 | 452.29 | 487.44 | 517.14 | 542.66 | 564.8 | 584.1 | 602.5 | 615.0 | 631.8 |
| 33mm8 | .00 | 164.18 | 235.77 | 237.07 | 305.72 | 365.60 | 415.89 | 458.57 | 494.55 | 525.09 | 551.87 | 574.5 | 595.0 | 615.0 | 627.6 | 644.3 |
| 3RS4SRmm8 | .00 | 152.42 | 228.78 | 230.12 | 298.82 | 358.11 | 407.94 | 449.78 | 484.93 | 515.05 | 540.57 | 562.7 | 582.4 | 598.3 | 615.0 | 631.8 |
| 3RS4RSmm8 | .00 | 151.08 | 227.15 | 228.49 | 297.78 | 357.73 | 407.94 | 449.78 | 485.34 | 515.47 | 540.99 | 563.2 | 582.4 | 598.3 | 615.0 | 631.8 |
| 3RS5RSmm8 | .00 | 159.79 | 236.06 | 237.40 | 305.56 | 364.01 | 412.96 | 453.96 | 488.69 | 518.40 | 543.50 | 565.3 | 584.5 | 602.5 | 615.0 | 631.8 |
| 3RS5SRmm8 | .00 | 161.88 | 237.94 | 239.28 | 306.65 | 364.55 | 413.38 | 453.96 | 488.69 | 518.40 | 543.50 | 565.3 | 584.5 | 602.5 | 615.0 | 631.8 |
| 3RS6RSmm8 | .00 | 154.35 | 228.32 | 229.62 | 297.86 | 357.40 | 407.52 | 449.36 | 484.93 | 515.05 | 540.99 | 563.2 | 582.4 | 598.3 | 615.0 | 631.8 |
| 3R6Smm8 | .00 | 154.35 | 228.32 | 229.62 | 297.86 | 357.40 | 407.52 | 449.36 | 484.93 | 515.05 | 540.99 | 563.2 | 582.4 | 598.3 | 615.0 | 631.8 |
| 44mm8 | .00 | 162.59 | 237.94 | 239.28 | 309.49 | 369.41 | 419.24 | 461.08 | 496.64 | 527.18 | 553.12 | 575.7 | 595.8 | 615.0 | 631.8 | 644.3 |
| 4RS5RSmm8 | .00 | 149.87 | 227.90 | 229.28 | 299.53 | 359.70 | 410.03 | 451.87 | 487.02 | 516.72 | 542.25 | 564.0 | 583.2 | 602.5 | 615.0 | 631.8 |
| 4R5Smm8 | .00 | 151.25 | 229.70 | 231.04 | 300.62 | 360.12 | 410.03 | 451.45 | 486.60 | 516.31 | 541.83 | 564.0 | 583.2 | 598.3 | 615.0 | 631.8 |
| 4p7 | .00 | 175.02 | 236.52 | 237.73 | 303.09 | 361.20 | 410.03 | 450.62 | 484.51 | 513.38 | 537.64 | 558.6 | 576.6 | 594.1 | 606.7 | 623.4 |
| 41p7 | .00 | 167.36 | 238.03 | 239.24 | 303.72 | 360.58 | 409.20 | 450.20 | 485.34 | 515.05 | 540.57 | 562.3 | 582.0 | 598.3 | 615.0 | 627.6 |
| 3RSe2m7 | .00 | 167.99 | 237.32 | 238.53 | 302.63 | 359.45 | 407.94 | 449.36 | 484.51 | 514.21 | 539.74 | 561.9 | 581.6 | 598.3 | 615.0 | 627.6 |
| 4RSe2m7 | .00 | 174.35 | 242.17 | 243.43 | 308.61 | 365.77 | 414.22 | 454.80 | 489.11 | 518.40 | 543.92 | 565.3 | 584.5 | 602.5 | 615.0 | 631.8 |
| 5e2m7 | .00 | 166.90 | 233.05 | 234.26 | 299.87 | 358.19 | 407.52 | 449.36 | 484.51 | 514.63 | 540.15 | 562.3 | 582.0 | 598.3 | 615.0 | 627.6 |
| 3e3m7 | .00 | 161.42 | 234.85 | 236.19 | 304.89 | 364.55 | 415.05 | 457.31 | 493.29 | 524.26 | 550.61 | 573.6 | 594.1 | 610.9 | 627.6 | 644.3 |
| 4RSe3RSm7 | .00 | 162.55 | 237.02 | 238.28 | 303.30 | 360.08 | 408.78 | 449.78 | 484.51 | 514.63 | 540.15 | 562.3 | 581.6 | 598.3 | 615.0 | 627.6 |
| 4RSe3SRm7 | .00 | 162.55 | 237.02 | 238.28 | 303.30 | 360.08 | 408.78 | 449.78 | 484.51 | 514.63 | 540.15 | 562.3 | 581.6 | 598.3 | 615.0 | 627.6 |
| 3e5RSm7 | .00 | 172.30 | 239.70 | 240.91 | 305.01 | 361.96 | 410.45 | 451.87 | 486.60 | 516.31 | 541.83 | 563.6 | 582.8 | 598.3 | 615.0 | 631.8 |
| 3e4RSm7 | .00 | 162.72 | 237.27 | 238.57 | 303.67 | 360.45 | 408.78 | 450.20 | 484.93 | 514.63 | 540.15 | 562.3 | 581.6 | 598.3 | 615.0 | 627.6 |
| 4e4m7 | .00 | 158.78 | 237.78 | 239.20 | 310.37 | 370.28 | 420.07 | 461.50 | 497.06 | 527.18 | 553.12 | 575.7 | 595.8 | 615.0 | 631.8 | 644.3 |
| 223RSmmm7 | .00 | 156.44 | 231.17 | 232.50 | 301.79 | 362.00 | 412.96 | 456.47 | 493.71 | 525.51 | 553.54 | 577.8 | 599.1 | 619.2 | 636.0 | 652.7 |
| 224RSmmm7 | .00 | 161.13 | 233.38 | 234.72 | 303.67 | 363.97 | 415.05 | 458.15 | 495.39 | 527.18 | 554.80 | 579.1 | 600.4 | 619.2 | 636.0 | 652.7 |
| 225RSmmm7 | .00 | 155.94 | 229.16 | 230.50 | 299.57 | 360.20 | 411.71 | 455.64 | 492.88 | 525.09 | 553.12 | 577.4 | 598.7 | 619.2 | 636.0 | 652.7 |
| 226mmm7 | .00 | 159.37 | 233.47 | 234.81 | 304.55 | 364.89 | 415.89 | 458.98 | 495.80 | 527.60 | 555.22 | 579.1 | 600.4 | 619.2 | 636.0 | 652.7 |
| 233mmm7 | .00 | 154.56 | 233.76 | 235.14 | 305.43 | 365.77 | 416.73 | 459.82 | 496.64 | 528.44 | 556.05 | 579.9 | 601.2 | 619.2 | 636.0 | 652.7 |
| 23RS4SRmmm7 | .00 | 154.89 | 237.86 | 239.24 | 306.90 | 364.59 | 413.38 | 455.22 | 490.78 | 521.33 | 547.69 | 570.3 | 590.8 | 606.7 | 623.4 | 640.2 |
| 23RS4RSmmm7 | .00 | 151.50 | 234.72 | 236.10 | 305.47 | 364.22 | 413.80 | 455.22 | 491.20 | 521.74 | 548.10 | 570.7 | 590.8 | 610.9 | 623.4 | 640.2 |
| 23RS5RSmmm7 | .00 | 148.41 | 230.83 | 232.25 | 302.50 | 362.21 | 412.12 | 454.38 | 490.36 | 521.33 | 547.69 | 570.7 | 590.8 | 606.7 | 623.4 | 640.2 |
| 23RS5SRmmm7 | .00 | 152.13 | 234.43 | 235.77 | 304.18 | 362.50 | 411.71 | 453.55 | 489.53 | 520.49 | 546.85 | 569.9 | 589.9 | 606.7 | 623.4 | 640.2 |
| 23RS6mmm7 | .00 | 146.06 | 227.11 | 228.49 | 298.78 | 358.86 | 409.61 | 451.87 | 488.27 | 519.23 | 546.01 | 569.0 | 589.1 | 606.7 | 623.4 | 640.2 |
| 244mmm7 | .00 | 158.11 | 237.48 | 238.91 | 309.78 | 370.20 | 420.91 | 463.59 | 499.99 | 531.37 | 558.98 | 582.4 | 603.3 | 623.4 | 640.2 | 656.9 |
| 24RS5SRmmm7 | .00 | 147.99 | 233.43 | 234.85 | 305.60 | 364.76 | 414.22 | 456.06 | 491.20 | 521.74 | 548.10 | 570.7 | 590.8 | 610.9 | 623.4 | 640.2 |
| 24RS5RSmmm7 | .00 | 146.82 | 231.88 | 233.30 | 304.60 | 364.30 | 414.22 | 456.06 | 491.20 | 522.16 | 548.10 | 571.1 | 591.2 | 610.9 | 623.4 | 640.2 |
| 246mmm7 | .00 | 160.46 | 244.85 | 246.27 | 315.64 | 372.96 | 420.91 | 461.08 | 495.80 | 525.51 | 551.45 | 573.6 | 593.7 | 610.9 | 627.6 | 640.2 |
| 255mmm7 | .00 | 155.56 | 232.84 | 234.18 | 303.13 | 363.21 | 414.22 | 457.73 | 494.97 | 527.18 | 554.80 | 579.1 | 600.4 | 619.2 | 636.0 | 652.7 |
| 334RSmmm7 | .00 | 148.99 | 232.17 | 233.59 | 304.80 | 365.35 | 416.31 | 459.40 | 496.22 | 528.44 | 556.05 | 579.9 | 601.2 | 619.2 | 636.0 | 652.7 |
| 335RSmmm7 | .00 | 156.36 | 232.80 | 234.14 | 303.38 | 363.84 | 415.05 | 458.57 | 496.22 | 528.02 | 556.05 | 579.9 | 601.2 | 619.2 | 636.0 | 652.7 |
| 3RS44mmm7 | .00 | 147.19 | 234.18 | 235.64 | 308.70 | 369.32 | 419.66 | 462.33 | 498.73 | 530.11 | 557.31 | 581.2 | 602.1 | 619.2 | 640.2 | 652.7 |
| 3RS45RSmmm7 | .00 | 148.91 | 233.47 | 234.85 | 303.97 | 362.67 | 412.12 | 454.38 | 489.95 | 520.49 | 547.27 | 569.9 | 590.4 | 606.7 | 623.4 | 640.2 |
| s3R45Smmm7 | .00 | 152.55 | 237.23 | 238.61 | 305.85 | 363.21 | 412.12 | 453.55 | 489.53 | 520.07 | 546.43 | 569.4 | 589.5 | 606.7 | 623.4 | 640.2 |
| r3R45Smmm7 | .00 | 146.73 | 230.96 | 232.34 | 302.42 | 361.92 | 412.12 | 453.96 | 489.95 | 520.91 | 547.27 | 570.3 | 590.4 | 606.7 | 623.4 | 640.2 |
| 3ip2m6 | .00 | 156.15 | 230.50 | 231.79 | 299.70 | 358.82 | 408.78 | 451.45 | 487.44 | 518.40 | 545.18 | 568.2 | 588.7 | 606.7 | 623.4 | 640.2 |
| 33ee6 | .00 | 169.28 | 241.25 | 242.55 | 308.65 | 366.52 | 415.89 | 457.73 | 493.29 | 523.84 | 550.61 | 573.2 | 593.7 | 610.9 | 627.6 | 644.3 |
| 34ee6 | .00 | 175.06 | 245.73 | 246.94 | 307.31 | 361.12 | 408.36 | 448.52 | 483.25 | 512.96 | 538.90 | 560.7 | 580.3 | 598.3 | 615.0 | 627.6 |
| 3RSe22mm6 | .00 | 157.11 | 226.35 | 227.65 | 296.14 | 356.90 | 408.78 | 452.71 | 490.36 | 523.00 | 551.03 | 575.7 | 597.1 | 615.0 | 636.0 | 648.5 |
| 4e22mm6 | .00 | 171.13 | 234.89 | 236.14 | 301.96 | 361.25 | 412.12 | 455.64 | 492.88 | 525.09 | 553.12 | 577.4 | 598.7 | 619.2 | 636.0 | 652.7 |
| 3RSe23mm6 | .00 | 152.00 | 236.77 | 238.20 | 308.11 | 367.27 | 417.56 | 459.82 | 496.64 | 528.02 | 555.64 | 579.5 | 600.8 | 619.2 | 636.0 | 652.7 |
| 4e23RSmm6 | .00 | 166.27 | 241.79 | 243.05 | 307.40 | 363.76 | 412.12 | 453.55 | 489.11 | 519.65 | 546.01 | 569.0 | 589.1 | 606.7 | 623.4 | 640.2 |
| 3RSe24SRmm6 | .00 | 154.22 | 230.45 | 231.79 | 299.83 | 358.78 | 408.78 | 451.04 | 487.02 | 518.40 | 545.18 | 568.2 | 588.3 | 606.7 | 623.4 | 640.2 |
| 3RSe24RSmm6 | .00 | 153.55 | 229.33 | 230.66 | 298.95 | 358.32 | 408.78 | 451.04 | 487.44 | 518.40 | 545.18 | 568.2 | 588.7 | 606.7 | 623.4 | 640.2 |
| 4e24mm6 | .00 | 156.31 | 233.59 | 234.97 | 304.68 | 365.05 | 416.31 | 459.40 | 496.64 | 528.44 | 556.47 | 580.3 | 601.7 | 619.2 | 636.0 | 652.7 |
| 3e25mm6 | .00 | 161.00 | 239.49 | 240.79 | 306.65 | 363.55 | 412.12 | 453.55 | 489.11 | 519.65 | 546.01 | 569.0 | 589.1 | 606.7 | 623.4 | 640.2 |
| 4e33mm6 | .00 | 150.12 | 226.86 | 228.24 | 298.44 | 359.49 | 411.29 | 455.22 | 492.88 | 525.09 | 553.12 | 577.4 | 599.1 | 618.4 | 635.5 | 651.9 |
| 3e34RSmm6 | .00 | 147.23 | 234.09 | 235.48 | 305.68 | 364.97 | 415.47 | 458.15 | 494.97 | 526.77 | 554.38 | 578.6 | 600.0 | 619.2 | 636.0 | 652.7 |
| 2233mmmm6 | .00 | 153.93 | 236.77 | 238.24 | 309.78 | 370.54 | 422.17 | 466.52 | 505.43 | 538.90 | 568.61 | 594.5 | 618.0 | 640.2 | 656.9 | 673.6 |
| 223RS4RSmmmm6 | .00 | 148.78 | 229.62 | 231.00 | 301.25 | 361.75 | 413.38 | 457.73 | 495.80 | 528.86 | 557.73 | 583.2 | 605.4 | 627.6 | 644.3 | 661.1 |
| 223RS4SRmmmm6 | .00 | 146.19 | 226.56 | 227.99 | 299.07 | 360.49 | 412.96 | 457.31 | 495.80 | 528.86 | 558.15 | 583.2 | 605.8 | 627.6 | 644.3 | 661.1 |
| 223RS5mmmm6 | .00 | 152.93 | 234.39 | 235.81 | 306.06 | 366.06 | 417.14 | 460.66 | 498.31 | 530.95 | 559.82 | 584.9 | 607.1 | 627.6 | 644.3 | 661.1 |
| 2244mmmm6 | .00 | 165.48 | 237.90 | 239.24 | 307.65 | 368.23 | 420.49 | 465.68 | 504.59 | 538.90 | 568.61 | 595.0 | 618.4 | 640.2 | 656.9 | 677.8 |
| 224RS5mmmm6 | .00 | 150.08 | 227.86 | 229.24 | 299.32 | 360.37 | 412.54 | 457.31 | 495.39 | 528.86 | 558.15 | 583.2 | 605.8 | 627.6 | 644.3 | 661.1 |
| 2255mmmm6 | .00 | 157.49 | 228.45 | 229.79 | 298.99 | 360.58 | 413.80 | 459.40 | 499.15 | 533.88 | 564.00 | 590.8 | 614.2 | 636.0 | 656.9 | 673.6 |
| 2334RSmmmm6 | .00 | 151.04 | 240.04 | 241.50 | 312.25 | 371.46 | 421.75 | 464.42 | 501.66 | 533.88 | 562.33 | 587.0 | 609.2 | 627.6 | 648.5 | 665.3 |
| 2335mmmm6 | .00 | 149.54 | 232.55 | 233.97 | 305.06 | 365.93 | 417.56 | 461.50 | 499.57 | 532.62 | 561.49 | 586.2 | 608.4 | 627.6 | 644.3 | 661.1 |
| 23RS44mmmm6 | .00 | 144.72 | 230.33 | 231.79 | 303.55 | 364.64 | 416.31 | 460.66 | 498.73 | 531.37 | 560.24 | 585.3 | 607.9 | 627.6 | 644.3 | 661.1 |
| 23RS4RS5mmmm6 | .00 | 151.29 | 239.16 | 240.58 | 309.49 | 367.31 | 416.31 | 458.57 | 494.55 | 525.93 | 553.12 | 577.0 | 598.3 | 615.0 | 631.8 | 648.5 |
| 23R4S5mmmm6 | .00 | 157.11 | 244.72 | 246.06 | 312.21 | 368.36 | 416.73 | 458.15 | 494.55 | 525.51 | 553.12 | 576.6 | 597.9 | 615.0 | 631.8 | 648.5 |
| 3344mmmm6 | .00 | 147.07 | 236.52 | 237.99 | 310.33 | 371.12 | 423.00 | 467.35 | 505.85 | 539.74 | 569.02 | 595.4 | 618.4 | 640.2 | 656.9 | 677.8 |
| 3ip24mm5 | .00 | 156.86 | 233.17 | 234.51 | 302.63 | 361.96 | 412.54 | 455.64 | 492.46 | 524.26 | 552.29 | 576.1 | 597.5 | 615.0 | 631.8 | 648.5 |
| 33ee2m5 | .00 | 146.11 | 223.43 | 224.81 | 295.73 | 357.27 | 409.61 | 453.55 | 491.20 | 523.84 | 551.87 | 576.1 | 597.9 | 619.2 | 636.0 | 652.7 |
| 3e223mmm5 | .00 | 140.83 | 222.25 | 223.68 | 296.69 | 359.82 | 413.80 | 459.82 | 499.57 | 534.30 | 564.42 | 591.2 | 614.6 | 636.0 | 656.9 | 673.6 |
| 3RSe224mmm5 | .00 | 151.84 | 225.94 | 227.32 | 296.73 | 357.82 | 410.03 | 454.80 | 493.71 | 527.18 | 556.47 | 581.6 | 604.2 | 623.4 | 644.3 | 661.1 |
| 3e234mmm5 | .00 | 142.00 | 227.57 | 228.99 | 301.21 | 362.67 | 414.63 | 458.98 | 497.48 | 530.53 | 559.40 | 584.5 | 607.1 | 627.6 | 644.3 | 661.1 |
| 22334mmmmm5 | .00 | 150.62 | 232.84 | 234.30 | 305.85 | 367.61 | 420.91 | 466.52 | 506.26 | 541.41 | 572.79 | 600.0 | 624.3 | 644.3 | 665.3 | 686.2 |
| 22344mmmmm5 | .00 | 157.82 | 232.80 | 234.18 | 303.72 | 364.97 | 417.98 | 464.01 | 504.17 | 539.74 | 570.70 | 598.3 | 622.6 | 644.3 | 665.3 | 682.0 |

Table A2. Standard entropy of alkanes in J/K mol

| T/K | 0 | 200 | 298.15 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| methane | .00 | 172.70 | 186.38 | 186.59 | 197.51 | 207.18 | 216.00 | 224.79 | 232.74 | 240.69 | 248.22 | 255.3 | 262.0 | 268.3 | 275.0 | 280.9 |
| ethane | .00 | 210.57 | 229.23 | 229.56 | 246.59 | 262.82 | 278.76 | 293.83 | 309.73 | 322.28 | 336.09 | 349.1 | 361.6 | 373.3 | 385.0 | 396.3 |
| propane | .00 | 245.17 | 270.02 | 270.48 | 294.41 | 317.47 | 339.43 | 360.77 | 381.27 | 400.94 | 419.35 | 436.9 | 454.1 | 470.4 | 485.9 | 500.9 |
| butanes | | | | | | | | | | | | | | | | |
| 4 | .00 | 276.17 | 310.44 | 311.06 | 342.65 | 372.78 | 401.36 | 428.97 | 455.33 | 480.43 | 503.86 | 526.5 | 547.8 | 568.3 | 588.0 | 606.4 |
| 2m3 | .00 | 261.65 | 294.71 | 295.25 | 326.96 | 357.26 | 386.29 | 414.33 | 440.69 | 465.79 | 490.06 | 513.1 | 535.2 | 556.2 | 576.2 | 595.5 |
| pentanes | | | | | | | | | | | | | | | | |
| 5 | .00 | 307.59 | 349.56 | 350.31 | 389.35 | 426.67 | 462.44 | 496.33 | 528.55 | 559.09 | 587.96 | 615.2 | 641.1 | 666.2 | 689.6 | 712.2 |
| 2m4 | .00 | 303.45 | 343.74 | 344.45 | 383.49 | 420.89 | 456.58 | 490.89 | 523.11 | 554.07 | 583.36 | 611.4 | 637.8 | 663.3 | 687.5 | 710.6 |
| 22mm3 | .00 | 258.47 | 306.00 | 306.76 | 347.59 | 385.79 | 422.28 | 457.00 | 490.06 | 521.85 | 551.98 | 581.3 | 608.9 | 635.7 | 661.2 | 685.4 |
| hexanes | | | | | | | | | | | | | | | | |
| 6 | .00 | 339.06 | 388.85 | 389.72 | 436.17 | 480.60 | 523.11 | 563.28 | 601.35 | 637.33 | 671.64 | 703.9 | 734.4 | 763.3 | 790.9 | 817.7 |
| 2m5 | .00 | 332.86 | 380.98 | 381.86 | 428.64 | 473.53 | 516.42 | 557.00 | 595.91 | 632.31 | 667.04 | 699.7 | 731.1 | 760.8 | 788.8 | 816.0 |
| 3m5 | .00 | 335.79 | 383.03 | 383.87 | 430.02 | 474.41 | 516.83 | 557.42 | 595.91 | 631.89 | 666.62 | 699.3 | 730.6 | 759.9 | 788.4 | 815.2 |
| 22mm4 | .00 | 310.44 | 358.34 | 359.18 | 405.79 | 450.68 | 493.82 | 535.24 | 574.15 | 611.81 | 647.37 | 681.3 | 713.5 | 744.9 | 774.6 | 803.0 |
| 23mm4 | .00 | 319.85 | 365.92 | 366.75 | 412.90 | 457.46 | 500.10 | 540.68 | 579.59 | 616.41 | 651.14 | 684.2 | 716.0 | 746.5 | 775.0 | 802.6 |
| heptanes | | | | | | | | | | | | | | | | |
| 7 | .00 | 370.52 | 428.09 | 429.10 | 482.99 | 534.49 | 583.78 | 630.22 | 674.57 | 715.99 | 755.32 | 792.1 | 827.3 | 860.8 | 892.6 | 922.7 |
| 2m6 | .00 | 364.62 | 420.52 | 421.52 | 475.54 | 527.42 | 577.08 | 623.94 | 668.29 | 710.55 | 750.30 | 788.0 | 823.5 | 857.4 | 889.6 | 920.6 |
| 3RSm6 | 5.77 | 370.94 | 426.04 | 427.05 | 480.94 | 532.78 | 582.52 | 629.38 | 673.73 | 715.57 | 755.32 | 793.0 | 829.0 | 862.9 | 895.1 | 926.0 |
| 3e5 | .00 | 354.24 | 411.65 | 412.65 | 466.79 | 518.47 | 567.88 | 614.32 | 658.67 | 700.51 | 740.26 | 777.9 | 813.1 | 847.4 | 879.2 | 910.1 |
| 22mm5 | .00 | 336.80 | 392.69 | 393.70 | 448.80 | 501.86 | 552.40 | 600.93 | 646.54 | 689.63 | 730.64 | 769.5 | 806.8 | 841.9 | 875.8 | 908.5 |
| 23RSmm5 | 5.77 | 361.94 | 414.66 | 415.62 | 469.09 | 521.02 | 570.39 | 617.67 | 662.44 | 704.70 | 744.44 | 782.9 | 818.9 | 853.6 | 886.3 | 917.7 |
| 24mm5 | .00 | 340.27 | 397.00 | 398.05 | 454.24 | 507.88 | 558.67 | 606.79 | 651.98 | 694.65 | 735.24 | 773.7 | 810.1 | 844.9 | 877.9 | 909.3 |
| 33mm5 | .00 | 342.95 | 398.26 | 399.26 | 453.99 | 506.75 | 557.00 | 605.12 | 650.72 | 694.24 | 735.24 | 774.1 | 811.4 | 847.0 | 880.8 | 913.5 |
| 223mmm4 | .00 | 329.14 | 383.45 | 384.41 | 438.47 | 490.64 | 540.68 | 588.38 | 633.99 | 677.50 | 718.50 | 758.3 | 795.5 | 831.5 | 865.8 | 898.4 |
| octanes | | | | | | | | | | | | | | | | |
| 8 | .00 | 401.98 | 467.34 | 468.47 | 529.76 | 588.42 | 644.45 | 697.58 | 747.37 | 794.23 | 838.58 | 880.8 | 920.6 | 958.2 | 993.8 | 1028.1 |
| 2m7 | .00 | 396.00 | 459.68 | 460.81 | 522.32 | 581.35 | 637.75 | 690.89 | 741.51 | 789.21 | 833.98 | 876.2 | 916.8 | 954.9 | 991.3 | 1026.0 |
| 3RSm7 | 5.77 | 402.74 | 465.62 | 466.75 | 527.88 | 586.71 | 642.77 | 695.91 | 746.54 | 793.81 | 839.00 | 881.3 | 921.4 | 959.9 | 995.9 | 1030.6 |
| 4m7 | .00 | 394.54 | 457.50 | 458.68 | 520.31 | 579.64 | 636.08 | 689.63 | 740.26 | 787.96 | 833.14 | 875.4 | 916.0 | 954.1 | 990.5 | 1025.2 |
| 3e6 | .00 | 392.61 | 457.97 | 459.09 | 521.02 | 580.10 | 636.50 | 689.63 | 739.84 | 787.54 | 831.89 | 874.6 | 914.7 | 952.8 | 989.2 | 1023.9 |
| 22mm6 | .00 | 369.18 | 432.82 | 433.99 | 496.04 | 555.75 | 613.07 | 667.04 | 718.50 | 767.04 | 813.48 | 857.0 | 898.8 | 938.2 | 976.2 | 1012.2 |
| 23RSmm6 | 5.77 | 391.44 | 452.07 | 453.15 | 514.24 | 573.32 | 629.80 | 684.61 | 733.98 | 782.10 | 827.29 | 870.4 | 911.0 | 949.9 | 986.7 | 1022.3 |
| 24RSmm6 | 5.77 | 383.82 | 447.71 | 448.89 | 512.19 | 572.65 | 629.80 | 684.19 | 735.24 | 783.35 | 828.96 | 872.1 | 913.1 | 952.4 | 989.2 | 1024.4 |
| 25mm6 | .00 | 380.77 | 442.44 | 443.57 | 504.87 | 563.99 | 620.60 | 674.15 | 724.78 | 772.48 | 818.08 | 860.8 | 901.8 | 940.7 | 977.5 | 1012.6 |
| 33mm6 | .00 | 375.08 | 438.34 | 439.51 | 502.69 | 563.53 | 621.43 | 676.66 | 728.54 | 777.50 | 823.94 | 867.9 | 909.7 | 949.5 | 987.5 | 1023.9 |
| 3RS4RSmm6 | 5.77 | 387.05 | 446.08 | 447.17 | 507.75 | 566.62 | 623.11 | 676.66 | 727.29 | 774.99 | 820.17 | 863.3 | 904.3 | 943.2 | 979.6 | 1015.1 |
| 3R4Smm6 | .00 | 386.08 | 445.75 | 446.88 | 507.84 | 566.83 | 623.11 | 676.66 | 727.29 | 775.41 | 820.59 | 863.7 | 904.3 | 943.2 | 980.0 | 1015.1 |
| 3e2m5 | .00 | 379.14 | 443.87 | 444.99 | 507.75 | 567.33 | 623.94 | 677.50 | 728.13 | 775.82 | 821.01 | 863.7 | 904.3 | 943.2 | 980.0 | 1015.1 |
| 3e3m5 | .00 | 362.19 | 424.70 | 425.83 | 488.01 | 547.88 | 605.12 | 659.51 | 710.97 | 759.92 | 805.95 | 849.9 | 891.7 | 931.0 | 969.1 | 1005.5 |
| 223RSmmm5 | 5.77 | 363.11 | 423.99 | 425.12 | 486.88 | 546.62 | 603.86 | 658.25 | 709.72 | 759.09 | 805.53 | 849.5 | 891.7 | 931.9 | 970.4 | 1007.2 |
| 224mmm5 | .00 | 360.06 | 423.07 | 424.20 | 486.42 | 546.33 | 603.44 | 658.25 | 709.72 | 759.09 | 805.53 | 849.9 | 892.1 | 932.7 | 970.8 | 1007.6 |
| 233mmm5 | .00 | 365.96 | 427.13 | 428.26 | 490.43 | 550.52 | 608.05 | 662.44 | 714.32 | 763.69 | 810.55 | 854.9 | 897.2 | 937.3 | 975.8 | 1012.6 |
| 234mmm5 | .00 | 365.75 | 428.51 | 429.68 | 492.90 | 553.28 | 610.56 | 664.95 | 715.99 | 764.53 | 810.55 | 854.1 | 895.5 | 935.2 | 972.5 | 1008.5 |
| 2233mmmm4 | .00 | 326.92 | 389.47 | 390.60 | 452.53 | 512.40 | 569.97 | 624.78 | 677.08 | 727.29 | 774.57 | 820.2 | 863.7 | 905.1 | 944.9 | 983.3 |
| nonanes | | | | | | | | | | | | | | | | |
| 9 | .00 | 433.41 | 506.54 | 507.84 | 576.54 | 642.31 | 705.11 | 764.11 | 820.17 | 872.89 | 922.26 | 969.1 | 1013.5 | 1055.3 | 1095.1 | 1133.1 |
| 2m8 | .00 | 427.42 | 498.93 | 500.18 | 569.09 | 635.24 | 698.42 | 758.25 | 814.32 | 867.45 | 917.66 | 964.9 | 1009.7 | 1052.4 | 1092.6 | 1131.5 |
| 3RSm8 | 5.77 | 434.07 | 504.78 | 506.04 | 574.66 | 640.64 | 703.44 | 763.27 | 819.34 | 872.47 | 922.68 | 970.0 | 1014.7 | 1057.4 | 1097.6 | 1136.1 |
| 4RSm8 | 5.77 | 432.07 | 502.82 | 504.07 | 572.98 | 639.26 | 702.60 | 762.43 | 818.50 | 871.64 | 921.85 | 969.5 | 1014.3 | 1056.6 | 1097.2 | 1135.6 |
| 3e7 | .00 | 424.37 | 497.46 | 498.76 | 567.96 | 633.99 | 696.75 | 756.16 | 812.22 | 865.36 | 915.15 | 962.4 | 1007.2 | 1049.9 | 1090.0 | 1128.5 |
| 4e7 | .00 | 421.86 | 495.12 | 496.42 | 566.12 | 632.61 | 695.91 | 755.32 | 811.81 | 864.94 | 914.73 | 962.0 | 1006.8 | 1049.5 | 1089.6 | 1128.1 |
| 22mm7 | .00 | 400.39 | 471.90 | 473.19 | 542.77 | 609.76 | 673.73 | 734.40 | 791.72 | 846.11 | 897.16 | 946.1 | 992.1 | 1036.1 | 1077.9 | 1118.1 |
| 23RSmm7 | 5.77 | 423.78 | 492.36 | 493.61 | 561.94 | 627.84 | 690.89 | 750.72 | 807.20 | 860.34 | 910.97 | 958.7 | 1003.9 | 1046.9 | 1087.9 | 1127.3 |
| 24RSmm7 | 5.77 | 412.78 | 484.53 | 485.83 | 556.96 | 624.95 | 689.63 | 750.30 | 807.20 | 861.18 | 912.22 | 960.3 | 1005.9 | 1049.0 | 1090.0 | 1129.4 |
| 25RSmm7 | 5.77 | 425.12 | 493.86 | 495.12 | 563.61 | 629.63 | 692.56 | 752.39 | 809.30 | 862.43 | 913.06 | 960.8 | 1006.4 | 1049.5 | 1090.5 | 1129.4 |
| 26mm7 | .00 | 411.86 | 481.60 | 482.90 | 552.02 | 618.59 | 682.10 | 742.35 | 798.84 | 852.81 | 903.02 | 951.1 | 996.7 | 1039.8 | 1080.8 | 1120.2 |
| 33mm7 | .00 | 407.51 | 478.63 | 479.93 | 550.18 | 617.75 | 682.10 | 743.19 | 800.51 | 855.32 | 906.78 | 955.3 | 1001.8 | 1046.1 | 1087.9 | 1128.1 |
| 3RS4SRmm7 | 5.77 | 421.44 | 489.01 | 490.27 | 558.84 | 625.16 | 688.38 | 748.63 | 805.11 | 858.25 | 908.87 | 957.0 | 1002.2 | 1045.3 | 1086.3 | 1125.6 |
| 3RS4RSmm7 | 5.77 | 422.40 | 489.30 | 490.56 | 558.76 | 624.91 | 688.38 | 748.21 | 804.69 | 858.25 | 908.87 | 956.6 | 1001.8 | 1045.3 | 1086.3 | 1125.2 |
| 3RS5RSmm7 | 5.77 | 411.86 | 482.44 | 483.74 | 553.74 | 620.81 | 684.61 | 744.86 | 801.76 | 855.32 | 905.95 | 954.1 | 999.2 | 1042.3 | 1083.3 | 1122.7 |
| 3R5Smm7 | .00 | 409.93 | 481.35 | 482.65 | 553.15 | 620.39 | 684.19 | 744.44 | 801.35 | 854.90 | 905.53 | 953.2 | 998.8 | 1041.9 | 1082.9 | 1122.3 |
| 44mm7 | .00 | 395.67 | 466.92 | 468.22 | 539.85 | 608.80 | 674.15 | 736.08 | 794.23 | 849.04 | 900.93 | 950.3 | 996.7 | 1040.7 | 1082.9 | 1123.1 |
| 3RSe2m6 | 5.77 | 424.24 | 492.57 | 493.86 | 564.20 | 630.97 | 694.15 | 753.98 | 810.47 | 864.11 | 914.31 | 962.4 | 1007.6 | 1050.7 | 1091.3 | 1130.6 |
| 4e2m6 | .00 | 405.04 | 479.55 | 480.89 | 552.19 | 619.76 | 683.78 | 744.03 | 800.93 | 854.90 | 905.53 | 953.2 | 998.8 | 1041.9 | 1082.9 | 1121.8 |
| 3e3m6 | .00 | 397.67 | 468.13 | 469.43 | 539.93 | 607.79 | 672.48 | 733.57 | 791.30 | 846.11 | 897.16 | 946.1 | 992.6 | 1036.5 | 1078.7 | 1118.9 |
| 3e4RSm6 | 5.77 | 415.04 | 486.50 | 487.80 | 557.92 | 624.61 | 687.96 | 747.79 | 804.27 | 857.41 | 907.62 | 955.3 | 1000.5 | 1043.6 | 1084.6 | 1123.5 |
| 223RSmmm6 | 5.77 | 392.82 | 461.65 | 462.90 | 532.11 | 598.97 | 662.86 | 723.52 | 781.26 | 835.65 | 887.54 | 936.5 | 983.3 | 1027.7 | 1070.0 | 1110.5 |
| 224RSmmm6 | 5.77 | 397.67 | 467.67 | 468.93 | 538.13 | 604.87 | 668.71 | 729.38 | 787.12 | 841.51 | 892.98 | 942.3 | 988.8 | 1033.6 | 1075.8 | 1116.4 |
| 225mmm6 | .00 | 392.69 | 461.77 | 463.03 | 531.85 | 598.42 | 662.02 | 722.69 | 780.43 | 834.82 | 886.28 | 935.7 | 982.1 | 1026.4 | 1069.1 | 1109.7 |
| 233mmm6 | .00 | 392.19 | 461.35 | 462.65 | 533.15 | 601.23 | 666.20 | 727.71 | 785.45 | 840.68 | 892.56 | 941.9 | 989.2 | 1033.6 | 1076.2 | 1116.8 |
| 23RS4SRmmm6 | 5.77 | 401.19 | 471.44 | 472.73 | 543.36 | 610.76 | 674.57 | 735.24 | 792.56 | 846.11 | 897.16 | 945.7 | 991.7 | 1035.6 | 1077.1 | 1116.8 |
| 23RS4RSmmm6 | 5.77 | 402.95 | 471.77 | 473.07 | 543.07 | 610.30 | 674.15 | 734.82 | 791.72 | 846.11 | 897.16 | 945.7 | 991.3 | 1035.2 | 1076.7 | 1116.4 |
| 23RS5mmm6 | 5.77 | 405.67 | 474.62 | 475.87 | 545.95 | 613.36 | 677.50 | 738.17 | 795.49 | 849.46 | 900.51 | 949.0 | 995.1 | 1039.0 | 1080.4 | 1120.6 |
| 244mmm6 | .00 | 398.13 | 468.47 | 469.72 | 539.97 | 607.58 | 672.06 | 733.57 | 791.30 | 846.53 | 898.41 | 947.8 | 994.6 | 1039.4 | 1082.1 | 1122.7 |
| 334RSmmm6 | 5.77 | 400.06 | 467.71 | 468.97 | 538.72 | 606.29 | 670.81 | 731.89 | 790.05 | 844.86 | 896.74 | 945.7 | 992.6 | 1037.3 | 1080.0 | 1120.6 |
| 33ee5 | .00 | 363.24 | 436.63 | 437.92 | 508.76 | 576.12 | 639.84 | 700.51 | 757.83 | 812.22 | 863.27 | 912.2 | 958.2 | 1002.2 | 1044.0 | 1084.2 |
| 3e22mm5 | .00 | 393.15 | 461.10 | 462.32 | 529.93 | 595.54 | 658.67 | 718.50 | 775.82 | 829.80 | 881.26 | 930.2 | 976.7 | 1021.0 | 1063.3 | 1103.4 |
| 3e23mm5 | .00 | 385.54 | 455.37 | 456.21 | 526.42 | 593.78 | 657.83 | 718.92 | 776.66 | 831.05 | 882.93 | 931.9 | 978.7 | 1023.5 | 1065.8 | 1106.4 |
| 3e24mm5 | .00 | 402.36 | 471.19 | 472.44 | 541.18 | 607.33 | 670.39 | 730.64 | 787.12 | 841.09 | 891.72 | 940.3 | 985.9 | 1029.8 | 1071.2 | 1111.0 |
| 2233mmmm5 | .00 | 367.26 | 436.71 | 437.97 | 508.38 | 576.33 | 641.52 | 703.02 | 761.60 | 817.66 | 870.80 | 921.0 | 969.1 | 1015.1 | 1059.1 | 1101.3 |
| 223RS4mmmm5 | 5.77 | 383.41 | 451.31 | 452.57 | 521.48 | 588.17 | 651.98 | 713.06 | 770.80 | 825.61 | 877.49 | 927.3 | 974.6 | 1019.8 | 1062.4 | 1103.8 |
| 2244mmmm5 | .00 | 358.05 | 430.69 | 431.98 | 502.48 | 570.18 | 634.82 | 696.33 | 754.90 | 810.55 | 863.69 | 913.9 | 962.0 | 1008.0 | 1052.0 | 1094.2 |
| 2334mmmm5 | .00 | 365.54 | 437.00 | 438.30 | 510.35 | 579.18 | 644.45 | 706.37 | 764.95 | 820.17 | 872.47 | 922.7 | 970.4 | 1015.6 | 1058.7 | 1100.1 |

Table A2 continued

| T/K | 0 | 200 | 298.15 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| decanes | | | | | | | | | | | | | | | | |
| 10 | .00 | 464.83 | 545.79 | 547.21 | 623.32 | 696.24 | 765.78 | 831.47 | 893.39 | 951.55 | 1006.36 | 1057.8 | 1106.8 | 1153.2 | 1196.7 | 1238.6 |
| 2m9 | .00 | 458.84 | 538.13 | 539.55 | 615.91 | 689.17 | 759.09 | 825.19 | 887.54 | 946.11 | 1001.34 | 1053.6 | 1103.0 | 1149.9 | 1194.2 | 1236.9 |
| 3RSm9 | 5.77 | 465.50 | 543.99 | 545.41 | 621.43 | 694.53 | 764.11 | 830.22 | 892.56 | 951.13 | 1006.36 | 1058.7 | 1107.6 | 1154.5 | 1199.2 | 1241.5 |
| 4RSm9 | 5.77 | 463.45 | 541.98 | 543.40 | 619.76 | 693.19 | 763.27 | 829.38 | 891.72 | 950.30 | 1005.94 | 1057.8 | 1107.6 | 1154.5 | 1198.8 | 1241.1 |
| 5m9 | .00 | 458.17 | 536.62 | 538.05 | 614.20 | 687.46 | 757.41 | 823.52 | 885.86 | 944.44 | 999.67 | 1052.0 | 1101.3 | 1148.2 | 1192.5 | 1234.8 |
| 3e8 | .00 | 455.75 | 536.67 | 538.09 | 614.74 | 687.92 | 757.83 | 823.52 | 885.44 | 944.02 | 999.25 | 1051.1 | 1100.5 | 1147.4 | 1191.7 | 1234.0 |
| 4RSe8 | 5.77 | 459.56 | 540.52 | 541.98 | 618.92 | 692.39 | 762.43 | 828.12 | 890.47 | 949.04 | 1004.27 | 1056.6 | 1105.9 | 1152.4 | 1196.7 | 1239.4 |
| 22mm8 | .00 | 431.82 | 511.14 | 512.57 | 589.55 | 663.61 | 734.40 | 801.35 | 864.52 | 924.36 | 980.84 | 1034.4 | 1085.0 | 1133.1 | 1179.2 | 1223.1 |
| 23RSmm8 | 5.77 | 455.12 | 531.52 | 532.90 | 608.67 | 681.81 | 751.56 | 817.66 | 880.01 | 939.00 | 994.65 | 1047.4 | 1097.2 | 1144.9 | 1189.6 | 1232.7 |
| 24RSmm8 | 5.77 | 444.58 | 524.07 | 525.54 | 603.94 | 678.88 | 749.88 | 817.25 | 880.01 | 939.42 | 995.48 | 1048.6 | 1098.4 | 1146.1 | 1191.3 | 1234.4 |
| 25RSmm8 | 5.77 | 454.49 | 531.10 | 532.48 | 608.71 | 682.27 | 752.39 | 818.92 | 881.68 | 940.67 | 996.32 | 1049.0 | 1099.2 | 1146.5 | 1191.7 | 1234.4 |
| 26RSmm8 | 5.77 | 455.71 | 532.48 | 533.86 | 610.14 | 683.65 | 753.65 | 820.17 | 882.93 | 941.93 | 997.58 | 1050.3 | 1100.5 | 1147.8 | 1193.0 | 1235.6 |
| 27mm8 | .00 | 443.24 | 520.85 | 522.27 | 598.84 | 672.52 | 742.77 | 809.30 | 872.06 | 931.47 | 987.12 | 1039.8 | 1089.6 | 1137.3 | 1182.5 | 1225.6 |
| 33mm8 | .00 | 438.72 | 517.71 | 519.18 | 596.96 | 671.73 | 743.19 | 810.55 | 874.15 | 933.98 | 990.88 | 1044.4 | 1095.5 | 1143.6 | 1189.6 | 1233.6 |
| 3RS4SRmm8 | 5.77 | 453.78 | 529.30 | 530.72 | 606.54 | 679.72 | 749.46 | 815.57 | 877.91 | 936.91 | 992.55 | 1045.3 | 1095.1 | 1142.3 | 1187.5 | 1230.2 |
| 3RS4RSmm8 | 5.77 | 454.74 | 529.60 | 530.98 | 606.41 | 679.47 | 749.05 | 815.57 | 877.91 | 936.91 | 992.55 | 1045.3 | 1095.1 | 1142.3 | 1187.1 | 1230.2 |
| 3RS5RSmm8 | 5.77 | 446.58 | 524.99 | 526.46 | 604.28 | 678.88 | 749.88 | 816.41 | 879.59 | 939.00 | 994.65 | 1047.8 | 1097.6 | 1145.3 | 1190.5 | 1233.6 |
| 3RS5SRmm8 | 5.77 | 444.66 | 523.95 | 525.37 | 603.69 | 678.46 | 749.46 | 816.41 | 879.17 | 938.58 | 994.23 | 1047.4 | 1097.2 | 1144.9 | 1190.0 | 1233.1 |
| 3RS6RSmm8 | 5.77 | 451.69 | 527.42 | 528.84 | 604.41 | 677.42 | 746.95 | 813.48 | 875.82 | 934.40 | 990.04 | 1042.8 | 1092.6 | 1140.2 | 1185.0 | 1227.7 |
| 3R6Smm8 | .00 | 451.69 | 527.42 | 528.84 | 604.41 | 677.42 | 746.95 | 813.48 | 875.82 | 934.40 | 990.04 | 1042.8 | 1092.6 | 1140.2 | 1185.0 | 1227.7 |
| 44mm8 | .00 | 433.87 | 512.98 | 514.45 | 593.11 | 668.76 | 740.68 | 808.46 | 872.47 | 932.72 | 989.63 | 1043.6 | 1094.6 | 1142.8 | 1188.8 | 1233.1 |
| 4RS5RSmm8 | 5.77 | 446.21 | 521.02 | 522.40 | 598.21 | 671.68 | 741.93 | 808.46 | 870.80 | 930.21 | 985.86 | 1038.6 | 1088.4 | 1136.1 | 1180.8 | 1223.9 |
| 4R5Smm8 | .00 | 445.25 | 520.73 | 522.15 | 598.38 | 671.98 | 742.35 | 808.88 | 871.22 | 930.21 | 985.86 | 1039.0 | 1088.8 | 1136.1 | 1181.3 | 1224.3 |
| 4p7 | .00 | 442.23 | 523.28 | 524.74 | 602.19 | 676.20 | 746.54 | 812.64 | 875.40 | 933.98 | 989.63 | 1041.9 | 1091.3 | 1138.2 | 1182.5 | 1224.8 |
| 4ip7 | .00 | 437.92 | 518.26 | 519.68 | 597.50 | 671.52 | 741.51 | 808.04 | 870.38 | 929.38 | 985.02 | 1037.3 | 1087.5 | 1134.8 | 1179.6 | 1222.7 |
| 3RSe2m7 | 5.77 | 446.04 | 526.33 | 527.80 | 605.33 | 679.09 | 749.05 | 815.15 | 877.49 | 936.49 | 991.72 | 1044.4 | 1094.2 | 1141.5 | 1186.3 | 1229.4 |
| 4RSe2m7 | 5.77 | 439.76 | 522.15 | 523.61 | 602.73 | 677.83 | 749.05 | 815.99 | 879.17 | 938.16 | 994.23 | 1047.4 | 1097.2 | 1144.9 | 1189.6 | 1232.7 |
| 5e2m7 | .00 | 446.79 | 525.75 | 527.17 | 603.69 | 677.00 | 746.95 | 813.06 | 875.40 | 933.98 | 989.63 | 1042.3 | 1092.1 | 1139.4 | 1184.2 | 1227.3 |
| 3e3m7 | .00 | 430.10 | 508.42 | 509.85 | 587.42 | 662.02 | 733.15 | 800.09 | 863.69 | 923.52 | 980.42 | 1034.0 | 1084.6 | 1133.1 | 1178.7 | 1222.7 |
| 4RSe3RSm7 | 5.77 | 444.41 | 523.70 | 525.16 | 602.82 | 676.70 | 746.95 | 813.06 | 875.40 | 933.98 | 989.63 | 1042.3 | 1092.1 | 1139.4 | 1184.2 | 1227.3 |
| 4RSe3SRm7 | 5.77 | 444.41 | 523.70 | 525.16 | 602.82 | 676.70 | 746.95 | 813.06 | 875.40 | 933.98 | 989.63 | 1042.3 | 1092.1 | 1139.4 | 1184.2 | 1227.3 |
| 3e5RSm7 | 5.77 | 443.70 | 525.24 | 526.71 | 604.95 | 679.22 | 749.88 | 815.99 | 878.75 | 937.74 | 993.39 | 1046.1 | 1096.3 | 1143.6 | 1188.8 | 1231.5 |
| 3e4RSm7 | 5.77 | 444.49 | 523.86 | 525.33 | 603.07 | 677.08 | 747.37 | 813.48 | 875.82 | 934.82 | 990.46 | 1042.8 | 1092.6 | 1139.8 | 1185.0 | 1227.7 |
| 4e4m7 | .00 | 424.03 | 502.44 | 503.91 | 582.73 | 658.59 | 730.64 | 798.42 | 862.43 | 923.10 | 979.58 | 1033.6 | 1084.6 | 1133.1 | 1179.2 | 1223.1 |
| 223RSmmm7 | 5.77 | 424.41 | 501.06 | 502.44 | 579.05 | 652.98 | 723.52 | 790.89 | 854.06 | 914.31 | 970.80 | 1024.8 | 1076.2 | 1124.8 | 1171.2 | 1215.6 |
| 224RSmmm7 | 5.77 | 426.88 | 504.83 | 506.25 | 583.40 | 657.75 | 728.96 | 796.33 | 859.92 | 920.17 | 977.07 | 1031.0 | 1082.5 | 1131.0 | 1177.9 | 1222.3 |
| 225RSmmm7 | 5.77 | 430.69 | 506.79 | 508.17 | 584.15 | 657.63 | 728.13 | 795.07 | 858.25 | 918.08 | 974.98 | 1029.0 | 1080.0 | 1129.0 | 1175.0 | 1219.7 |
| 226mmm7 | .00 | 421.90 | 499.51 | 500.93 | 578.26 | 652.81 | 723.94 | 791.30 | 855.32 | 915.57 | 972.47 | 1026.4 | 1077.9 | 1126.9 | 1173.3 | 1217.7 |
| 233mmm7 | .00 | 424.53 | 501.44 | 502.86 | 580.39 | 655.16 | 726.45 | 794.23 | 857.83 | 918.08 | 975.40 | 1029.8 | 1080.8 | 1129.8 | 1176.7 | 1221.0 |
| 23RS4SRmmm7 | 5.77 | 430.39 | 508.59 | 510.01 | 588.38 | 663.19 | 733.98 | 800.93 | 864.11 | 923.94 | 980.00 | 1034.0 | 1084.2 | 1132.3 | 1177.5 | 1221.4 |
| 23RS4RSmmm7 | 5.77 | 432.28 | 509.05 | 510.47 | 588.21 | 662.81 | 733.57 | 800.93 | 864.11 | 923.52 | 980.00 | 1033.1 | 1083.8 | 1131.9 | 1177.5 | 1221.0 |
| 23RS5RSmmm7 | 5.77 | 439.05 | 514.37 | 515.75 | 592.48 | 666.54 | 737.33 | 803.86 | 867.03 | 926.45 | 982.93 | 1036.1 | 1086.7 | 1134.8 | 1180.4 | 1223.9 |
| 23RS5SRmmm7 | 5.77 | 437.05 | 513.91 | 515.33 | 592.82 | 667.08 | 737.75 | 804.27 | 867.45 | 926.87 | 982.93 | 1036.5 | 1086.7 | 1134.8 | 1180.4 | 1223.9 |
| 23RS6mmm7 | 5.77 | 445.87 | 519.89 | 521.27 | 596.87 | 670.14 | 740.26 | 806.79 | 869.55 | 928.54 | 984.61 | 1037.7 | 1088.4 | 1136.5 | 1181.7 | 1225.6 |
| 244mmm7 | .00 | 424.41 | 502.73 | 504.20 | 582.90 | 658.63 | 730.64 | 798.84 | 863.27 | 923.94 | 981.26 | 1036.1 | 1087.5 | 1136.5 | 1183.3 | 1227.7 |
| 24RS5SRmmm7 | 5.77 | 435.54 | 511.31 | 512.69 | 590.26 | 664.99 | 736.08 | 803.02 | 866.20 | 926.03 | 982.51 | 1035.6 | 1086.3 | 1134.4 | 1180.0 | 1223.5 |
| 24RS5RSmmm7 | 5.77 | 436.58 | 511.77 | 513.19 | 590.39 | 664.91 | 736.08 | 803.02 | 866.20 | 926.03 | 982.09 | 1035.6 | 1086.3 | 1134.4 | 1180.0 | 1223.5 |
| 246mmm7 | .00 | 420.48 | 500.98 | 502.44 | 583.15 | 659.88 | 732.31 | 800.09 | 864.11 | 924.36 | 980.84 | 1034.8 | 1085.4 | 1134.0 | 1179.6 | 1223.5 |
| 255mmm7 | .00 | 431.77 | 508.76 | 510.18 | 587.21 | 661.43 | 732.31 | 799.67 | 863.27 | 923.52 | 980.42 | 1034.4 | 1085.9 | 1134.8 | 1181.3 | 1225.6 |
| 334RSmmm7 | 5.77 | 429.76 | 505.37 | 506.79 | 584.03 | 658.67 | 729.80 | 797.58 | 861.18 | 921.43 | 978.75 | 1032.7 | 1084.2 | 1133.1 | 1179.6 | 1224.3 |
| 335RSmmm7 | 5.77 | 436.42 | 513.53 | 514.95 | 591.98 | 666.29 | 737.33 | 804.69 | 868.29 | 928.96 | 985.86 | 1039.8 | 1091.3 | 1140.2 | 1187.1 | 1231.5 |
| 3RS44mmm7 | 5.77 | 426.29 | 501.94 | 503.36 | 581.52 | 657.08 | 728.96 | 797.16 | 861.18 | 921.85 | 979.17 | 1033.1 | 1084.6 | 1133.6 | 1180.4 | 1224.8 |
| 3RS45RSmmm7 | 5.77 | 432.78 | 508.93 | 510.31 | 587.63 | 661.89 | 732.73 | 799.25 | 862.43 | 921.85 | 977.91 | 1031.5 | 1082.1 | 1129.8 | 1175.4 | 1219.3 |
| s3R45Smmm7 | .00 | 424.83 | 502.57 | 503.99 | 582.15 | 656.66 | 727.29 | 794.23 | 856.99 | 916.41 | 972.47 | 1026.0 | 1076.2 | 1124.4 | 1170.0 | 1213.5 |
| r3R45Smmm7 | .00 | 428.72 | 503.82 | 505.24 | 581.94 | 655.95 | 726.45 | 793.40 | 856.16 | 915.99 | 972.05 | 1025.2 | 1075.8 | 1123.9 | 1169.5 | 1213.1 |
| 3ip2m6 | .00 | 431.61 | 508.13 | 509.51 | 585.70 | 659.05 | 728.96 | 795.49 | 858.25 | 917.24 | 973.31 | 1026.4 | 1076.7 | 1124.8 | 1170.4 | 1213.9 |
| 33ee6 | .00 | 401.10 | 482.36 | 483.86 | 562.86 | 638.09 | 709.30 | 776.66 | 840.26 | 900.09 | 956.57 | 1010.1 | 1061.2 | 1109.3 | 1155.3 | 1199.2 |
| 34ee6 | .00 | 426.17 | 509.80 | 511.31 | 590.81 | 665.24 | 735.24 | 801.35 | 863.69 | 922.26 | 977.49 | 1030.2 | 1079.6 | 1126.9 | 1171.6 | 1214.7 |
| 3RSe22mm6 | 5.77 | 428.30 | 503.95 | 505.29 | 580.31 | 653.07 | 722.69 | 789.21 | 852.39 | 911.80 | 968.29 | 1022.3 | 1073.3 | 1121.8 | 1168.3 | 1212.6 |
| 4e22mm6 | .00 | 418.30 | 498.34 | 499.76 | 576.83 | 650.68 | 721.01 | 787.96 | 851.55 | 911.39 | 968.29 | 1021.8 | 1073.3 | 1121.8 | 1168.3 | 1212.6 |
| 3RSe23mm6 | 5.77 | 417.59 | 494.87 | 496.29 | 574.70 | 649.97 | 721.43 | 789.21 | 852.81 | 913.48 | 970.38 | 1024.8 | 1075.8 | 1124.8 | 1171.2 | 1216.0 |
| 4e23RSmm6 | 5.77 | 425.54 | 506.71 | 508.17 | 587.08 | 661.85 | 732.73 | 799.25 | 862.01 | 921.85 | 977.91 | 1031.0 | 1081.3 | 1129.4 | 1175.0 | 1218.5 |
| 3RSe24SRmm6 | 5.77 | 434.70 | 510.93 | 512.32 | 588.55 | 661.89 | 731.89 | 798.00 | 860.76 | 920.17 | 975.82 | 1029.0 | 1079.6 | 1127.3 | 1172.9 | 1216.4 |
| 3RSe24RSmm6 | 5.77 | 435.37 | 511.23 | 512.61 | 588.55 | 661.77 | 731.47 | 798.00 | 860.76 | 919.75 | 975.82 | 1029.0 | 1079.2 | 1127.3 | 1172.9 | 1216.4 |
| 4e24mm6 | .00 | 420.43 | 497.67 | 499.09 | 576.46 | 651.06 | 722.27 | 789.63 | 853.65 | 913.90 | 971.22 | 1025.2 | 1076.7 | 1125.6 | 1172.5 | 1216.8 |
| 3e25mm6 | 5.77 | 429.43 | 509.05 | 510.52 | 589.05 | 663.69 | 734.40 | 800.93 | 864.11 | 923.52 | 979.58 | 1032.7 | 1083.3 | 1131.0 | 1176.7 | 1220.2 |
| 4e33mm6 | .00 | 430.02 | 504.62 | 506.00 | 581.48 | 654.74 | 724.78 | 791.72 | 854.90 | 915.15 | 971.63 | 1026.0 | 1077.1 | 1125.6 | 1172.0 | 1216.4 |
| 3e34RSmm6 | 5.77 | 419.68 | 495.54 | 496.96 | 574.66 | 649.34 | 720.59 | 787.96 | 851.55 | 911.80 | 968.29 | 1022.7 | 1073.7 | 1122.7 | 1169.1 | 1213.5 |
| 2233mmmm6 | .00 | 393.49 | 470.89 | 472.32 | 550.93 | 626.71 | 698.84 | 767.46 | 832.31 | 893.81 | 952.39 | 1007.6 | 1060.3 | 1111.0 | 1158.7 | 1204.7 |
| 223RS4RSmmmm6 | 5.77 | 412.53 | 487.55 | 488.93 | 565.24 | 639.09 | 709.72 | 777.08 | 840.68 | 900.93 | 958.25 | 1012.6 | 1064.1 | 1113.5 | 1160.3 | 1205.5 |
| 223RS4SRmmmm6 | 5.77 | 414.66 | 488.51 | 489.89 | 565.45 | 638.92 | 709.30 | 776.66 | 840.26 | 900.51 | 957.83 | 1012.2 | 1063.7 | 1113.5 | 1160.3 | 1205.1 |
| 223RS5mmmm6 | 5.77 | 407.63 | 484.45 | 485.83 | 563.61 | 638.46 | 709.72 | 777.50 | 841.51 | 902.18 | 959.50 | 1014.3 | 1065.8 | 1115.6 | 1162.4 | 1207.6 |
| 2244mmmm6 | .00 | 401.77 | 481.56 | 482.99 | 561.35 | 636.62 | 708.46 | 776.66 | 841.51 | 903.02 | 961.17 | 1016.8 | 1069.5 | 1119.7 | 1167.9 | 1214.3 |
| 224RS5mmmm6 | 5.77 | 419.43 | 494.28 | 495.66 | 571.44 | 644.91 | 715.16 | 782.52 | 846.11 | 906.36 | 963.27 | 1018.1 | 1069.5 | 1118.9 | 1166.2 | 1211.0 |
| 2255mmmm6 | .00 | 393.99 | 470.14 | 471.48 | 547.25 | 620.68 | 691.31 | 758.67 | 822.68 | 883.35 | 941.09 | 996.3 | 1048.6 | 1098.8 | 1146.5 | 1192.5 |
| 2334RSmmmm6 | 5.77 | 405.20 | 483.07 | 484.53 | 564.03 | 640.22 | 712.65 | 780.84 | 845.28 | 906.36 | 964.10 | 1018.9 | 1070.8 | 1120.6 | 1167.4 | 1213.1 |
| 2335mmmm6 | .00 | 415.71 | 491.56 | 492.99 | 570.31 | 645.03 | 716.41 | 784.19 | 848.63 | 909.29 | 966.61 | 1021.4 | 1073.7 | 1123.1 | 1170.4 | 1215.6 |
| 23RS44mmmm6 | 5.77 | 420.10 | 494.62 | 496.00 | 572.77 | 647.21 | 718.50 | 785.87 | 849.88 | 910.55 | 968.29 | 1022.7 | 1075.0 | 1124.4 | 1171.2 | 1216.4 |
| 23RS4RS5mmmm6 | 5.77 | 408.51 | 486.37 | 487.80 | 566.79 | 642.19 | 713.48 | 781.26 | 844.44 | 904.69 | 961.59 | 1015.6 | 1066.6 | 1115.6 | 1161.6 | 1205.9 |
| 23R4S5mmmm6 | .00 | 404.66 | 484.99 | 486.46 | 566.67 | 642.44 | 713.90 | 781.68 | 845.28 | 905.11 | 961.59 | 1015.6 | 1067.0 | 1115.6 | 1161.6 | 1205.9 |
| 3344mmmm6 | .00 | 396.08 | 472.36 | 473.82 | 552.52 | 628.42 | 700.93 | 769.55 | 834.40 | 895.90 | 954.06 | 1009.7 | 1062.8 | 1113.1 | 1161.2 | 1207.2 |
| 3ip24mm5 | .00 | 405.37 | 482.69 | 484.12 | 561.14 | 635.16 | 705.95 | 772.48 | 836.07 | 895.90 | 952.39 | 1006.4 | 1057.4 | 1105.9 | 1152.4 | 1196.3 |
| 33ee2m5 | .00 | 412.78 | 485.83 | 487.17 | 561.77 | 634.49 | 704.28 | 770.80 | 833.98 | 893.81 | 950.30 | 1004.3 | 1055.3 | 1103.8 | 1150.3 | 1194.6 |
| 3e223mmm5 | .00 | 400.35 | 472.15 | 473.53 | 548.09 | 621.22 | 691.73 | 759.09 | 823.10 | 883.77 | 941.93 | 996.7 | 1049.5 | 1099.2 | 1147.4 | 1193.4 |
| 3RSe224mmm5 | 5.77 | 417.00 | 491.65 | 492.99 | 568.09 | 640.97 | 710.97 | 777.92 | 841.09 | 900.93 | 958.25 | 1012.2 | 1064.1 | 1113.5 | 1159.9 | 1205.1 |
| 3e234mmm5 | .00 | 404.79 | 478.17 | 479.55 | 555.62 | 629.55 | 700.51 | 767.87 | 831.47 | 892.14 | 949.46 | 1004.3 | 1056.2 | 1105.5 | 1152.4 | 1197.6 |
| 22334mmmmm5 | .00 | 383.78 | 459.76 | 461.14 | 538.63 | 613.61 | 685.45 | 754.07 | 818.92 | 880.42 | 939.00 | 995.1 | 1048.2 | 1099.2 | 1147.8 | 1194.6 |
| 22344mmmmm5 | .00 | 377.84 | 455.04 | 456.46 | 533.57 | 608.00 | 679.59 | 747.37 | 811.81 | 873.31 | 931.89 | 987.5 | 1040.7 | 1091.3 | 1139.8 | 1186.7 |

Table A3. Standard enthalpy of formation of alkanes in kJ/mol

| T/K | 0 | 200 | 298.15 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| methane | -66.7 | -71.9 | -74.7 | -74.8 | -77.8 | -80.7 | -83.3 | -85.4 | -87.0 | -88.3 | -89.5 | -90.4 | -90.8 | -91.2 | -91.2 | -91.2 |
| ethane | -68.0 | -78.7 | -83.7 | -83.8 | -88.6 | -92.7 | -96.2 | -98.7 | -99.2 | -101.3 | -101.7 | -101.7 | -100.8 | -100.0 | -98.3 | -96.7 |
| propane | -82.6 | -98.0 | -104.9 | -105.0 | -111.3 | -116.7 | -120.9 | -124.3 | -126.4 | -128.0 | -128.9 | -128.9 | -128.4 | -127.2 | -125.9 | -124.3 |
| butanes | | | | | | | | | | | | | | | | |
| 4 | -98.9 | -117.7 | -125.7 | -125.9 | -133.5 | -139.9 | -145.2 | -149.0 | -151.9 | -153.6 | -154.8 | -154.8 | -154.8 | -154.0 | -152.3 | -151.0 |
| 2m3 | -106.0 | -126.2 | -134.6 | -134.7 | -142.3 | -148.6 | -153.6 | -157.3 | -159.8 | -161.5 | -161.9 | -161.9 | -160.7 | -159.4 | -157.3 | -154.8 |
| pentanes | | | | | | | | | | | | | | | | |
| 5 | -114.4 | -136.8 | -146.4 | -146.5 | -155.5 | -162.9 | -168.6 | -173.2 | -176.6 | -178.7 | -179.9 | -180.3 | -179.9 | -179.1 | -177.8 | -176.1 |
| 2m4 | -119.0 | -143.1 | -153.1 | -153.4 | -162.2 | -169.6 | -175.3 | -179.9 | -182.8 | -184.5 | -185.4 | -185.4 | -184.5 | -182.8 | -180.7 | -178.2 |
| 22mm3 | -135.5 | -160.4 | -168.4 | -168.6 | -176.6 | -183.3 | -188.3 | -192.0 | -194.6 | -195.4 | -195.0 | -193.7 | -191.2 | -187.9 | -184.1 | -179.5 |
| hexanes | | | | | | | | | | | | | | | | |
| 6 | -130.1 | -155.9 | -167.0 | -167.2 | -177.5 | -186.0 | -192.5 | -197.9 | -201.3 | -203.8 | -205.0 | -205.9 | -205.4 | -205.0 | -203.3 | -201.7 |
| 2m5 | -134.6 | -162.4 | -173.8 | -174.1 | -184.2 | -192.5 | -198.7 | -203.8 | -207.1 | -208.8 | -209.6 | -209.6 | -208.8 | -207.1 | -205.0 | -202.5 |
| 3m5 | -131.7 | -159.6 | -171.3 | -171.5 | -181.8 | -190.4 | -197.1 | -202.1 | -205.4 | -207.5 | -208.4 | -208.8 | -207.9 | -206.3 | -204.2 | -201.7 |
| 22mm4 | -143.4 | -172.4 | -183.9 | -184.1 | -194.3 | -202.6 | -208.8 | -213.4 | -216.3 | -217.6 | -217.1 | -215.9 | -213.8 | -210.5 | -206.7 | -202.1 |
| 23mm4 | -135.1 | -164.3 | -176.2 | -176.4 | -186.8 | -195.3 | -201.7 | -206.7 | -209.6 | -211.7 | -212.1 | -211.7 | -210.5 | -208.4 | -205.4 | -202.1 |
| heptanes | | | | | | | | | | | | | | | | |
| 7 | -145.7 | -175.0 | -187.6 | -187.9 | -199.5 | -209.0 | -216.3 | -222.2 | -226.4 | -228.9 | -230.5 | -231.4 | -231.0 | -230.5 | -229.3 | -227.6 |
| 2m6 | -150.2 | -181.5 | -194.5 | -194.7 | -206.3 | -215.7 | -223.0 | -228.4 | -232.2 | -234.7 | -235.6 | -236.0 | -235.1 | -233.5 | -231.4 | -228.9 |
| 3RSm6 | -147.4 | -178.9 | -192.1 | -192.3 | -203.9 | -213.3 | -220.5 | -225.9 | -229.7 | -232.2 | -233.5 | -233.5 | -232.6 | -231.4 | -229.3 | -226.4 |
| 3e5 | -145.8 | -176.9 | -189.5 | -189.7 | -201.3 | -210.7 | -218.0 | -223.8 | -227.6 | -230.1 | -231.4 | -231.8 | -231.0 | -229.7 | -227.6 | -225.1 |
| 22mm5 | -159.1 | -192.0 | -205.0 | -205.3 | -216.4 | -225.3 | -231.8 | -236.8 | -239.3 | -241.0 | -240.6 | -239.3 | -236.8 | -233.9 | -229.7 | -225.1 |
| 23RSmm5 | -147.3 | -180.4 | -194.1 | -194.3 | -206.1 | -215.6 | -223.0 | -228.0 | -231.8 | -233.9 | -234.7 | -234.3 | -233.0 | -230.5 | -228.0 | -224.3 |
| 24mm5 | -155.7 | -188.8 | -201.5 | -201.8 | -212.5 | -221.2 | -227.6 | -232.6 | -235.6 | -237.2 | -237.7 | -237.2 | -235.6 | -233.0 | -230.1 | -226.4 |
| 33mm5 | -153.3 | -186.3 | -199.4 | -199.7 | -211.0 | -220.0 | -226.8 | -231.4 | -234.3 | -235.6 | -235.6 | -234.3 | -231.8 | -228.4 | -224.3 | -219.2 |
| 223mmm4 | -156.6 | -190.4 | -203.7 | -204.0 | -215.5 | -224.8 | -231.8 | -236.8 | -239.7 | -241.0 | -240.6 | -238.9 | -236.0 | -232.2 | -227.2 | -221.8 |
| octanes | | | | | | | | | | | | | | | | |
| 8 | -161.4 | -194.1 | -208.2 | -208.5 | -221.5 | -232.1 | -240.2 | -246.4 | -251.0 | -254.4 | -256.1 | -256.9 | -256.9 | -256.1 | -254.8 | -253.1 |
| 2m7 | -165.9 | -200.6 | -215.1 | -215.4 | -228.2 | -238.7 | -246.9 | -252.7 | -256.9 | -259.4 | -261.1 | -261.1 | -260.2 | -259.0 | -256.9 | -254.4 |
| 3RSm7 | -163.1 | -198.1 | -212.7 | -213.0 | -226.0 | -236.5 | -244.8 | -250.6 | -254.8 | -257.7 | -259.0 | -259.4 | -258.6 | -257.3 | -255.2 | -252.7 |
| 4m7 | -163.0 | -198.3 | -212.9 | -213.2 | -226.0 | -236.3 | -244.3 | -250.2 | -254.4 | -256.9 | -258.2 | -258.2 | -257.3 | -256.1 | -254.0 | -251.0 |
| 3e6 | -161.5 | -196.3 | -210.4 | -210.6 | -223.4 | -233.8 | -241.8 | -248.1 | -252.3 | -255.2 | -256.5 | -256.9 | -256.1 | -254.8 | -253.1 | -250.6 |
| 22mm6 | -174.8 | -211.1 | -225.6 | -225.8 | -238.5 | -248.7 | -256.1 | -261.9 | -265.3 | -266.9 | -266.9 | -266.1 | -263.6 | -260.7 | -256.5 | -251.9 |
| 23RSmm6 | -163.0 | -199.7 | -214.9 | -215.2 | -228.2 | -238.7 | -246.4 | -252.7 | -256.5 | -259.0 | -259.8 | -259.4 | -258.2 | -256.1 | -253.1 | -249.8 |
| 24RSmm6 | -168.6 | -205.4 | -219.8 | -220.1 | -232.3 | -242.1 | -249.8 | -255.2 | -258.6 | -261.1 | -261.5 | -261.1 | -259.8 | -257.3 | -254.4 | -251.0 |
| 25mm6 | -170.2 | -206.9 | -221.9 | -222.2 | -235.1 | -245.5 | -253.6 | -259.4 | -263.2 | -265.7 | -266.5 | -266.5 | -264.8 | -262.8 | -260.2 | -256.5 |
| 33mm6 | -168.9 | -206.0 | -220.5 | -220.8 | -233.1 | -242.7 | -249.8 | -254.8 | -257.7 | -259.4 | -259.0 | -257.7 | -255.2 | -251.9 | -247.7 | -242.7 |
| 3RS4RSmm6 | -159.4 | -196.4 | -212.0 | -212.3 | -225.5 | -236.0 | -243.9 | -249.8 | -254.0 | -256.5 | -257.3 | -257.3 | -255.6 | -253.6 | -251.0 | -247.3 |
| 3R4Smm6 | -159.6 | -196.6 | -212.0 | -212.3 | -225.4 | -235.8 | -243.9 | -249.8 | -253.6 | -256.1 | -257.3 | -256.9 | -255.6 | -253.6 | -250.6 | -247.3 |
| 3e2m5 | -161.6 | -198.1 | -212.3 | -212.5 | -225.0 | -235.2 | -243.1 | -248.9 | -253.1 | -255.6 | -256.5 | -256.5 | -255.2 | -253.6 | -250.6 | -247.3 |
| 3e3m5 | -162.8 | -199.8 | -214.6 | -214.8 | -227.4 | -237.5 | -245.2 | -250.6 | -254.0 | -255.6 | -255.6 | -254.4 | -251.9 | -248.9 | -244.8 | -239.7 |
| 223RSmmm5 | -168.0 | -205.8 | -220.9 | -221.2 | -234.0 | -244.1 | -251.5 | -256.9 | -260.2 | -261.9 | -261.5 | -259.8 | -256.9 | -253.1 | -248.5 | -243.1 |
| 224mmm5 | -172.5 | -210.4 | -225.0 | -225.2 | -237.9 | -247.9 | -255.2 | -260.7 | -264.0 | -265.3 | -264.8 | -263.2 | -260.2 | -256.5 | -251.5 | -245.6 |
| 233mmm5 | -165.1 | -202.9 | -218.0 | -218.2 | -230.9 | -240.9 | -248.1 | -253.6 | -256.5 | -257.7 | -257.3 | -255.6 | -252.7 | -248.5 | -243.9 | -238.1 |
| 234mmm5 | -163.9 | -201.8 | -216.4 | -216.6 | -228.9 | -238.8 | -246.4 | -251.9 | -255.2 | -257.3 | -257.3 | -256.9 | -254.8 | -251.9 | 248.1 | -243.5 |
| 2233mmmm4 | -172.6 | -211.0 | -225.7 | -226.0 | -238.7 | -248.8 | -256.1 | -261.1 | -264.0 | -264.4 | -263.2 | -260.7 | -256.1 | -250.6 | -243.9 | -236.4 |
| nonanes | | | | | | | | | | | | | | | | |
| 9 | -177.1 | -213.3 | -228.9 | -229.2 | -243.5 | -255.2 | -264.4 | -271.1 | -276.1 | -279.5 | -281.6 | -282.4 | -282.4 | -282.0 | -280.7 | -279.1 |
| 2m8 | -181.6 | -219.8 | -235.8 | -236.1 | -250.3 | -261.8 | -270.7 | -277.4 | -282.0 | -284.9 | -286.2 | -286.6 | -286.2 | -284.9 | -282.8 | -279.9 |
| 3RSm8 | -178.7 | -217.2 | -233.3 | -233.6 | -247.9 | -259.5 | -268.6 | -275.3 | -279.9 | -282.8 | -284.5 | -284.9 | -284.1 | -282.8 | -280.7 | -278.2 |
| 4RSm8 | -178.7 | -217.4 | -233.5 | -233.8 | -248.0 | -259.5 | -268.2 | -274.9 | -279.5 | -282.4 | -283.7 | -284.1 | -283.7 | -282.0 | -279.9 | -277.4 |
| 3e7 | -177.2 | -215.4 | -231.0 | -231.3 | -245.4 | -257.0 | -266.1 | -272.8 | -277.4 | -280.7 | -282.4 | -282.8 | -282.4 | -281.2 | -279.1 | -276.6 |
| 4e7 | -177.2 | -215.7 | -231.2 | -231.5 | -245.5 | -256.9 | -265.7 | -272.4 | -277.0 | -279.9 | -281.6 | -282.0 | -281.6 | -280.3 | -278.2 | -275.7 |
| 22mm7 | -190.5 | -230.3 | -246.2 | -246.5 | -260.5 | -271.6 | -279.9 | -286.2 | -290.0 | -292.0 | -292.0 | -291.2 | -289.1 | -285.8 | -282.0 | -277.0 |
| 23RSmm7 | -178.7 | -218.8 | -235.5 | -235.8 | -250.2 | -261.8 | -270.7 | -277.4 | -281.6 | -284.5 | -285.8 | -285.8 | -284.5 | -282.4 | -279.9 | -276.1 |
| 24RSmm7 | -184.2 | -224.8 | -240.7 | -241.0 | -254.4 | -265.1 | -273.2 | -279.1 | -282.8 | -285.3 | -286.2 | -285.8 | -284.1 | -282.0 | -279.1 | -275.3 |
| 25RSmm7 | -183.1 | -223.5 | -240.1 | -240.4 | -254.8 | -266.3 | -275.3 | -281.6 | -286.2 | -288.7 | -290.0 | -290.0 | -288.7 | -286.6 | -284.1 | -280.3 |
| 26mm7 | -186.0 | -226.2 | -242.6 | -242.9 | -257.0 | -268.3 | -277.0 | -283.3 | -287.4 | -290.0 | -291.2 | -291.2 | -289.5 | -287.4 | -284.5 | -281.2 |
| 33mm7 | -184.7 | -225.1 | -241.1 | -241.4 | -255.1 | -266.0 | -274.1 | -279.9 | -283.7 | -285.3 | -285.3 | -284.5 | -282.0 | -278.7 | -274.5 | -269.9 |
| 3RS4SRmm7 | -175.3 | -215.9 | -232.8 | -233.1 | -247.4 | -258.9 | -267.8 | -274.1 | -278.2 | -281.2 | -282.0 | -282.0 | -280.7 | -279.1 | -276.1 | -272.8 |
| 3RS4RSmm7 | -175.1 | -215.8 | -232.8 | -233.1 | -247.6 | -259.1 | -267.8 | -274.5 | -278.7 | -281.2 | -282.4 | -282.4 | -281.2 | -279.1 | -276.1 | -272.8 |
| 3RS5RSmm7 | -181.3 | -222.0 | -238.2 | -238.5 | -252.3 | -263.4 | -272.0 | -278.2 | -282.4 | -284.9 | -285.8 | -285.8 | -284.5 | -282.4 | -279.5 | -275.7 |
| 3R5Smm7 | -181.6 | -222.1 | -238.1 | -238.4 | -252.0 | -263.0 | -271.5 | -277.8 | -282.0 | -284.5 | -285.3 | -285.3 | -284.1 | -282.0 | -279.1 | -275.3 |
| 44mm7 | -184.6 | -225.7 | -241.7 | -242.0 | -255.2 | -265.5 | -272.8 | -278.2 | -281.6 | -282.8 | -282.8 | -281.6 | -278.7 | -275.3 | -271.1 | -266.1 |
| 3RSe2m6 | -177.2 | -216.7 | -233.1 | -233.4 | -247.1 | -258.4 | -266.9 | -273.6 | -278.2 | -280.7 | -282.0 | -282.0 | -281.2 | -279.1 | -276.1 | -272.8 |
| 4e2m6 | -182.8 | -222.9 | -238.2 | -238.4 | -251.8 | -262.7 | -271.1 | -277.4 | -281.2 | -284.1 | -284.9 | -284.9 | -283.3 | -281.2 | -278.2 | -274.9 |
| 3e3m6 | -178.5 | -219.5 | -235.7 | -236.0 | -249.7 | -260.4 | -268.2 | -274.1 | -277.4 | -279.5 | -279.5 | -278.2 | -276.1 | -272.8 | -268.6 | -263.6 |
| 3e4RSm6 | -173.9 | -214.5 | -230.4 | -230.7 | -244.5 | -255.8 | -264.4 | -271.1 | -275.7 | -278.7 | -279.9 | -279.9 | -278.7 | -277.0 | -274.1 | -270.7 |
| 223RSmmm6 | -183.8 | -225.2 | -241.8 | -242.0 | -256.1 | -267.3 | -275.7 | -281.6 | -285.3 | -287.0 | -287.0 | -285.8 | -282.8 | -279.1 | -274.5 | -269.0 |
| 224RSmmm6 | -185.4 | -227.0 | -243.3 | -243.6 | -257.7 | -268.9 | -277.4 | -283.3 | -287.0 | -288.7 | -288.7 | -287.4 | -284.5 | -280.7 | -276.1 | -270.3 |
| 225mmm6 | -194.7 | -236.4 | -252.9 | -253.2 | -267.4 | -278.8 | -287.4 | -293.3 | -297.1 | -298.7 | -298.7 | -297.5 | -294.6 | -290.8 | -286.2 | -280.7 |
| 233mmm6 | -180.8 | -222.6 | -239.1 | -239.4 | -253.0 | -263.7 | -271.5 | -277.0 | -280.3 | -281.6 | -281.2 | -279.9 | -276.6 | -272.8 | -267.8 | -261.9 |
| 23RS4SRmmm6 | -176.4 | -217.9 | -234.1 | -234.4 | -248.0 | -259.0 | -267.4 | -273.6 | -277.4 | -279.9 | -280.3 | -279.9 | -277.8 | -274.9 | -271.1 | -266.9 |
| 23RS4RSmmm6 | -176.0 | -217.7 | -234.3 | -234.6 | -248.4 | -259.4 | -267.8 | -274.1 | -277.8 | -279.9 | -280.7 | -279.9 | -277.8 | -275.3 | -271.5 | -266.9 |
| 23RS5mmm6 | -184.0 | -226.0 | -242.5 | -242.8 | -256.6 | -267.6 | -275.7 | -282.0 | -285.8 | -287.9 | -288.3 | -287.9 | -285.8 | -282.8 | -279.1 | -274.5 |
| 244mmm6 | -182.4 | -224.3 | -240.5 | -240.8 | -254.6 | -265.4 | -273.6 | -279.1 | -282.4 | -284.1 | -283.7 | -282.0 | -278.7 | -274.9 | -269.9 | -264.0 |
| 334RSmmm6 | -176.6 | -218.3 | -235.2 | -235.5 | -249.4 | -260.2 | -268.2 | -274.1 | -277.4 | -279.1 | -278.7 | -277.0 | -274.1 | -270.3 | -265.3 | -259.4 |
| 33ee5 | -173.8 | -214.6 | -230.0 | -230.3 | -243.9 | -254.8 | -263.2 | -269.0 | -273.2 | -275.3 | -275.7 | -274.9 | -272.4 | -269.4 | -265.3 | -260.7 |
| 3e22mm5 | -172.9 | -214.5 | -231.3 | -231.6 | -246.3 | -258.0 | -266.9 | -273.2 | -277.4 | -279.5 | -279.5 | -278.7 | -276.1 | -272.4 | -267.8 | -262.3 |
| 3e23mm5 | -174.0 | -215.5 | -231.9 | -232.2 | -246.0 | -256.9 | -265.3 | -271.1 | -274.5 | -276.6 | -276.1 | -274.9 | -272.0 | -268.2 | -263.2 | -257.7 |
| 3e24mm5 | -168.6 | -210.5 | -227.1 | -227.3 | -241.6 | -253.1 | -261.9 | -268.2 | -272.8 | -275.3 | -275.7 | -275.3 | -273.6 | -270.7 | -267.4 | -263.2 |
| 2233mmmm5 | -178.4 | -220.7 | -237.1 | -237.4 | -251.0 | -261.8 | -269.4 | -274.9 | -277.4 | -278.2 | -277.0 | -274.5 | -269.9 | -264.0 | -257.3 | -249.4 |
| 223RS4mmmm5 | -175.6 | -218.2 | -235.1 | -235.3 | -249.6 | -260.8 | -269.0 | -274.9 | -278.7 | -279.9 | -279.5 | -277.8 | -274.5 | -269.9 | -264.4 | -257.7 |
| 2244mmmm5 | -183.4 | -225.9 | -241.6 | -241.9 | -255.5 | -266.4 | -274.5 | -279.5 | -282.4 | -283.3 | -282.0 | -279.5 | -274.9 | -269.4 | -262.8 | -254.8 |
| 2334mmmm5 | -177.0 | -219.4 | -235.3 | -235.6 | -248.7 | -259.0 | -266.5 | -272.0 | -274.9 | -275.7 | -274.9 | -272.8 | -269.0 | -264.4 | -258.6 | -251.9 |

Table A3 continued

| T/K | 0 | 200 | 298.15 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| decanes | | | | | | | | | | | | | | | | |
| 10 | -192.7 | -232.5 | -249.5 | -249.9 | -265.5 | -278.2 | -287.9 | -295.4 | -300.8 | -304.6 | -306.7 | -307.9 | -307.9 | -307.5 | -306.3 | -304.6 |
| 2m9 | -197.3 | -238.9 | -256.4 | -256.7 | -272.3 | -284.8 | -294.6 | -301.7 | -306.7 | -310.0 | -311.7 | -312.1 | -311.7 | -310.0 | -308.4 | -305.4 |
| 3RSm9 | -194.3 | -236.3 | -254.0 | -254.3 | -270.0 | -282.6 | -292.5 | -299.6 | -304.6 | -307.9 | -309.6 | -310.5 | -309.6 | -308.4 | -306.7 | -303.8 |
| 4RSm9 | -194.3 | -236.5 | -254.2 | -254.5 | -270.0 | -282.5 | -292.0 | -299.2 | -304.2 | -307.5 | -309.2 | -309.6 | -308.8 | -307.5 | -305.4 | -302.9 |
| 5m9 | -194.3 | -236.4 | -254.1 | -254.4 | -270.0 | -282.6 | -292.0 | -299.6 | -304.6 | -307.5 | -309.2 | -310.0 | -309.2 | -307.9 | -305.9 | -303.3 |
| 3e8 | -192.8 | -234.6 | -251.7 | -252.0 | -267.4 | -280.0 | -290.0 | -297.1 | -302.1 | -305.9 | -307.5 | -308.4 | -307.9 | -306.7 | -304.6 | -302.1 |
| 4RSe8 | -192.8 | -234.8 | -251.8 | -252.2 | -267.5 | -280.0 | -289.5 | -296.6 | -301.7 | -305.4 | -307.1 | -307.5 | -307.1 | -305.9 | -304.2 | -301.2 |
| 22mm8 | -206.2 | -249.5 | -266.9 | -267.2 | -282.5 | -294.8 | -303.8 | -310.5 | -314.6 | -317.1 | -317.6 | -317.1 | -314.6 | -311.7 | -307.9 | -302.9 |
| 23RSmm8 | -194.4 | -237.9 | -256.1 | -256.4 | -272.2 | -284.8 | -294.6 | -301.7 | -306.7 | -309.6 | -310.9 | -311.3 | -310.0 | -307.9 | -305.0 | -301.7 |
| 24RSmm8 | -199.9 | -243.9 | -261.3 | -261.6 | -276.4 | -288.2 | -297.1 | -303.8 | -308.4 | -310.9 | -311.7 | -311.7 | -310.5 | -308.4 | -305.0 | -301.7 |
| 25RSmm8 | -198.7 | -242.8 | -261.0 | -261.3 | -276.9 | -289.3 | -298.7 | -305.9 | -310.5 | -313.4 | -314.6 | -314.6 | -313.4 | -311.3 | -308.8 | -305.0 |
| 26RSmm8 | -198.8 | -242.8 | -260.8 | -261.2 | -276.7 | -289.2 | -298.7 | -305.9 | -310.5 | -313.4 | -314.6 | -314.6 | -313.4 | -311.3 | -308.4 | -305.0 |
| 27mm8 | -201.7 | -245.3 | -263.2 | -263.6 | -279.0 | -291.4 | -300.8 | -307.5 | -312.1 | -315.1 | -316.3 | -316.3 | -315.1 | -313.0 | -310.0 | -306.7 |
| 33mm8 | -200.4 | -244.2 | -261.8 | -262.1 | -277.1 | -289.0 | -297.9 | -304.2 | -308.4 | -310.5 | -310.5 | -309.6 | -307.5 | -304.2 | -300.0 | -295.0 |
| 3RS4SRmm8 | -191.0 | -235.0 | -253.3 | -253.7 | -269.4 | -282.0 | -291.6 | -298.7 | -303.8 | -306.7 | -308.4 | -308.4 | -307.1 | -305.4 | -302.5 | -299.2 |
| 3RS4RSmm8 | -190.8 | -234.8 | -253.4 | -253.7 | -269.6 | -282.3 | -292.0 | -299.2 | -303.8 | -307.1 | -308.4 | -308.4 | -307.5 | -305.4 | -302.5 | -299.2 |
| 3RS5RSmm8 | -197.0 | -241.4 | -259.0 | -259.4 | -274.4 | -286.4 | -295.4 | -302.1 | -306.7 | -309.2 | -310.5 | -310.5 | -308.8 | -306.7 | -303.8 | -300.4 |
| 3RS5SRmm8 | -197.2 | -241.5 | -258.9 | -259.2 | -274.1 | -286.0 | -295.0 | -301.7 | -306.3 | -308.8 | -310.0 | -310.0 | -308.8 | -306.3 | -303.3 | -300.0 |
| 3RS6RSmm8 | -195.9 | -240.0 | -258.4 | -258.7 | -274.5 | -287.2 | -297.1 | -304.2 | -308.8 | -312.1 | -313.4 | -313.8 | -312.5 | -310.5 | -307.9 | -304.2 |
| 3R6Smm8 | -195.9 | -240.0 | -258.4 | -258.7 | -274.5 | -287.2 | -297.1 | -304.2 | -308.8 | -312.1 | -313.4 | -313.8 | -312.5 | -310.5 | -307.9 | -304.2 |
| 44mm8 | -200.4 | -244.7 | -262.2 | -262.5 | -277.2 | -288.7 | -297.1 | -303.3 | -307.1 | -308.8 | -309.2 | -307.9 | -305.4 | -302.1 | -297.9 | -292.9 |
| 4RS5RSmm8 | -190.7 | -235.1 | -253.6 | -254.0 | -269.7 | -282.2 | -291.6 | -298.7 | -303.3 | -306.3 | -307.5 | -307.5 | -306.3 | -304.2 | -301.2 | -297.9 |
| 4R5Smm8 | -191.0 | -235.3 | -253.6 | -254.0 | -269.5 | -282.0 | -291.2 | -298.3 | -302.9 | -306.3 | -307.5 | -307.5 | -306.3 | -304.2 | -301.2 | -297.9 |
| 4p7 | -192.8 | -235.0 | -252.0 | -252.4 | -267.5 | -279.8 | -289.1 | -296.2 | -300.8 | -304.2 | -305.9 | -306.3 | -305.9 | -304.6 | -302.5 | -300.0 |
| 4ip7 | -193.0 | -236.8 | -254.0 | -254.3 | -269.4 | -281.6 | -291.2 | -298.3 | -302.9 | -306.3 | -307.5 | -307.5 | -306.7 | -304.6 | -302.1 | -298.7 |
| 3RSe2m7 | -192.9 | -236.6 | -253.8 | -254.1 | -269.2 | -281.6 | -291.2 | -298.3 | -303.3 | -306.3 | -307.9 | -308.4 | -307.1 | -305.4 | -302.5 | -299.2 |
| 4RSe2m7 | -198.5 | -242.3 | -259.0 | -259.3 | -273.9 | -285.6 | -294.6 | -301.2 | -305.4 | -308.4 | -309.2 | -309.2 | -307.9 | -305.9 | -302.9 | -299.2 |
| 5e2m7 | -197.2 | -240.9 | -258.4 | -258.7 | -274.2 | -286.8 | -296.2 | -303.8 | -308.4 | -311.7 | -313.0 | -313.4 | -312.1 | -310.5 | -307.5 | -304.2 |
| 3e3m7 | -194.3 | -238.6 | -256.3 | -256.6 | -271.7 | -283.7 | -292.5 | -299.2 | -303.3 | -305.4 | -305.9 | -305.0 | -302.9 | -299.6 | -295.4 | -290.8 |
| 4RSe3RSm7 | -189.6 | -233.8 | -251.2 | -251.6 | -266.6 | -278.9 | -288.3 | -295.4 | -300.4 | -303.8 | -305.0 | -305.4 | -304.2 | -302.5 | -300.0 | -296.6 |
| 4RSe3SRm7 | -189.6 | -233.8 | -251.2 | -251.6 | -266.6 | -278.9 | -288.3 | -295.4 | -300.4 | -303.8 | -305.0 | -305.4 | -304.2 | -302.5 | -300.0 | -296.6 |
| 3e5RSm7 | -195.7 | -239.6 | -256.5 | -256.8 | -271.7 | -283.8 | -293.3 | -300.0 | -304.6 | -307.9 | -309.2 | -309.2 | -307.9 | -305.9 | -303.3 | -299.6 |
| 3e4RSm7 | -189.6 | -233.8 | -251.2 | -251.5 | -266.6 | -278.8 | -288.3 | -295.4 | -300.4 | -303.3 | -305.0 | -305.0 | -304.2 | -302.1 | -299.6 | -296.2 |
| 4e4m7 | -194.1 | -239.2 | -256.8 | -257.1 | -271.8 | -283.2 | -291.6 | -297.5 | -301.2 | -303.3 | -303.3 | -302.5 | -300.0 | -296.6 | -292.5 | -287.4 |
| 223RSmmm7 | -199.5 | -244.3 | -262.4 | -262.7 | -278.2 | -290.4 | -299.6 | -306.3 | -310.5 | -312.5 | -312.5 | -311.3 | -308.8 | -305.0 | -300.4 | -295.0 |
| 224RSmmm7 | -201.0 | -246.3 | -264.1 | -264.4 | -279.7 | -291.8 | -300.8 | -307.1 | -310.9 | -313.0 | -313.0 | -311.7 | -308.8 | -305.0 | -300.4 | -294.6 |
| 225RSmmm7 | -207.5 | -252.9 | -271.2 | -271.5 | -287.2 | -299.6 | -308.8 | -315.9 | -320.1 | -322.2 | -322.2 | -321.3 | -318.4 | -314.6 | -310.0 | -304.6 |
| 226mmm7 | -210.5 | -255.9 | -273.7 | -274.1 | -289.2 | -301.2 | -310.0 | -316.3 | -320.5 | -322.2 | -322.2 | -320.9 | -318.0 | -314.2 | -309.6 | -303.8 |
| 233mmm7 | -196.6 | -241.7 | -259.7 | -260.0 | -275.1 | -287.0 | -295.8 | -302.1 | -305.9 | -307.9 | -307.5 | -306.3 | -303.3 | -299.6 | -294.6 | -288.7 |
| 23RS4SRmmm7 | -192.3 | -237.4 | -255.1 | -255.5 | -270.3 | -282.2 | -291.2 | -297.9 | -302.1 | -304.6 | -305.4 | -305.0 | -302.9 | -300.0 | -296.6 | -292.0 |
| 23RS4RSmmm7 | -191.7 | -237.1 | -255.1 | -255.4 | -270.5 | -282.5 | -291.6 | -297.9 | -302.5 | -305.0 | -305.4 | -305.0 | -302.9 | -300.4 | -296.6 | -292.0 |
| 23RS5RSmmm7 | -196.6 | -242.5 | -260.9 | -261.2 | -276.6 | -288.9 | -297.9 | -304.6 | -309.2 | -311.7 | -312.5 | -312.1 | -310.0 | -307.1 | -303.3 | -299.2 |
| 23RS5SRmmm7 | -197.2 | -242.8 | -260.8 | -261.2 | -276.3 | -288.4 | -297.5 | -304.6 | -308.8 | -311.7 | -312.1 | -311.7 | -310.0 | -307.1 | -303.8 | -299.2 |
| 23RS6mmm7 | -198.6 | -244.3 | -263.0 | -263.3 | -279.1 | -291.7 | -301.2 | -308.4 | -313.0 | -315.5 | -316.3 | -316.3 | -314.2 | -311.7 | -307.9 | -303.8 |
| 244mmm7 | -198.1 | -244.0 | -261.7 | -262.0 | -276.7 | -288.2 | -296.6 | -302.5 | -305.9 | -307.5 | -307.1 | -305.4 | -302.1 | -297.9 | -292.9 | -287.0 |
| 24RS5SRmmm7 | -196.3 | -242.2 | -260.5 | -260.8 | -275.9 | -287.8 | -296.6 | -303.3 | -307.5 | -310.0 | -310.9 | -310.0 | -308.4 | -305.4 | -301.7 | -297.1 |
| 24RS5RSmmm7 | -196.1 | -242.0 | -260.5 | -260.8 | -276.0 | -288.0 | -297.1 | -303.8 | -307.9 | -310.5 | -310.9 | -310.5 | -308.4 | -305.4 | -301.7 | -297.5 |
| 246mmm7 | -205.4 | -251.3 | -268.4 | -268.7 | -282.8 | -293.8 | -302.1 | -307.9 | -311.7 | -313.8 | -314.2 | -313.4 | -310.9 | -307.9 | -304.2 | -299.6 |
| 255mmm7 | -204.8 | -250.4 | -268.4 | -268.7 | -284.1 | -296.2 | -305.4 | -311.7 | -315.5 | -317.6 | -317.6 | -316.3 | -313.4 | -309.6 | -305.0 | -299.2 |
| 334RSmmm7 | -192.4 | -237.7 | -256.0 | -256.4 | -271.6 | -283.5 | -292.5 | -298.7 | -302.5 | -304.2 | -304.2 | -302.9 | -300.0 | -296.2 | -291.2 | -285.3 |
| 335RSmmm7 | -195.1 | -240.8 | -258.8 | -259.2 | -274.4 | -286.5 | -295.4 | -302.1 | -305.9 | -307.5 | -307.5 | -306.3 | -303.3 | -299.2 | -294.6 | -288.7 |
| 3RS44mmm7 | -192.3 | -238.1 | -256.4 | -256.7 | -271.6 | -283.1 | -291.6 | -297.5 | -301.2 | -302.9 | -302.5 | -301.2 | -297.9 | -294.1 | -289.1 | -283.3 |
| 3RS45RSmmm7 | -188.4 | -233.7 | -251.9 | -252.3 | -267.4 | -279.6 | -288.7 | -295.4 | -300.0 | -302.5 | -303.3 | -302.9 | -300.8 | -298.3 | -294.6 | -290.0 |
| s3R45Smmm7 | -188.9 | -234.1 | -251.9 | -252.3 | -267.1 | -279.2 | -288.3 | -295.0 | -299.6 | -302.1 | -302.9 | -302.5 | -300.8 | -298.3 | -294.6 | -290.4 |
| r3R45Smmm7 | -188.0 | -233.5 | -252.0 | -252.3 | -267.7 | -279.9 | -289.1 | -295.8 | -300.4 | -302.9 | -303.8 | -303.3 | -301.2 | -298.7 | -295.0 | -290.4 |
| 3ip2m6 | -184.3 | -229.8 | -247.9 | -248.3 | -263.9 | -276.4 | -285.8 | -292.9 | -297.5 | -300.4 | -301.2 | -301.2 | -299.6 | -296.6 | -293.3 | -289.1 |
| 33ee6 | -189.5 | -234.2 | -251.2 | -251.5 | -266.1 | -277.8 | -286.6 | -292.9 | -297.1 | -299.2 | -299.6 | -299.2 | -296.6 | -293.7 | -289.5 | -284.9 |
| 34ee6 | -188.3 | -232.4 | -248.8 | -249.1 | -263.6 | -275.6 | -284.9 | -292.5 | -297.5 | -300.8 | -302.1 | -302.5 | -301.7 | -300.0 | -297.5 | -294.1 |
| 3RSe22mm6 | -188.6 | -233.8 | -252.2 | -252.5 | -268.5 | -281.3 | -290.8 | -297.9 | -302.5 | -305.0 | -305.4 | -304.2 | -301.7 | -298.3 | -293.7 | -288.3 |
| 4e22mm6 | -199.5 | -244.4 | -261.7 | -262.0 | -277.3 | -289.6 | -298.7 | -305.4 | -309.6 | -312.1 | -312.1 | -310.9 | -308.4 | -304.6 | -300.0 | -294.6 |
| 3RSe23mm6 | -189.7 | -235.2 | -253.1 | -253.4 | -268.2 | -279.9 | -288.7 | -295.0 | -298.7 | -300.4 | -300.4 | -299.2 | -296.2 | -292.5 | -287.4 | -282.0 |
| 4e23RSmm6 | -190.3 | -235.1 | -252.0 | -252.3 | -267.0 | -278.9 | -288.3 | -295.0 | -299.2 | -302.1 | -302.9 | -302.5 | -300.8 | -297.9 | -294.6 | -290.4 |
| 3RSe24SRmm6 | -181.2 | -226.9 | -245.1 | -245.5 | -261.0 | -273.6 | -283.3 | -290.4 | -295.0 | -297.9 | -298.7 | -298.3 | -296.6 | -294.1 | -290.8 | -286.6 |
| 3RSe24RSmm6 | -181.0 | -226.8 | -245.1 | -245.4 | -261.1 | -273.7 | -283.3 | -290.4 | -295.0 | -297.9 | -298.7 | -298.7 | -297.1 | -294.1 | -290.8 | -286.6 |
| 4e24mm6 | -191.9 | -237.8 | -255.7 | -256.1 | -271.2 | -283.2 | -292.0 | -298.3 | -302.1 | -304.2 | -303.8 | -302.5 | -299.6 | -295.4 | -290.8 | -284.9 |
| 3e25mm6 | -197.7 | -243.2 | -260.5 | -260.8 | -275.6 | -287.6 | -296.6 | -303.3 | -307.9 | -310.9 | -311.7 | -311.3 | -309.2 | -306.7 | -303.3 | -298.7 |
| 4e33mm6 | -181.4 | -227.0 | -245.6 | -245.9 | -261.8 | -274.3 | -283.7 | -290.4 | -294.6 | -297.1 | -297.1 | -295.8 | -293.3 | -289.5 | -284.9 | -279.5 |
| 3e34RSmm6 | -185.4 | -230.9 | -249.2 | -249.5 | -264.6 | -276.5 | -285.3 | -291.6 | -295.8 | -297.9 | -297.9 | -296.6 | -293.7 | -290.0 | -285.3 | -279.5 |
| 3233mmm6 | -184.1 | -230.4 | -248.3 | -248.6 | -263.9 | -275.8 | -284.8 | -292.0 | -298.7 | -301.7 | -302.5 | -301.2 | -298.7 | -294.1 | -288.7 | -281.6 | -273.6 |
| 223RS4RSmmmm6 | -187.9 | -234.4 | -252.8 | -253.2 | -268.7 | -281.0 | -290.4 | -296.6 | -300.8 | -302.5 | -302.5 | -300.8 | -297.5 | -292.9 | -287.4 | -281.2 |
| 223RS4SRmmmm6 | -187.6 | -234.2 | -252.9 | -253.3 | -269.1 | -281.5 | -290.8 | -297.5 | -301.2 | -303.3 | -302.9 | -301.2 | -297.9 | -293.7 | -287.9 | -281.6 |
| 223RS5mmmm6 | -204.7 | -251.3 | -269.3 | -269.7 | -284.7 | -296.6 | -305.4 | -311.7 | -315.1 | -316.7 | -316.3 | -314.6 | -311.3 | -306.7 | -300.8 | -294.6 |
| 2244mmmm6 | -193.3 | -239.8 | -257.1 | -257.5 | -272.3 | -284.0 | -292.5 | -298.3 | -301.2 | -302.5 | -301.2 | -298.3 | -293.7 | -287.9 | -281.2 | -273.2 |
| 224RS5mmmm6 | -200.7 | -247.5 | -266.0 | -266.4 | -282.1 | -294.6 | -303.8 | -310.5 | -314.6 | -316.3 | -316.3 | -314.6 | -311.3 | -306.7 | -301.2 | -294.6 |
| 2255mmmm6 | -219.0 | -265.6 | -283.8 | -284.1 | -299.9 | -312.4 | -321.7 | -328.0 | -331.8 | -333.0 | -332.6 | -330.1 | -325.9 | -320.5 | -314.2 | -306.7 |
| 2334RSmmmm6 | -188.5 | -234.8 | -252.6 | -252.9 | -267.4 | -278.6 | -287.0 | -292.5 | -295.8 | -297.5 | -296.6 | -294.6 | -290.8 | -286.2 | -280.3 | -273.6 |
| 2335mmmm6 | -194.1 | -240.9 | -259.1 | -259.4 | -274.6 | -286.5 | -295.4 | -301.2 | -305.0 | -306.7 | -305.9 | -303.8 | -300.4 | -295.8 | -290.0 | -283.3 |
| 23RS44mmmm6 | -184.1 | -230.8 | -249.4 | -249.7 | -265.1 | -277.1 | -286.2 | -292.0 | -295.8 | -297.5 | -297.1 | -295.0 | -291.6 | -287.0 | -281.2 | -274.9 |
| 23RS4RS5mmmm6 | -192.3 | -238.9 | -256.6 | -257.0 | -271.6 | -283.2 | -292.0 | -298.3 | -302.1 | -304.2 | -304.6 | -303.3 | -300.8 | -297.1 | -292.5 | -287.4 |
| 23R4S5mmmm6 | -193.1 | -239.4 | -256.6 | -256.9 | -271.1 | -282.5 | -291.2 | -297.5 | -301.7 | -303.8 | -303.8 | -302.9 | -300.0 | -296.6 | -292.0 | -286.6 |
| 3344mmmm6 | -184.1 | -230.3 | -248.4 | -248.7 | -263.4 | -274.8 | -283.3 | -288.7 | -291.6 | -292.5 | -291.2 | -288.3 | -283.7 | -277.8 | -271.1 | -263.2 |
| 3ip24mm5 | -191.2 | -238.2 | -256.1 | -256.4 | -271.8 | -284.0 | -293.3 | -300.0 | -304.2 | -306.3 | -306.7 | -305.9 | -302.9 | -299.6 | -295.0 | -290.0 |
| 33ee2m5 | -174.2 | -220.1 | -239.0 | -239.4 | -255.5 | -268.3 | -277.8 | -284.9 | -289.1 | -291.6 | -292.0 | -290.8 | -288.3 | -284.9 | -280.3 | -274.5 |
| 3e223mmm5 | -175.2 | -221.7 | -241.0 | -241.3 | -257.4 | -270.1 | -279.5 | -285.8 | -289.5 | -290.8 | -290.0 | -287.4 | -283.3 | -278.2 | -271.5 | -264.0 |
| 3RSe224mmm5 | -179.8 | -226.5 | -245.1 | -245.4 | -261.4 | -274.1 | -283.7 | -290.4 | -294.6 | -296.6 | -296.6 | -295.4 | -292.0 | -287.9 | -282.4 | -276.1 |
| 3e234mmm5 | -175.4 | -222.0 | -240.9 | -241.2 | -256.9 | -269.1 | -278.2 | -284.5 | -288.3 | -290.0 | -289.5 | -287.9 | -284.5 | -279.9 | -274.5 | -267.8 |
| 22334mmmmm5 | -178.3 | -225.6 | -243.8 | -244.1 | -259.3 | -271.0 | -279.5 | -285.3 | -288.3 | -289.1 | -287.4 | -284.1 | -279.1 | -272.8 | -265.3 | -256.5 |
| 22344mmmmm5 | -180.7 | -228.0 | -245.9 | -246.3 | -261.5 | -273.5 | -282.4 | -288.3 | -291.6 | -292.5 | -291.2 | -288.3 | -283.3 | -277.0 | -269.4 | -261.1 |

Table A4. Standard Gibbs energy of formation of alkanes in kJ/mol

| T/K | 0 | 200 | 298.15 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| methane | -66.73 | -58.05 | -50.68 | -50.51 | -41.96 | -32.66 | -22.95 | -12.48 | -2.00 | 8.47 | 19.36 | 30.2 | 41.1 | 52.4 | 63.3 | 74.2 |
| ethane | -68.03 | -47.91 | -31.73 | -31.44 | -13.22 | 6.09 | 26.07 | 46.59 | 67.54 | 88.90 | 109.84 | 131.2 | 152.1 | 173.1 | 194.0 | 215.0 |
| propane | -82.59 | -49.64 | -24.46 | -23.96 | 4.06 | 33.55 | 63.79 | 95.21 | 126.62 | 158.45 | 190.28 | 222.1 | 253.9 | 285.8 | 317.6 | 349.0 |
| butanes | | | | | | | | | | | | | | | | |
| 4 | -98.87 | -51.08 | -16.69 | -16.02 | 21.81 | 61.39 | 101.93 | 143.82 | 185.70 | 228.00 | 270.30 | 313.0 | 355.3 | 398.0 | 440.3 | 482.7 |
| 2m3 | -106.02 | -56.73 | -20.79 | -20.12 | 19.25 | 60.43 | 102.77 | 145.91 | 189.05 | 233.02 | 277.00 | 320.6 | 364.5 | 408.1 | 451.6 | 495.2 |
| pentanes | | | | | | | | | | | | | | | | |
| 5 | -114.43 | -51.98 | -8.33 | -7.45 | 40.30 | 90.10 | 141.33 | 193.26 | 246.04 | 298.81 | 352.00 | 405.2 | 458.4 | 511.6 | 564.8 | 617.5 |
| 2m4 | -118.99 | -57.46 | -13.27 | -12.43 | 35.91 | 86.34 | 137.98 | 190.75 | 243.94 | 297.14 | 350.75 | 404.4 | 458.0 | 511.6 | 564.8 | 618.0 |
| 22mm3 | -135.48 | -65.75 | -17.37 | -16.57 | 35.91 | 90.19 | 145.51 | 202.05 | 258.59 | 315.55 | 372.50 | 429.5 | 486.0 | 542.5 | 598.7 | 654.4 |
| hexanes | | | | | | | | | | | | | | | | |
| 6 | -130.08 | -52.92 | -.01 | 1.03 | 58.71 | 118.78 | 180.30 | 243.13 | 306.37 | 369.62 | 433.70 | 497.4 | 561.4 | 625.1 | 689.2 | 752.8 |
| 2m5 | -134.56 | -58.15 | -4.53 | -3.44 | 54.99 | 115.81 | 178.21 | 241.46 | 305.12 | 369.20 | 433.70 | 497.8 | 562.3 | 626.4 | 690.4 | 754.1 |
| 3m5 | -131.71 | -55.93 | -2.52 | -1.48 | 56.79 | 117.48 | 179.89 | 242.71 | 306.79 | 370.87 | 435.37 | 499.5 | 564.0 | 628.0 | 692.1 | 756.2 |
| 22mm4 | -143.43 | -63.63 | -7.80 | -6.71 | 54.03 | 117.10 | 181.56 | 246.90 | 313.07 | 379.24 | 445.83 | 512.0 | 577.8 | 643.9 | 709.3 | 774.6 |
| 23mm4 | -135.10 | -57.44 | -2.40 | -1.35 | 58.67 | 121.04 | 184.91 | 249.82 | 315.16 | 380.91 | 447.09 | 512.8 | 578.6 | 643.9 | 709.7 | 775.4 |
| heptanes | | | | | | | | | | | | | | | | |
| 7 | -145.73 | -53.82 | 8.34 | 9.56 | 77.17 | 147.45 | 219.70 | 292.58 | 366.29 | 440.84 | 515.39 | 589.9 | 664.5 | 739.0 | 813.6 | 888.2 |
| 2m6 | -150.25 | -59.13 | 3.74 | 4.96 | 73.32 | 144.35 | 217.19 | 290.90 | 365.46 | 440.01 | 515.39 | 590.4 | 665.3 | 740.3 | 815.3 | 889.8 |
| 3RSm6 | -147.36 | -57.80 | 4.45 | 5.67 | 73.53 | 143.98 | 216.35 | 289.23 | 363.36 | 437.50 | 512.05 | 586.6 | 661.2 | 735.7 | 809.8 | 884.0 |
| 3e5 | -145.77 | -52.40 | 11.36 | 12.61 | 81.85 | 153.77 | 227.23 | 302.20 | 377.59 | 453.40 | 529.20 | 605.4 | 681.2 | 757.5 | 833.3 | 909.1 |
| 22mm5 | -159.08 | -64.11 | 1.48 | 2.78 | 73.86 | 147.49 | 222.63 | 298.85 | 375.50 | 452.56 | 529.62 | 606.7 | 683.3 | 760.0 | 836.2 | 912.4 |
| 23RSmm5 | -147.28 | -57.46 | 5.83 | 7.09 | 76.08 | 147.78 | 220.95 | 295.51 | 370.48 | 445.86 | 521.67 | 597.5 | 672.9 | 748.3 | 823.6 | 898.2 |
| 24mm5 | -155.69 | -61.56 | 3.66 | 4.96 | 75.53 | 148.62 | 223.05 | 298.85 | 375.08 | 451.30 | 527.95 | 604.2 | 680.8 | 757.0 | 833.3 | 909.1 |
| 33mm5 | -153.30 | -59.59 | 5.42 | 6.71 | 77.25 | 150.42 | 225.14 | 300.95 | 377.17 | 453.40 | 530.46 | 606.7 | 682.9 | 759.1 | 834.9 | 910.3 |
| 223mmm4 | -156.57 | -60.89 | 5.54 | 6.84 | 78.92 | 153.64 | 230.16 | 307.22 | 385.12 | 463.44 | 541.75 | 620.1 | 698.0 | 775.5 | 852.9 | 930.0 |
| octanes | | | | | | | | | | | | | | | | |
| 8 | -161.38 | -54.72 | 16.66 | 18.04 | 95.62 | 176.16 | 258.68 | 342.44 | 426.63 | 511.65 | 596.67 | 682.1 | 767.6 | 853.0 | 938.0 | 1023.5 |
| 2m7 | -165.90 | -60.03 | 12.06 | 13.48 | 91.81 | 173.07 | 256.17 | 340.35 | 425.37 | 511.23 | 596.67 | 682.5 | 768.4 | 853.8 | 939.7 | 1024.7 |
| 3RSm7 | -163.05 | -58.78 | 12.69 | 14.11 | 91.81 | 172.57 | 255.33 | 339.10 | 423.28 | 508.30 | 593.74 | 679.2 | 764.2 | 849.6 | 934.7 | 1019.7 |
| 4m7 | -163.01 | -57.40 | 14.90 | 16.33 | 94.82 | 176.29 | 259.51 | 344.12 | 429.14 | 514.58 | 600.86 | 686.3 | 772.2 | 858.0 | 943.9 | 1029.3 |
| 3e6 | -161.46 | -55.01 | 17.33 | 18.75 | 97.21 | 178.59 | 262.02 | 346.21 | 431.65 | 517.09 | 602.95 | 688.8 | 775.1 | 860.9 | 946.8 | 1032.2 |
| 22mm6 | -174.77 | -65.14 | 9.63 | 11.10 | 92.06 | 175.91 | 261.60 | 348.30 | 435.83 | 523.37 | 611.32 | 698.9 | 786.8 | 873.9 | 961.4 | 1048.1 |
| 23RSmm6 | -163.01 | -58.23 | 14.53 | 15.95 | 95.07 | 177.13 | 261.19 | 346.21 | 432.07 | 517.93 | 604.62 | 690.9 | 777.2 | 863.5 | 949.7 | 1035.6 |
| 24RSmm6 | -168.57 | -62.42 | 10.93 | 12.35 | 91.77 | 173.99 | 257.84 | 342.86 | 428.72 | 514.58 | 600.86 | 687.1 | 773.4 | 859.3 | 945.1 | 1030.6 |
| 25mm6 | -170.25 | -63.30 | 10.43 | 11.89 | 91.94 | 174.91 | 259.93 | 345.79 | 432.49 | 519.60 | 607.13 | 694.2 | 781.8 | 868.9 | 956.0 | 1042.7 |
| 33mm6 | -168.95 | -61.20 | 13.02 | 14.45 | 94.82 | 177.96 | 262.86 | 348.72 | 435.00 | 521.69 | 608.81 | 695.1 | 781.8 | 868.1 | 954.3 | 1039.8 |
| 3RS4RSmm6 | -159.37 | -54.05 | 19.21 | 20.68 | 100.39 | 183.15 | 267.88 | 353.32 | 440.02 | 526.71 | 614.25 | 700.9 | 788.1 | 874.8 | 961.9 | 1048.1 |
| 3R4Smm6 | -159.58 | -54.01 | 19.34 | 20.76 | 100.51 | 183.23 | 267.88 | 353.74 | 440.02 | 526.71 | 614.25 | 700.9 | 788.1 | 874.8 | 961.9 | 1048.1 |
| 3e2m5 | -161.59 | -54.13 | 19.59 | 21.06 | 100.85 | 183.57 | 267.88 | 353.74 | 440.02 | 527.13 | 614.25 | 700.9 | 788.1 | 874.8 | 961.9 | 1048.1 |
| 3e3m5 | -162.84 | -52.46 | 23.06 | 24.53 | 106.33 | 190.98 | 277.50 | 365.04 | 452.99 | 541.36 | 630.15 | 718.5 | 806.9 | 895.3 | 982.8 | 1070.3 |
| 223RSmmm5 | -168.03 | -58.61 | 16.91 | 18.38 | 100.26 | 185.03 | 271.65 | 359.18 | 447.55 | 535.92 | 624.71 | 713.1 | 801.4 | 889.8 | 977.3 | 1064.9 |
| 224mmm5 | -172.51 | -62.59 | 13.10 | 14.61 | 96.54 | 181.35 | 267.88 | 355.41 | 443.78 | 532.57 | 620.94 | 709.7 | 797.7 | 885.6 | 973.6 | 1060.7 |
| 233mmm5 | -165.14 | -56.31 | 18.88 | 20.39 | 101.89 | 186.33 | 272.48 | 359.60 | 447.55 | 535.50 | 623.87 | 711.8 | 799.8 | 887.3 | 974.4 | 1061.1 |
| 234mmm5 | -163.93 | -55.10 | 20.09 | 21.56 | 102.90 | 187.04 | 272.90 | 360.02 | 447.55 | 535.50 | 623.45 | 711.8 | 799.8 | 887.3 | 974.8 | 1062.0 |
| 2233mmmm4 | -172.59 | -56.56 | 22.39 | 23.94 | 109.26 | 197.46 | 287.55 | 378.43 | 470.14 | 561.86 | 653.58 | 744.9 | 836.2 | 927.1 | 1017.5 | 1107.6 |
| nonanes | | | | | | | | | | | | | | | | |
| 9 | -177.07 | -55.70 | 24.98 | 26.53 | 114.03 | 204.80 | 297.65 | 391.89 | 486.97 | 582.46 | 678.37 | 774.3 | 870.6 | 966.5 | 1062.4 | 1158.3 |
| 2m8 | -181.59 | -60.97 | 20.38 | 21.97 | 110.22 | 201.70 | 295.14 | 390.22 | 485.71 | 582.04 | 678.37 | 774.7 | 871.4 | 967.8 | 1064.1 | 1160.0 |
| 3RSm8 | -178.70 | -59.72 | 21.05 | 22.64 | 110.31 | 201.24 | 294.31 | 388.54 | 483.62 | 579.53 | 675.02 | 771.4 | 867.3 | 963.2 | 1059.1 | 1154.6 |
| 4RSm8 | -178.66 | -59.47 | 21.46 | 23.06 | 110.93 | 202.03 | 295.14 | 389.80 | 484.87 | 580.37 | 676.70 | 772.6 | 868.5 | 964.4 | 1060.3 | 1156.3 |
| 3e7 | -177.15 | -55.99 | 25.56 | 27.16 | 115.54 | 207.14 | 301.00 | 395.66 | 491.57 | 587.90 | 684.65 | 781.4 | 878.1 | 974.9 | 1071.2 | 1168.0 |
| 4e7 | -177.15 | -55.79 | 26.02 | 27.62 | 116.21 | 207.98 | 301.84 | 396.91 | 492.82 | 589.15 | 685.90 | 782.7 | 879.4 | 976.1 | 1072.9 | 1169.2 |
| 22mm7 | -190.50 | -66.04 | 17.95 | 19.62 | 110.52 | 204.63 | 300.58 | 397.75 | 495.75 | 594.17 | 693.01 | 791.0 | 889.4 | 987.9 | 1085.4 | 1183.0 |
| 23RSmm7 | -178.74 | -59.26 | 22.64 | 24.23 | 113.15 | 205.42 | 299.74 | 395.24 | 491.57 | 588.73 | 685.90 | 782.7 | 879.8 | 976.6 | 1073.7 | 1170.1 |
| 24RSmm7 | -184.22 | -63.07 | 19.75 | 21.38 | 110.93 | 203.58 | 298.07 | 393.98 | 490.31 | 587.06 | 683.81 | 781.0 | 877.7 | 974.5 | 1071.2 | 1167.6 |
| 25RSmm7 | -183.09 | -64.24 | 17.53 | 19.12 | 107.92 | 199.98 | 293.89 | 389.38 | 485.71 | 582.46 | 679.21 | 776.0 | 873.1 | 969.5 | 1066.2 | 1162.5 |
| 26mm7 | -186.02 | -64.28 | 18.70 | 20.34 | 110.31 | 203.50 | 298.49 | 395.24 | 492.40 | 589.99 | 687.99 | 786.0 | 883.6 | 981.2 | 1078.8 | 1176.3 |
| 33mm7 | -184.68 | -62.27 | 21.09 | 22.72 | 112.94 | 206.26 | 301.42 | 397.75 | 494.92 | 592.50 | 690.09 | 787.7 | 884.8 | 982.0 | 1078.8 | 1175.5 |
| 3RS4SRmm7 | -175.27 | -55.91 | 26.32 | 27.91 | 117.17 | 209.69 | 304.35 | 400.26 | 496.59 | 593.76 | 690.92 | 788.5 | 885.7 | 982.8 | 1079.6 | 1176.3 |
| 3RS4RSmm7 | -175.06 | -55.95 | 26.15 | 27.78 | 117.04 | 209.56 | 304.35 | 399.84 | 496.59 | 593.76 | 690.92 | 788.5 | 885.7 | 982.8 | 1080.0 | 1176.3 |
| 3RS5RSmm7 | -181.33 | -60.10 | 22.84 | 24.48 | 114.32 | 207.31 | 302.25 | 398.59 | 495.33 | 592.92 | 690.50 | 788.1 | 885.7 | 982.8 | 1080.4 | 1177.2 |
| 3R5Smm7 | -181.59 | -59.80 | 23.30 | 24.94 | 114.87 | 207.89 | 303.09 | 399.00 | 496.17 | 593.34 | 691.34 | 788.9 | 886.5 | 983.7 | 1081.3 | 1178.4 |
| 44mm7 | -184.60 | -60.51 | 24.02 | 25.65 | 116.96 | 211.28 | 307.28 | 404.44 | 502.03 | 600.45 | 698.45 | 796.5 | 894.5 | 992.0 | 1089.2 | 1186.4 |
| 3RSe2m6 | -177.23 | -57.17 | 24.89 | 26.53 | 115.33 | 207.26 | 301.29 | 396.62 | 492.40 | 588.99 | 685.99 | 782.6 | 879.1 | 975.8 | 1072.4 | 1168.5 |
| 4e2m6 | -182.84 | -59.63 | 23.76 | 25.40 | 115.45 | 208.56 | 303.51 | 399.84 | 497.01 | 594.17 | 692.18 | 789.8 | 887.3 | 984.5 | 1082.1 | 1179.3 |
| 3e3m6 | -178.53 | -54.78 | 29.58 | 31.26 | 122.48 | 216.80 | 313.13 | 410.30 | 508.30 | 606.73 | 705.57 | 803.6 | 902.0 | 1000.0 | 1098.0 | 1195.2 |
| 3e4RSm6 | -173.89 | -53.19 | 29.41 | 31.05 | 120.47 | 213.04 | 307.69 | 403.61 | 500.35 | 597.52 | 694.69 | 792.3 | 889.9 | 987.0 | 1084.2 | 1180.9 |
| 223RSmmm6 | -183.80 | -59.43 | 25.52 | 27.16 | 119.13 | 214.29 | 311.46 | 409.88 | 508.72 | 608.40 | 707.66 | 806.9 | 906.2 | 1005.4 | 1103.9 | 1202.3 |
| 224RSmmm6 | -185.35 | -62.23 | 22.17 | 23.81 | 115.16 | 209.73 | 306.44 | 404.02 | 502.45 | 601.29 | 700.55 | 799.4 | 897.8 | 996.2 | 1094.2 | 1191.8 |
| 225mmm6 | -194.72 | -70.64 | 14.31 | 15.94 | 107.92 | 203.12 | 300.16 | 398.59 | 497.84 | 597.52 | 697.20 | 796.5 | 895.7 | 995.0 | 1093.8 | 1192.2 |
| 233mmm6 | -180.83 | -56.79 | 28.24 | 29.88 | 121.81 | 216.80 | 313.55 | 411.56 | 510.40 | 609.24 | 708.08 | 806.9 | 905.8 | 1004.2 | 1102.2 | 1199.8 |
| 23RS4SRmmm6 | -176.44 | -53.86 | 30.21 | 31.84 | 122.73 | 216.76 | 312.71 | 409.88 | 507.89 | 605.89 | 704.73 | 803.2 | 901.6 | 999.2 | 1097.6 | 1195.2 |
| 23RS4RSmmm6 | -175.98 | -53.99 | 29.96 | 31.63 | 122.52 | 216.55 | 312.71 | 409.88 | 507.89 | 605.89 | 704.73 | 803.2 | 901.6 | 999.6 | 1097.6 | 1195.2 |
| 23RS5mmm6 | -184.01 | -62.86 | 20.84 | 22.47 | 113.11 | 206.85 | 302.67 | 399.42 | 497.01 | 595.01 | 693.43 | 791.4 | 889.4 | 987.0 | 1084.6 | 1182.2 |
| 244mmm6 | -182.42 | -59.63 | 24.69 | 26.32 | 117.54 | 211.91 | 308.11 | 405.70 | 503.70 | 601.71 | 700.55 | 798.5 | 896.6 | 994.6 | 1092.1 | 1189.3 |
| 334RSmmm6 | -176.61 | -54.03 | 30.25 | 31.93 | 123.23 | 217.72 | 313.97 | 411.56 | 509.98 | 608.40 | 706.82 | 805.2 | 903.7 | 1001.7 | 1099.3 | 1196.8 |
| 33ee5 | -173.85 | -42.90 | 44.68 | 46.40 | 140.77 | 238.23 | 337.82 | 438.33 | 539.68 | 641.45 | 743.22 | 845.0 | 946.8 | 1048.1 | 1149.5 | 1250.4 |
| 3e22mm5 | -172.88 | -48.80 | 36.11 | 37.78 | 129.89 | 225.34 | 322.76 | 421.60 | 521.27 | 621.37 | 721.47 | 821.6 | 921.2 | 1020.9 | 1120.2 | 1219.4 |
| 3e23mm5 | -173.97 | -48.30 | 37.32 | 39.00 | 131.60 | 227.31 | 324.85 | 423.69 | 523.37 | 623.04 | 723.14 | 822.8 | 922.5 | 1022.2 | 1121.0 | 1219.9 |
| 3e24mm5 | -168.57 | -46.66 | 37.36 | 39.00 | 130.01 | 224.33 | 320.66 | 418.25 | 516.67 | 615.51 | 714.77 | 813.6 | 912.5 | 1010.9 | 1109.7 | 1207.7 |
| 2233mmmm5 | -178.36 | -49.80 | 37.61 | 39.33 | 133.74 | 231.24 | 330.71 | 430.80 | 532.15 | 633.50 | 734.85 | 835.8 | 936.3 | 1036.4 | 1136.5 | 1235.8 |
| 223RS4mmmm5 | -175.56 | -50.64 | 35.27 | 36.95 | 129.97 | 226.22 | 324.43 | 423.69 | 523.78 | 624.30 | 724.81 | 825.3 | 925.4 | 1025.1 | 1124.8 | 1223.6 |
| 2244mmmm5 | -183.43 | -53.23 | 34.89 | 36.61 | 131.60 | 229.69 | 329.87 | 430.80 | 532.57 | 634.34 | 736.53 | 838.3 | 939.6 | 1040.6 | 1141.1 | 1241.2 |
| 2334mmmm5 | -176.98 | -48.25 | 39.25 | 40.96 | 135.24 | 232.49 | 331.54 | 431.64 | 532.57 | 633.50 | 734.44 | 835.4 | 935.9 | 1036.0 | 1136.1 | 1235.3 |

Table A4 continued

| T/K | 0 | 200 | 298.15 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| decanes | | | | | | | | | | | | | | | | |
| 10 | -192.72 | -56.60 | 33.29 | 35.05 | 132.48 | 233.47 | 336.63 | 441.34 | 547.30 | 653.27 | 760.07 | 866.9 | 973.7 | 1080.1 | 1186.9 | 1293.7 |
| 2m9 | -197.28 | -61.91 | 28.69 | 30.49 | 128.63 | 230.37 | 334.54 | 439.66 | 546.05 | 652.85 | 760.07 | 867.3 | 974.1 | 1081.3 | 1188.5 | 1295.3 |
| 3RSm9 | -194.35 | -60.62 | 29.40 | 31.16 | 128.76 | 229.95 | 333.28 | 438.41 | 543.96 | 650.34 | 757.14 | 863.5 | 970.3 | 1076.7 | 1183.5 | 1289.9 |
| 4RSm9 | -194.35 | -60.45 | 29.78 | 31.54 | 129.35 | 230.66 | 334.12 | 439.25 | 545.21 | 651.59 | 757.98 | 864.8 | 971.6 | 1078.0 | 1184.8 | 1291.1 |
| 5m9 | -194.26 | -59.28 | 31.45 | 33.26 | 131.56 | 233.51 | 337.47 | 443.43 | 549.81 | 656.61 | 763.83 | 871.1 | 978.7 | 1085.9 | 1193.1 | 1299.9 |
| 3e8 | -192.84 | -56.94 | 33.88 | 35.64 | 133.95 | 235.81 | 339.98 | 445.52 | 551.90 | 658.71 | 766.34 | 873.6 | 981.2 | 1088.4 | 1195.6 | 1302.9 |
| 4RSe8 | -192.80 | -57.90 | 32.54 | 34.34 | 132.23 | 233.64 | 337.47 | 442.59 | 548.14 | 654.94 | 761.74 | 868.5 | 975.3 | 1082.1 | 1188.9 | 1295.3 |
| 22mm8 | -206.19 | -67.02 | 26.27 | 28.07 | 128.93 | 233.26 | 339.56 | 447.61 | 556.09 | 665.40 | 774.29 | 883.6 | 992.5 | 1101.4 | 1209.9 | 1318.3 |
| 23RSmm8 | -194.39 | -60.20 | 30.99 | 32.75 | 131.65 | 234.10 | 338.72 | 445.10 | 551.90 | 659.54 | 767.18 | 875.2 | 982.9 | 1090.5 | 1198.1 | 1305.4 |
| 24RSmm8 | -199.91 | -64.05 | 28.02 | 29.82 | 129.26 | 232.13 | 337.05 | 443.43 | 550.23 | 657.87 | 765.51 | 873.1 | 980.8 | 1088.4 | 1196.1 | 1302.9 |
| 25RSmm8 | -198.74 | -64.97 | 26.27 | 28.03 | 126.92 | 229.37 | 334.96 | 440.08 | 546.88 | 654.52 | 762.16 | 869.8 | 977.0 | 1084.7 | 1191.9 | 1299.1 |
| 26RSmm8 | -198.78 | -65.14 | 25.97 | 27.73 | 126.50 | 228.82 | 333.28 | 439.25 | 546.05 | 653.27 | 760.90 | 868.1 | 975.8 | 1083.0 | 1190.2 | 1297.0 |
| 27mm8 | -201.67 | -65.22 | 27.06 | 28.86 | 128.76 | 232.17 | 337.88 | 444.69 | 552.74 | 660.80 | 769.69 | 878.2 | 986.6 | 1094.7 | 1203.2 | 1311.2 |
| 33mm8 | -200.41 | -63.21 | 29.45 | 31.25 | 131.40 | 234.97 | 340.81 | 447.61 | 555.25 | 663.31 | 771.36 | 879.8 | 987.5 | 1095.5 | 1203.2 | 1310.4 |
| 3RS4SRmm8 | -191.04 | -56.94 | 34.38 | 36.18 | 135.29 | 237.95 | 342.91 | 449.29 | 556.51 | 664.14 | 772.20 | 880.3 | 988.3 | 1096.0 | 1204.0 | 1311.2 |
| 3RS4RSmm8 | -190.83 | -57.02 | 34.26 | 36.06 | 135.16 | 237.86 | 342.91 | 449.29 | 556.51 | 664.14 | 772.20 | 880.3 | 988.3 | 1096.0 | 1204.0 | 1311.2 |
| 3RS5RSmm8 | -196.98 | -61.91 | 29.99 | 31.79 | 131.19 | 234.05 | 339.14 | 445.10 | 552.32 | 659.96 | 767.60 | 875.7 | 983.3 | 1090.9 | 1198.1 | 1305.4 |
| 3RS5SRmm8 | -197.23 | -61.62 | 30.45 | 32.25 | 131.73 | 234.60 | 339.56 | 445.94 | 553.16 | 660.80 | 768.44 | 876.5 | 984.1 | 1091.8 | 1199.0 | 1306.2 |
| 3RS6RSmm8 | -195.85 | -61.62 | 29.95 | 31.75 | 131.02 | 233.93 | 339.14 | 445.52 | 553.16 | 661.22 | 769.27 | 877.7 | 985.8 | 1093.9 | 1201.9 | 1309.6 |
| 3R6Smm8 | -195.85 | -61.62 | 29.95 | 31.75 | 131.02 | 233.93 | 339.14 | 445.52 | 553.16 | 661.22 | 769.27 | 877.7 | 985.8 | 1093.9 | 1201.9 | 1309.6 |
| 44mm8 | -200.37 | -62.71 | 30.41 | 32.21 | 132.78 | 236.69 | 342.49 | 449.71 | 557.76 | 665.82 | 774.29 | 882.3 | 990.4 | 1098.5 | 1206.1 | 1313.3 |
| 4RS5RSmm8 | -190.75 | -55.55 | 36.56 | 38.40 | 138.30 | 241.79 | 347.51 | 454.73 | 562.36 | 670.84 | 779.73 | 888.2 | 997.1 | 1105.6 | 1214.0 | 1322.1 |
| 4R5Smm8 | -191.00 | -55.51 | 36.64 | 38.49 | 138.38 | 241.88 | 347.51 | 454.73 | 562.36 | 670.84 | 779.73 | 888.2 | 996.7 | 1105.2 | 1213.6 | 1322.1 |
| 4p7 | -192.76 | -54.68 | 37.48 | 39.28 | 138.88 | 241.96 | 347.09 | 453.89 | 561.53 | 669.17 | 777.64 | 886.1 | 994.2 | 1102.6 | 1210.7 | 1318.8 |
| 41p7 | -192.97 | -55.60 | 37.02 | 38.82 | 138.93 | 242.46 | 348.34 | 455.15 | 563.20 | 671.68 | 780.57 | 889.5 | 997.9 | 1106.8 | 1215.3 | 1323.4 |
| 3RSe2m7 | -192.92 | -56.98 | 34.88 | 36.64 | 135.96 | 238.70 | 343.74 | 450.12 | 557.34 | 664.98 | 773.46 | 881.5 | 989.6 | 1097.2 | 1205.3 | 1312.9 |
| 4RSe2m7 | -198.49 | -61.45 | 30.87 | 32.71 | 132.32 | 235.27 | 340.39 | 446.78 | 554.00 | 661.22 | 769.27 | 877.3 | 985.0 | 1092.6 | 1200.2 | 1307.5 |
| 5e2m7 | -197.19 | -61.41 | 30.41 | 32.21 | 131.60 | 234.56 | 339.56 | 446.36 | 554.00 | 662.05 | 770.11 | 878.6 | 986.6 | 1094.7 | 1203.2 | 1310.8 |
| 3e3m7 | -194.26 | -55.85 | 37.69 | 39.53 | 140.60 | 245.14 | 351.69 | 459.75 | 568.22 | 677.53 | 786.85 | 895.7 | 1005.0 | 1113.9 | 1222.4 | 1330.9 |
| 4RSe3RSm7 | -189.58 | -53.92 | 38.15 | 39.95 | 139.51 | 242.51 | 347.93 | 454.31 | 561.95 | 670.00 | 778.06 | 886.5 | 994.6 | 1102.6 | 1211.1 | 1318.8 |
| 4RSe3SRm7 | -189.58 | -53.92 | 38.15 | 39.95 | 139.51 | 242.51 | 347.93 | 454.31 | 561.95 | 670.00 | 778.06 | 886.5 | 994.6 | 1102.6 | 1211.1 | 1318.8 |
| 3e5RSm7 | -195.69 | -59.53 | 32.46 | 34.26 | 133.61 | 236.40 | 341.23 | 447.61 | 554.83 | 662.47 | 770.53 | 878.2 | 986.2 | 1093.9 | 1201.5 | 1308.7 |
| 3e4RSm7 | -189.58 | -53.92 | 38.15 | 39.95 | 139.47 | 242.46 | 347.51 | 454.31 | 561.53 | 669.58 | 777.64 | 886.1 | 994.2 | 1102.2 | 1210.3 | 1317.9 |
| 4e4m7 | -194.14 | -55.18 | 38.94 | 40.79 | 142.40 | 247.32 | 354.20 | 462.26 | 571.15 | 680.46 | 789.77 | 899.1 | 1008.0 | 1116.9 | 1225.8 | 1333.8 |
| 223RSmmm7 | -199.53 | -60.37 | 33.80 | 35.64 | 137.50 | 242.92 | 350.44 | 459.33 | 569.06 | 679.21 | 789.36 | 899.5 | 1009.2 | 1119.0 | 1228.3 | 1337.6 |
| 224RSmmm7 | -201.00 | -62.92 | 30.95 | 32.79 | 134.24 | 239.20 | 346.25 | 454.73 | 563.62 | 673.35 | 783.08 | 892.4 | 1001.7 | 1110.6 | 1219.5 | 1328.0 |
| 225RSmmm7 | -207.53 | -70.28 | 23.30 | 25.14 | 126.46 | 231.38 | 338.30 | 446.78 | 556.09 | 665.82 | 775.55 | 885.3 | 995.0 | 1104.3 | 1213.2 | 1322.1 |
| 226mmm7 | -210.54 | -71.45 | 22.92 | 24.76 | 126.75 | 232.21 | 339.56 | 448.45 | 558.18 | 667.91 | 778.06 | 888.2 | 997.9 | 1107.2 | 1216.6 | 1325.5 |
| 233mmm7 | -196.56 | -57.81 | 36.35 | 38.19 | 139.97 | 245.18 | 352.53 | 461.00 | 570.31 | 680.04 | 789.77 | 899.5 | 1008.8 | 1118.1 | 1227.0 | 1335.5 |
| 23RS4SRmmm7 | -192.30 | -54.76 | 38.78 | 40.62 | 141.65 | 246.06 | 352.53 | 460.58 | 569.06 | 677.95 | 787.26 | 896.6 | 1005.9 | 1114.4 | 1223.3 | 1331.7 |
| 23RS4RSmmm7 | -191.71 | -54.76 | 38.69 | 40.49 | 141.52 | 245.98 | 352.53 | 460.58 | 569.06 | 677.95 | 787.68 | 896.6 | 1005.9 | 1114.8 | 1223.7 | 1332.1 |
| 23RS5RSmmm7 | -196.65 | -61.54 | 31.29 | 33.09 | 133.65 | 237.69 | 343.74 | 451.38 | 559.85 | 668.75 | 777.64 | 886.5 | 995.4 | 1103.9 | 1212.4 | 1320.9 |
| 23RS5SRmmm7 | -197.23 | -61.45 | 31.50 | 33.30 | 133.86 | 237.86 | 344.16 | 451.38 | 559.85 | 668.75 | 777.64 | 886.5 | 995.4 | 1103.9 | 1212.4 | 1320.4 |
| 23RS6mmm7 | -198.61 | -64.63 | 27.56 | 29.41 | 129.43 | 233.09 | 339.14 | 446.36 | 554.42 | 662.89 | 771.78 | 880.7 | 989.2 | 1097.6 | 1206.1 | 1314.2 |
| 244mmm7 | -198.07 | -60.12 | 34.01 | 35.85 | 137.42 | 242.34 | 349.18 | 457.24 | 566.13 | 675.44 | 784.33 | 893.6 | 1002.1 | 1111.0 | 1219.1 | 1327.1 |
| 24RS5SRmmm7 | -196.31 | -60.49 | 32.67 | 34.47 | 135.29 | 239.54 | 345.83 | 453.47 | 561.95 | 670.84 | 779.73 | 889.0 | 997.9 | 1106.4 | 1214.9 | 1323.4 |
| 24RS5RSmmm7 | -196.06 | -60.58 | 32.50 | 34.34 | 135.12 | 239.37 | 345.83 | 453.47 | 561.95 | 670.42 | 779.73 | 888.6 | 997.5 | 1106.0 | 1214.9 | 1322.9 |
| 246mmm7 | -205.43 | -66.64 | 27.73 | 29.57 | 131.27 | 236.10 | 342.91 | 450.96 | 559.44 | 668.75 | 777.64 | 887.0 | 995.8 | 1104.3 | 1213.2 | 1321.3 |
| 255mmm7 | -204.81 | -67.98 | 25.47 | 27.27 | 128.38 | 232.92 | 339.56 | 447.61 | 556.51 | 665.40 | 775.13 | 884.0 | 992.9 | 1101.8 | 1210.3 | 1318.3 |
| 334RSmmm7 | -192.38 | -54.89 | 38.86 | 40.70 | 142.11 | 246.98 | 353.78 | 462.26 | 571.15 | 680.46 | 789.77 | 899.1 | 1008.4 | 1117.7 | 1225.8 | 1333.8 |
| 335RSmmm7 | -195.14 | -59.36 | 33.63 | 35.43 | 136.04 | 240.12 | 346.25 | 453.89 | 561.95 | 670.84 | 779.31 | 888.2 | 996.3 | 1104.7 | 1212.4 | 1320.0 |
| 3RS44mmm7 | -192.30 | -54.55 | 39.53 | 41.37 | 143.11 | 248.15 | 355.46 | 463.51 | 572.41 | 681.72 | 791.45 | 900.8 | 1009.7 | 1118.5 | 1227.0 | 1335.1 |
| 3RS45RSmmm7 | -188.36 | -51.50 | 41.91 | 43.72 | 144.78 | 249.33 | 355.88 | 463.93 | 572.82 | 682.14 | 791.45 | 901.2 | 1010.5 | 1119.4 | 1228.3 | 1337.2 |
| s3R45Smmm7 | -188.95 | -50.32 | 43.80 | 45.64 | 147.29 | 252.34 | 359.64 | 468.12 | 577.43 | 687.16 | 797.31 | 907.0 | 1017.2 | 1126.5 | 1236.2 | 1345.5 |
| r3R45Smmm7 | -188.03 | -50.49 | 43.38 | 45.22 | 146.79 | 251.92 | 359.22 | 467.70 | 577.43 | 687.16 | 797.31 | 907.0 | 1017.2 | 1126.9 | 1236.6 | 1345.5 |
| 3ip2m6 | -184.31 | -47.35 | 46.10 | 47.94 | 149.14 | 253.89 | 360.90 | 469.37 | 578.26 | 687.99 | 798.14 | 907.9 | 1018.0 | 1127.3 | 1237.1 | 1346.4 |
| 33ee6 | -189.45 | -45.64 | 50.57 | 52.46 | 156.04 | 263.01 | 372.19 | 482.34 | 593.33 | 704.73 | 816.55 | 928.0 | 1039.4 | 1150.8 | 1261.7 | 1372.3 |
| 34ee6 | -188.28 | -48.86 | 44.76 | 46.60 | 147.42 | 251.58 | 357.97 | 465.61 | 574.50 | 683.39 | 793.12 | 902.4 | 1012.2 | 1121.5 | 1230.8 | 1339.7 |
| 3RSe22mm6 | -188.57 | -50.70 | 43.13 | 44.97 | 146.67 | 252.00 | 359.64 | 468.53 | 578.26 | 688.83 | 799.40 | 909.5 | 1019.7 | 1129.8 | 1239.6 | 1348.9 |
| 4e22mm6 | -199.45 | -59.24 | 35.30 | 37.15 | 139.26 | 244.89 | 352.53 | 461.84 | 571.57 | 682.14 | 792.70 | 902.9 | 1013.0 | 1123.1 | 1232.9 | 1342.2 |
| 3RSe23mm6 | -189.66 | -49.91 | 44.93 | 46.77 | 149.18 | 254.93 | 362.57 | 471.88 | 581.61 | 691.76 | 801.91 | 912.1 | 1022.2 | 1131.9 | 1241.2 | 1350.6 |
| 4e23RSmm6 | -190.33 | -51.37 | 42.42 | 44.26 | 145.45 | 250.00 | 356.71 | 464.77 | 573.66 | 682.97 | 792.28 | 901.6 | 1011.3 | 1120.2 | 1229.5 | 1338.0 |
| 3RSe24SRmm6 | -181.17 | -45.09 | 48.06 | 49.91 | 150.81 | 255.31 | 362.15 | 470.21 | 579.10 | 688.41 | 798.14 | 907.9 | 1017.2 | 1126.5 | 1235.8 | 1344.7 |
| 3RSe24RSmm6 | -181.04 | -45.09 | 48.02 | 49.87 | 150.77 | 255.23 | 362.15 | 470.21 | 579.10 | 688.41 | 798.14 | 907.9 | 1017.6 | 1126.9 | 1236.2 | 1345.1 |
| 4e24mm6 | -191.88 | -53.09 | 41.45 | 43.30 | 145.50 | 251.08 | 358.80 | 467.70 | 577.43 | 687.58 | 797.72 | 907.9 | 1018.0 | 1127.3 | 1236.6 | 1345.5 |
| 3e25mm6 | -197.74 | -60.28 | 33.25 | 35.05 | 136.04 | 240.37 | 346.67 | 454.73 | 563.20 | 672.51 | 781.82 | 891.1 | 1000.4 | 1109.3 | 1218.2 | 1326.7 |
| 4e33mm6 | -181.42 | -44.22 | 49.49 | 51.33 | 152.94 | 258.11 | 365.50 | 474.39 | 583.70 | 693.85 | 804.00 | 914.1 | 1023.9 | 1133.2 | 1242.9 | 1351.8 |
| 3e34RSmm6 | -185.43 | -46.06 | 48.65 | 50.49 | 152.86 | 258.66 | 366.75 | 475.65 | 585.80 | 695.94 | 806.51 | 916.7 | 1027.2 | 1137.0 | 1246.7 | 1356.0 |
| 2233mmmm6 | -194.14 | -50.32 | 46.89 | 48.78 | 153.57 | 261.71 | 371.77 | 483.18 | 595.00 | 707.24 | 819.48 | 931.3 | 1042.7 | 1154.1 | 1264.7 | 1374.8 |
| 223RS4RSmmmm6 | -187.95 | -48.07 | 47.35 | 49.24 | 152.48 | 259.24 | 368.01 | 478.58 | 589.56 | 700.96 | 812.37 | 923.8 | 1034.8 | 1145.7 | 1256.3 | 1366.5 |
| 223RS4SRmmmm6 | -187.57 | -48.32 | 46.98 | 48.86 | 152.06 | 258.82 | 367.59 | 478.16 | 589.14 | 700.55 | 812.37 | 923.8 | 1034.8 | 1145.7 | 1256.3 | 1366.5 |
| 223RS5mmmm6 | -204.72 | -64.05 | 31.79 | 33.67 | 137.17 | 244.05 | 352.95 | 463.09 | 574.08 | 685.48 | 796.89 | 908.3 | 1018.9 | 1129.4 | 1240.0 | 1349.7 |
| 2244mmmm6 | -193.30 | -51.41 | 44.84 | 46.69 | 150.43 | 257.53 | 366.75 | 476.90 | 587.89 | 699.29 | 810.69 | 921.7 | 1032.2 | 1142.4 | 1252.1 | 1361.4 |
| 224RS5mmmm6 | -200.71 | -62.58 | 32.17 | 34.01 | 136.63 | 242.80 | 351.27 | 461.00 | 571.57 | 682.14 | 793.12 | 904.1 | 1014.7 | 1124.8 | 1235.0 | 1344.3 |
| 2255mmmm6 | -219.03 | -75.60 | 21.58 | 23.51 | 128.51 | 237.11 | 347.93 | 460.17 | 572.82 | 685.90 | 799.40 | 912.5 | 1025.1 | 1137.4 | 1249.6 | 1361.0 |
| 2334RSmmmm6 | -188.49 | -47.10 | 48.94 | 50.83 | 154.32 | 261.12 | 369.68 | 479.83 | 590.40 | 701.38 | 812.37 | 922.9 | 1033.5 | 1143.6 | 1253.4 | 1362.7 |
| 2335mmmm6 | -194.14 | -55.22 | 39.86 | 41.75 | 144.53 | 250.75 | 359.22 | 468.53 | 579.10 | 689.67 | 800.23 | 910.8 | 1020.9 | 1130.7 | 1240.4 | 1349.3 |
| 23RS44mmmm6 | -184.10 | -46.02 | 48.73 | 50.58 | 153.11 | 259.12 | 367.17 | 476.48 | 586.63 | 697.20 | 807.77 | 917.9 | 1028.1 | 1137.8 | 1247.5 | 1356.4 |
| 23RS4RS5mmmm6 | -192.30 | -51.79 | 43.88 | 45.77 | 149.01 | 255.56 | 364.24 | 473.97 | 584.54 | 695.52 | 806.93 | 917.9 | 1028.9 | 1139.0 | 1249.6 | 1359.8 |
| 23R4S5mmmm6 | -193.13 | -51.58 | 44.38 | 46.27 | 149.55 | 256.10 | 364.66 | 474.39 | 584.96 | 695.94 | 807.35 | 918.3 | 1028.9 | 1139.5 | 1250.0 | 1359.8 |
| 3344mmmm6 | -184.14 | -40.70 | 56.31 | 58.19 | 162.86 | 270.79 | 380.56 | 491.96 | 603.37 | 715.61 | 827.43 | 939.3 | 1050.7 | 1161.6 | 1272.2 | 1381.9 |
| 3ip24mm5 | -191.21 | -50.49 | 45.51 | 47.40 | 151.10 | 258.28 | 367.59 | 478.16 | 589.98 | 701.80 | 813.62 | 925.9 | 1037.3 | 1148.7 | 1260.5 | 1371.5 |
| 33ee2m5 | -174.18 | -33.84 | 61.66 | 63.55 | 167.04 | 274.26 | 383.91 | 494.47 | 606.30 | 718.12 | 830.78 | 942.6 | 1054.8 | 1166.2 | 1278.1 | 1389.0 |
| 3e223mmm5 | -175.23 | -33.00 | 63.84 | 65.72 | 170.60 | 279.16 | 389.77 | 502.01 | 614.66 | 727.74 | 841.24 | 953.9 | 1066.6 | 1178.8 | 1291.0 | 1402.4 |
| 3RSe224mmm5 | -179.83 | -41.08 | 53.92 | 55.76 | 158.67 | 265.22 | 373.87 | 484.01 | 595.00 | 706.40 | 818.23 | 929.2 | 1040.6 | 1151.2 | 1262.2 | 1372.3 |
| 3e234mmm5 | -175.39 | -34.22 | 62.08 | 63.97 | 168.17 | 275.94 | 386.00 | 496.99 | 608.81 | 721.05 | 833.71 | 945.9 | 1057.8 | 1169.6 | 1281.0 | 1391.6 |
| 22334mmmmm5 | -178.28 | -33.55 | 64.67 | 66.60 | 172.57 | 281.96 | 393.53 | 506.19 | 619.27 | 732.76 | 846.26 | 959.3 | 1072.4 | 1184.7 | 1296.5 | 1407.9 |
| 22344mmmmm5 | -180.67 | -34.76 | 63.92 | 65.89 | 172.31 | 282.25 | 394.37 | 507.45 | 621.36 | 735.69 | 850.02 | 963.9 | 1077.4 | 1190.5 | 1303.2 | 1415.0 |