# Standard Chemical Thermodynamic Properties of Isomer Groups of Monochloroalkanes

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The chemical thermodynamic properties of isomer groups of monochloroalkanes from $C_2H_5Cl$ to $C_8H_{17}Cl$ in the ideal gas phase have been calculated from 298.15 to 1500 K using new Benson group values from Bozzelli. Increments in isomer group properties per $CH_2$ have been calculated to show the extent to which thermodynamic properties of higher isomer groups may be obtained by linear extrapolation. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state. Values of $C_p^\circ$, $S^\circ$, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ are given for all species of monochloroalkanes from $CH_3Cl$ to $C_8H_{17}Cl$ in SI units for a standard state pressure of 1 bar. The values calculated here are compared with values published by the Thermodynamics Research Center (Texas A&M University) on June 30, 1981.

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

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## 1. Introduction

Earlier papers in this series have presented isomer oup thermodynamic properties[1] for the alkanes[2], alkylnzenes[3], alkenes[4], alkylnaphthalenes[5], alkylcyclopenes and alkylcyclohexanes[6], alkynes[7], alkanethiols[8], canols[9], and polycyclic aromatic hydrocarbons[10,11] in e ideal gas state. This paper presents calculations on e monochloroalkanes. Chemical thermodynamic propties are given in Stull, Westrum, and Sinke[12] for all mers of monochloroalkanes through $C_4H_9Cl$ in the al gas state. More recently Rogers[13] has prepared tas on all isomers of the monochloroalkanes through $H_{13}Cl$ by a combination of statistical mechanics and e Benson group method[14]. Here we present calculans of the thermodynamic properties of all isomers ough $C_8H_{17}Cl$ using the Benson group method with w parameters from Bozzelli[15,16], who has studied curt literature sources, including Pedley, Naylor, and rby[17]. The principal objective of this article is to calcue the isomer group properties and to find the extent to ich the standard thermodynamic properties of higher mer groups can be obtained by linear extrapolation.

## . Standard Thermodynamic Properties f Isomer Groups of Monochloroalkanes

When isomers are in chemical equilibrium it has been own for some time[18,19] that they can be aggregated in culations of equilibrium mole fractions by use of the ndard Gibbs energy of formation $\Delta_f G°(I)$ of the iso- group defined by

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

ere $\Delta_f G_i°$ is the standard Gibbs energy of formation of ndividual isomer and $N_i$ is the number of isomers in group, including stereoisomers. The equilibrium e fractions $r_i$ of various isomers in a group can be ulated using

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

re $y_I$ is the sum of the mole fractions of the individ isomers. The corresponding equations for the other dard thermodynamic properties $C_p°(I)$, $S°(I)$, and °(I) can be derived by differentiating Eq. 1 with re t to temperature[1]. When standard Gibbs energies of ation of isomer groups are used to calculate equiim constants for reactions of ideal gases the equiim expression is written in terms of equilibrium mole ions of isomer groups.

or the monochloroalkanes the standard chemical nodynamic properties for an isomer group are intered by

$$\Delta_f G°(I) = \Delta_f H°(I) - T[S°(I) - nS°_{\text{graphite}} - ((2n+1)/2)S°_{H_2(g)} - (1/2)S°_{Cl_2(g)}] \qquad (3)$$

where $n$ is the number of carbon atoms.

To calculate the chemical thermodynamic properties for an isomer group a term must be included for each molecular species, including stereoisomers. Fortunately, the numbers of stereoisomers and non-stereoisomeric mono-substitution products of paraffins were calculated by Blair and Henze[20] in 1932. Their table was very helpful in identifyng all the isomers through $C_8H_{17}Cl$. An expanded version of their table of numbers of isomers through $C_8H_{17}Cl$ is given in Table 1. The isomers are classified according to whether chlorine is bonded to a primary, secondary, or tertiary carbon and according to the numbers of chiral centers (none, one, two, or three).

Table 1. Numbers of primary, secondary, and tertiary isomers of monochloroalkanes

| | Chiral Centers | Primary | Secondary | Tertiary | Total |
|---|---|---|---|---|---|
| CH3Cl | None | 1 | | | 1 |
| C2H5Cl | None | 1 | | | 1 |
| C3H7Cl | None | 1 | 1 | | 2 |
| C4H9Cl | None | 2 | | 1 | 3 |
| | One | | 2 | | 2 |
| | Total | 2 | 2 | 1 | 5 |
| C5H11Cl | None | 3 | 1 | 1 | 5 |
| | One | 2 | 4 | | 6 |
| | Total | 5 | 5 | 1 | 11 |
| C6H13Cl | None | 5 | | 3 | 8 |
| | One | 6 | 10 | | 16 |
| | Two | | 4 | | 4 |
| | Total | 11 | 14 | 3 | 28 |
| C7H15Cl | None | 8 | 2 | 4 | 14 |
| | One | 16 | 18 | 6 | 40 |
| | Two | 4 | 16 | | 20 |
| | Total | 28 | 36 | 10 | 74 |
| C8H17Cl | None | 14 | | 9 | 23 |
| | One | 40 | 38 | 14 | 92 |
| | Two | 20 | 52 | 4 | 76 |
| | Three | | 8 | | 8 |
| | Total | 74 | 98 | 27 | 199 |

Rather than having a line in a thermodynamic table for each stereoisomer, this article follows the standard practice of giving properties of racemates. When there is one chiral center $R\ln 2$ is added to the calculated standard entropy and $-RT\ln 2$ to the standard Gibbs energy of formation of one of the forms. For the monochloroalkanes with two chiral centers the adjustment of the entropy is $R\ln 4$ for two centers and $R\ln 8$ for three, since none of the species are internally compensated. Therefore, the numbers of lines in tables in this article is smaller than the total numbers of isomers. The number of lines in the tables for $CH_3Cl$, ..., $C_8H_{17}Cl$ are 1, 1, 2, 4, 8, 17, 39, and 89 respectively.

Stull, Westrum and Sinke[12] brought together a great deal of data in making their tables on the monochloroalkanes, and so those references are not given here. More recently Cox and Pilcher[21] and Pedley, Naylor, and Kirby[17] have evaluated enthalpy of formation data on monochloroalkanes at 298.15 K.

## 3. Calculations of Standard Thermodynamic Properties of Monochloroalkanes Using the Benson Method

In order to make these calculations, each monochloroalkane structure was divided into the following Benson groups; $C(H)_3(C)$, $C(H)_2(C)_2$, $C(H)(C)_3$, $C(C)_4$, $C(C)(H)_2Cl$, $C(C)_2(H)Cl$, $C(C)_3Cl$, and gauche. In addition the total symmetry number (TSN) and number of optical isomers (OPT) were tabulated. In view of the uncertainties in some of these group values indicated by Benson, the 1,5-H repulsions, which affect only several of the most highly branched species were omitted. In calculating symmetry numbers a report by Davies, Syverud, and Steiner[22] was very helpful.

Bozzelli[16] has recently provided the following Benson group values for monochloroalkanes up to 1500 K.

| Group | $\Delta_f H°$ | $S°$ | $C_p°$ | | | | |
|---|---|---|---|---|---|---|---|
| | 298 | 298 | 300 | 500 | 800 | 1000 | 1500 |
| $C-H_2,Cl,C$ | −16.80 | 37.86 | 8.65 | 12.08 | 15.15 | 16.47 | 18.46 |
| $C-H,Cl,C_2$ | −14.47 | 16.75 | 8.47 | 11.68 | 14.29 | 15.38 | 16.21 |
| $C-Cl,C_3$ | −14.41 | −6.65 | 8.09 | 11.69 | 13.47 | 13.53 | 13.32 |

(The group values for $S°$ and $C_p°$ are in cal $K^{-1}$ $mol^{-1}$ and for $\Delta_f H°$ in kcal $mol^{-1}$. The standard state pressure is 1 atmosphere.)

The assignment of Benson groups was checked by multiplying the matrix of numbers of groups by a matrix which had in its first column the number of carbon atoms in each group, in the second column the number of hydrogen atoms in each group, and in the third column the number of chlorine atoms in each group. Matrix multiplication yields a matrix with as many rows a lines in the table for that isomer group and three column giving the numbers of carbon atoms, hydrogen atom and chlorine atoms. This check prevents some possibl errors in the group assignments.

The procedures used in the estimation of chemica thermodynamic properties of the monochloroalkanes i the ideal gas state have been destribed in previous arti cles in this series. The function used to express the hea capacity as a function of temperature is that used in th paper on benzene-series polycyclic aromatic hydrocar bons[10,11]. The values of $H°-H°_{298}$ and $S°$ for graphite an $H_2(g)$, in their standard states were obtained from th JANAF[23] tables.

Table 2 shows how well the chemical thermodynami properties calculated using the group values fron Bozzelli agree with the values from Rogers[13]. The differ ences between the Rogers values and the values pre sented here at each temperature were squared, divide by the number of pairs of values, and the square root wa taken. This yields the root mean square deviations at var ious temperatures. These differences are distributec rather randomly and are about what would be expectec from the Benson method, except for $\Delta_f G°$ at 1000 K. The standard enthalpies of formation of twelve monochloroalkanes at 298.15 K are given by Pedley, Naylor and Kirby[17], and the values calculated here for eight of these species are within the uncertainty limits given by Pedley, Naylor, and Kirby.

Rogers[13] lists 2 (RR′)-chloro-3 (SS′)-methylpentane and 2(RS′)-chloro-(SR′)-methylpentane separately, but since they have the same thermodynamic properties, they are combined in the tables here with the name 2(RS)-chloro-3(RS)-methylpentane and $R$ ln 2 has been added to the entropy value given by Rogers.

Table 2. Root mean square deviations between chloroalkane thermodynamic properties from the Thermodynamics Research Center and the values presented here

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| | Standard heat capacity at constant pressure in J/K mol | | | | | | | | |
| C2H5Cl | .57 | .58 | .55 | .45 | .61 | .71 | .77 | .69 | .36 |
| C3H7Cl | .58 | .62 | 1.09 | 2.72 | 3.18 | 3.15 | 3.18 | 3.06 | 3.06 |
| C4H9Cl | .51 | .54 | 1.36 | 2.62 | 3.52 | 3.80 | 3.79 | 3.71 | 3.36 |
| C5H11Cl | .38 | .33 | 1.39 | 2.97 | 5.13 | 6.28 | 6.94 | 8.23 | 8.67 |
| C6H13Cl | .59 | .47 | 1.68 | 3.22 | 5.74 | 7.10 | 8.01 | 9.46 | 9.82 |
| | Standard entropy in J/K mol | | | | | | | | |
| C2H5Cl | .51 | .51 | .18 | .01 | .11 | .18 | .25 | .38 | .46 |
| C3H7Cl | .40 | .40 | .11 | .71 | 1.46 | 1.79 | 2.10 | 2.62 | 3.06 |
| C4H9Cl | 2.85 | 2.86 | 3.10 | 2.85 | 2.71 | 2.75 | 2.85 | 3.14 | 3.41 |
| C5H11Cl | 3.56 | 3.57 | 3.98 | 4.11 | 4.47 | 4.77 | 5.16 | 6.07 | 6.98 |
| C6H13Cl | 6.40 | 6.39 | 6.84 | 7.11 | 7.74 | 8.24 | 8.80 | 10.04 | 11.22 |
| | Standard enthalpy of formation in kJ/mol | | | | | | | | |
| C2H5Cl | .50 | .50 | .61 | .70 | .79 | .87 | .97 | 1.13 | 1.21 |
| C3H7Cl | .85 | .85 | .92 | .69 | .66 | .85 | 1.12 | 1.68 | 2.25 |
| C4H9Cl | 2.10 | 2.11 | 2.13 | 2.12 | 2.25 | 2.48 | 2.76 | 3.34 | 3.87 |
| C5H11Cl | 1.75 | 1.75 | 1.78 | 1.86 | 2.26 | 2.72 | 3.32 | 4.70 | 6.21 |
| C6H13Cl | 3.25 | 3.25 | 3.28 | 3.44 | 3.88 | 4.35 | 4.99 | 6.43 | 7.99 |
| | Standard Gibbs energy of formation in kJ/mol | | | | | | | | |
| C2H5Cl | .65 | .65 | .69 | .71 | .69 | 4.97 | .69 | .63 | 1.05 |
| C3H7Cl | .95 | .96 | .90 | .92 | 1.08 | 11.13 | 1.46 | 1.91 | 2.92 |
| C4H9Cl | 2.11 | 2.12 | 2.27 | 2.58 | 2.95 | 16.54 | 3.32 | 3.70 | 3.99 |
| C5H11Cl | 1.42 | 1.43 | 1.60 | 2.15 | 2.87 | 21.85 | 3.64 | 4.60 | 5.30 |
| C6H13Cl | 2.78 | 2.78 | 3.15 | 4.04 | 5.26 | 27.73 | 6.63 | 8.34 | 9.87 |

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

The conversion of thermodynamic properties from 1 tm to 1 bar is discussed in earlier papers in this series nd in the NBS Tables[24].

The remaining tables in this paper have all been calculated using values for $CH_3Cl$ from Chase, *et al.*[23]. The values in the tables here for $C_2H_5Cl$ to $C_8H_{17}Cl$ have been calculated with the Bozzelli group values. Tables 3 to 8 give isomer group properties and the increments per carbon atom. Table gives $H°(I,T)$-$H^0$(I,298.15 K), the standard enthalpy for an isomer group relative to the isomer group at 298.15 K. Table 8 gives values for $H°(I,T)$-$H°$(I,298.15 K) + $\Delta$[SB::*f*]$H°(I,298.15$ K), the standard enthalpy of formation 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 increments per carbon atom are of interest because they indicate the extent to which we can estimate thermodynamic properties of isomer groups of higher carbon numbers.

## 5. Equilibrium Mole Fractions Within Isomer Groups of Monochloroalkanes

The equilibrium mole fractions within isomer groups calculated from standard Gibbs energies of formation are given in Table 9 for the monochloroalkenes in the ideal gas state. Since the uncertainties in $\Delta_f G°(I)$ and $\Delta_f G_i°$ are about the same, the uncertainty in the difference is nearly independent of the relative values of the two parameters, but the absolute uncertainty does increase with temperature. The usual equation for the propagation of variance indicates that the equilibrium mole fractions are uncertain by about 15% at the lower temperature 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.

Compounds are named in tables according to the IUPAC Revised and Collected Recommendations for the Nomenclature of Organic Chemistry, 1979[25].

## 6. Standard Thermodynamic Properties of Individual Species of Monochloroalkanes

The values of $C_p°$, $S°$, $\Delta_f H°$, and $\Delta_f G°$ for all the monochloroalkane species through $C_8H_{17}Cl$ are given in Tables 10 to 13 in SI units for a standard state pressure of 1 bar. The values for chloromethane are from Chase, et al.[23], and the other values have been calculated using the Bozzelli values in the Benson method. The values for chiral forms are for the racemates.

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

| T/K | CH3Cl | C2H5Cl | C3H7Cl | C4H9Cl | C5H11Cl | C6H13Cl | C7H15Cl | C8H17Cl |
|---|---|---|---|---|---|---|---|---|
| 298.15 | 40.73 | 61.84 | 91.26 | 115.04 | 143.9 | 173.9 | 199.4 | 220.2 |
| 300.00 | 40.86 | 62.10 | 91.65 | 115.74 | 144.8 | 174.7 | 200.3 | 221.2 |
| 500.00 | 55.15 | 89.83 | 135.03 | 205.84 | 230.5 | 263.3 | 298.1 | 331.2 |
| 700.00 | 66.61 | 110.22 | 162.54 | 235.80 | 266.2 | 311.7 | 353.6 | 396.7 |
| 900.00 | 75.29 | 124.73 | 180.69 | 243.83 | 288.3 | 340.0 | 388.6 | 438.3 |
| 1000.00 | 78.85 | 130.52 | 187.90 | 248.94 | 297.9 | 351.7 | 403.0 | 455.1 |
| 1100.00 | 81.95 | 135.58 | 194.23 | 254.48 | 306.8 | 362.2 | 415.8 | 469.9 |
| 1300.00 | 87.04 | 144.03 | 204.92 | 265.47 | 322.3 | 380.6 | 437.8 | 495.2 |
| 1500.00 | 90.94 | 150.83 | 213.63 | 275.44 | 335.4 | 396.0 | 455.9 | 516.0 |

Table 3a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 |
|---|---|---|---|---|---|---|---|
| 298.15 | 21.11 | 29.42 | 23.78 | 28.9 | 30.0 | 25.6 | 20.7 |
| 300.00 | 21.24 | 29.55 | 24.10 | 29.0 | 29.9 | 25.6 | 20.8 |
| 500.00 | 34.68 | 45.20 | 70.81 | 24.6 | 32.8 | 34.8 | 33.2 |
| 700.00 | 43.61 | 52.32 | 73.26 | 30.4 | 45.4 | 41.9 | 43.2 |
| 900.00 | 49.44 | 55.96 | 63.14 | 44.4 | 51.8 | 48.6 | 49.7 |
| 1000.00 | 51.67 | 57.38 | 61.05 | 49.0 | 53.8 | 51.3 | 52.1 |
| 1100.00 | 53.63 | 58.65 | 60.25 | 52.3 | 55.5 | 53.5 | 54.2 |
| 1300.00 | 56.99 | 60.89 | 60.55 | 56.9 | 58.3 | 57.2 | 57.5 |
| 1500.00 | 59.89 | 62.79 | 61.81 | 60.0 | 60.6 | 59.9 | 60.1 |

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

| T/K | CH3Cl | C2H5Cl | C3H7Cl | C4H9Cl | C5H11Cl | C6H13Cl | C7H15Cl | C8H17Cl |
|---|---|---|---|---|---|---|---|---|
| 298.15 | 234.37 | 276.62 | 307.48 | 317.94 | 368.0 | 407.7 | 450.7 | 494.2 |
| 300.00 | 234.62 | 277.00 | 308.04 | 318.66 | 368.9 | 408.8 | 451.9 | 495.6 |
| 500.00 | 258.88 | 315.40 | 365.43 | 399.12 | 464.8 | 519.7 | 578.2 | 635.5 |
| 700.00 | 279.34 | 349.07 | 415.62 | 474.84 | 548.9 | 616.9 | 688.3 | 758.4 |
| 900.00 | 297.18 | 378.61 | 458.78 | 535.03 | 618.6 | 698.9 | 781.6 | 863.4 |
| 1000.00 | 305.30 | 392.06 | 478.20 | 560.98 | 649.4 | 735.3 | 823.3 | 910.5 |
| 1100.00 | 312.96 | 404.74 | 496.41 | 584.96 | 678.3 | 769.3 | 862.3 | 954.6 |
| 1300.00 | 327.08 | 428.10 | 529.76 | 628.38 | 730.8 | 831.4 | 933.7 | 1035.2 |
| 1500.00 | 339.82 | 449.21 | 559.71 | 667.08 | 777.9 | 887.0 | 997.6 | 1107.6 |

Table 4a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 |
|---|---|---|---|---|---|---|---|
| 298.15 | 42.25 | 30.86 | 10.47 | 50.1 | 39.7 | 43.0 | 43.6 |
| 300.00 | 42.38 | 31.04 | 10.62 | 50.3 | 39.9 | 43.1 | 43.7 |
| 500.00 | 56.52 | 50.03 | 33.69 | 65.7 | 54.8 | 58.6 | 57.3 |
| 700.00 | 69.73 | 66.55 | 59.22 | 74.1 | 68.1 | 71.4 | 70.1 |
| 900.00 | 81.43 | 80.17 | 76.25 | 83.5 | 80.3 | 82.7 | 81.8 |
| 1000.00 | 86.76 | 86.14 | 82.78 | 88.5 | 85.9 | 88.0 | 87.2 |
| 1100.00 | 91.78 | 91.67 | 88.55 | 93.3 | 91.1 | 93.0 | 92.2 |
| 1300.00 | 101.02 | 101.65 | 98.62 | 102.4 | 100.6 | 102.2 | 101.6 |
| 1500.00 | 109.39 | 110.50 | 107.37 | 110.8 | 109.1 | 110.6 | 110.0 |

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

| T/K | CH3Cl | C2H5Cl | C3H7Cl | C4H9Cl | C5H11Cl | C6H13Cl | C7H15Cl | C8H17Cl |
|---|---|---|---|---|---|---|---|---|
| 298.15 | -83.68 | -112.97 | -145.63 | -188.19 | -205.1 | -229.5 | -251.5 | -273.5 |
| 300.00 | -83.73 | -113.05 | -145.72 | -188.31 | -205.2 | -229.7 | -251.7 | -273.7 |
| 500.00 | -88.73 | -120.57 | -153.85 | -195.16 | -214.2 | -241.0 | -265.1 | -289.9 |
| 700.00 | -92.30 | -125.46 | -158.10 | -193.45 | -216.8 | -244.8 | -270.4 | -296.8 |
| 900.00 | -94.63 | -128.33 | -160.00 | -191.72 | -217.3 | -245.5 | -271.9 | -298.8 |
| 1000.00 | -95.41 | -129.19 | -160.31 | -190.96 | -217.0 | -245.0 | -271.5 | -298.5 |
| 1100.00 | -96.00 | -129.74 | -160.30 | -190.13 | -216.3 | -244.1 | -270.6 | -297.5 |
| 1300.00 | -96.69 | -130.11 | -159.46 | -187.99 | -214.0 | -241.1 | -267.3 | -293.7 |
| 1500.00 | -96.94 | -129.74 | -157.79 | -185.17 | -210.6 | -236.9 | -262.4 | -288.2 |

Table 5a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 |
|---|---|---|---|---|---|---|---|
| 298.15 | -29.29 | -32.66 | -42.56 | -16.9 | -24.5 | -22.0 | -22.0 |
| 300.00 | -29.32 | -32.67 | -42.59 | -16.9 | -24.5 | -22.0 | -22.1 |
| 500.00 | -31.84 | -33.28 | -41.31 | -19.1 | -26.8 | -24.0 | -24.8 |
| 700.00 | -33.16 | -32.64 | -35.35 | -23.3 | -28.1 | -25.6 | -26.3 |
| 900.00 | -33.70 | -31.67 | -31.72 | -25.6 | -28.2 | -26.4 | -26.9 |
| 1000.00 | -33.78 | -31.13 | -30.65 | -26.0 | -28.0 | -26.5 | -26.9 |
| 1100.00 | -33.74 | -30.56 | -29.83 | -26.2 | -27.8 | -26.5 | -26.8 |
| 1300.00 | -33.42 | -29.35 | -28.53 | -26.0 | -27.1 | -26.2 | -26.4 |
| 1500.00 | -32.80 | -28.06 | -27.38 | -25.4 | -26.3 | -25.5 | -25.7 |

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

| T/K | CH3Cl | C2H5Cl | C3H7Cl | C4H9Cl | C5H11Cl | C6H13Cl | C7H15Cl | C8H17Cl |
|---|---|---|---|---|---|---|---|---|
| 298.15 | -60.15 | -61.36 | -62.54 | -67.55 | -58.7 | -54.3 | -48.4 | -42.8 |
| 300.00 | -60.00 | -61.04 | -62.03 | -66.81 | -57.8 | -53.2 | -47.2 | -41.3 |
| 500.00 | -42.72 | -24.13 | -3.72 | 16.82 | 43.6 | 68.1 | 93.5 | 118.7 |
| 700.00 | -23.64 | 15.40 | 57.18 | 101.39 | 147.3 | 192.6 | 238.0 | 283.6 |
| 900.00 | -3.69 | 56.05 | 118.97 | 185.37 | 251.3 | 317.6 | 383.5 | 449.7 |
| 1000.00 | 6.46 | 84.61 | 162.02 | 243.27 | 323.5 | 404.2 | 484.4 | 565.0 |
| 1100.00 | 16.67 | 97.20 | 181.03 | 269.01 | 355.4 | 442.7 | 529.1 | 616.0 |
| 1300.00 | 37.23 | 138.51 | 243.05 | 352.35 | 459.2 | 567.3 | 674.3 | 781.9 |
| 1500.00 | 57.85 | 179.84 | 304.88 | 435.31 | 562.6 | 691.5 | 818.8 | 947.0 |

Table 6a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 |
|---|---|---|---|---|---|---|---|
| 298.15 | -1.21 | -1.19 | -5.01 | 8.8 | 4.4 | 5.9 | 5.7 |
| 300.00 | -1.04 | -.99 | -4.78 | 9.0 | 4.6 | 6.1 | 5.8 |
| 500.00 | 18.59 | 20.41 | 20.54 | 26.8 | 24.5 | 25.4 | 25.3 |
| 700.00 | 39.04 | 41.78 | 44.21 | 45.9 | 45.3 | 45.5 | 45.6 |
| 900.00 | 59.74 | 62.92 | 66.40 | 66.0 | 66.3 | 65.9 | 66.2 |
| 1000.00 | 78.15 | 77.41 | 81.25 | 80.2 | 80.8 | 80.1 | 80.6 |
| 1100.00 | 80.53 | 83.83 | 87.99 | 86.4 | 87.2 | 86.4 | 86.9 |
| 1300.00 | 101.28 | 104.53 | 109.30 | 106.9 | 108.1 | 106.9 | 107.6 |
| 1500.00 | 121.99 | 125.04 | 130.42 | 127.3 | 128.9 | 127.4 | 128.2 |

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

| T/K | CH3Cl | C2H5Cl | C3H7Cl | C4H9Cl | C5H11Cl | C6H13Cl | C7H15Cl | C8H17Cl |
|---|---|---|---|---|---|---|---|---|
| 298.15 | .00 | .00 | .00 | .00 | .0 | .0 | .0 | .0 |
| 300.00 | .08 | .11 | .17 | .21 | .3 | .3 | .4 | .4 |
| 500.00 | 9.69 | 15.39 | 23.02 | 32.51 | 38.6 | 44.5 | 50.7 | 56.1 |
| 700.00 | 21.92 | 35.51 | 53.00 | 77.68 | 88.7 | 102.6 | 116.4 | 129.6 |
| 900.00 | 36.15 | 59.08 | 87.42 | 125.61 | 144.3 | 167.9 | 190.8 | 213.3 |
| 1000.00 | 43.87 | 71.85 | 105.86 | 150.25 | 173.6 | 202.5 | 230.4 | 258.0 |
| 1100.00 | 51.91 | 85.17 | 124.97 | 175.42 | 203.8 | 238.2 | 271.4 | 304.2 |
| 1300.00 | 68.83 | 113.16 | 164.93 | 227.42 | 266.8 | 312.6 | 356.8 | 400.9 |
| 1500.00 | 86.64 | 142.67 | 206.81 | 281.54 | 332.6 | 390.3 | 446.2 | 502.0 |

Table 7a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 |
|---|---|---|---|---|---|---|---|
| 298.15 | .00 | .00 | .00 | .0 | .0 | .0 | .0 |
| 300.00 | .04 | .05 | .04 | .1 | .1 | .0 | .0 |
| 500.00 | 5.70 | 7.63 | 9.50 | 6.1 | 5.9 | 6.2 | 5.5 |
| 700.00 | 13.59 | 17.49 | 24.68 | 11.1 | 13.8 | 13.8 | 13.1 |
| 900.00 | 22.93 | 28.34 | 38.19 | 18.7 | 23.6 | 22.9 | 22.5 |
| 1000.00 | 27.99 | 34.01 | 44.39 | 23.3 | 28.9 | 27.9 | 27.6 |
| 1100.00 | 33.26 | 39.81 | 50.44 | 28.4 | 34.4 | 33.1 | 32.9 |
| 1300.00 | 44.32 | 51.77 | 62.50 | 39.4 | 45.8 | 44.2 | 44.1 |
| 1500.00 | 56.03 | 64.14 | 74.72 | 51.1 | 57.7 | 56.0 | 55.8 |

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

| T/K | CH3Cl | C2H5Cl | C3H7Cl | C4H9Cl | C5H11Cl | C6H13Cl | C7H15Cl | C8H17Cl |
|---|---|---|---|---|---|---|---|---|
| 298.15 | -83.68 | -112.97 | -145.63 | -188.19 | -205.1 | -229.5 | -251.5 | -273.5 |
| 300.00 | -83.60 | -112.85 | -145.46 | -187.98 | -204.8 | -229.2 | -251.1 | -273.1 |
| 500.00 | -73.99 | -97.58 | -122.61 | -155.68 | -166.5 | -185.0 | -200.8 | -217.4 |
| 700.00 | -61.76 | -77.45 | -92.63 | -110.51 | -116.4 | -127.0 | -135.1 | -144.0 |
| 900.00 | -47.53 | -53.89 | -58.21 | -62.58 | -60.8 | -61.6 | -60.7 | -60.2 |
| 1000.00 | -39.81 | -41.11 | -39.77 | -37.94 | -31.5 | -27.0 | -21.1 | -15.5 |
| 1100.00 | -31.77 | -27.80 | -20.65 | -12.77 | -1.3 | 8.7 | 19.9 | 30.7 |
| 1300.00 | -14.85 | .19 | 19.30 | 39.23 | 61.7 | 83.0 | 105.3 | 127.3 |
| 1500.00 | 2.96 | 29.70 | 61.18 | 93.35 | 127.5 | 160.7 | 194.7 | 228.5 |

Table 8a. Increments per carbon atom

| T/K | C2-C1 | C3-C2 | C4-C3 | C5-C4 | C6-C5 | C7-C6 | C8-C7 |
|---|---|---|---|---|---|---|---|
| 298.15 | -29.29 | -32.66 | -42.56 | -16.9 | -24.5 | -22.0 | -22.0 |
| 300.00 | -29.25 | -32.61 | -42.52 | -16.8 | -24.4 | -21.9 | -22.0 |
| 500.00 | -23.59 | -25.03 | -33.06 | -10.8 | -18.5 | -15.8 | -16.6 |
| 700.00 | -15.70 | -15.17 | -17.88 | -5.8 | -10.6 | -8.1 | -8.9 |
| 900.00 | -6.35 | -4.32 | -4.37 | 1.7 | -.8 | .9 | .5 |
| 1000.00 | -1.30 | 1.35 | 1.82 | 6.4 | 4.5 | 5.9 | 5.6 |
| 1100.00 | 3.97 | 7.15 | 7.88 | 11.5 | 9.9 | 11.2 | 10.9 |
| 1300.00 | 15.04 | 19.11 | 19.93 | 22.5 | 21.3 | 22.3 | 22.0 |
| 1500.00 | 26.74 | 31.48 | 32.16 | 34.2 | 33.2 | 34.0 | 33.8 |

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| C3H7Cl | | | | | | | | | |
| 1-chloropropane | .0218 | .0225 | .1386 | .2623 | .3480 | .3784 | .4027 | .4378 | .4609 |
| 2-chloropropane | .9782 | .9775 | .8614 | .7377 | .6520 | .6216 | .5973 | .5622 | .5391 |
| C4H9Cl | | | | | | | | | |
| 1-chlorobutane | .0001 | .0001 | .0199 | .1043 | .1927 | .2271 | .2554 | .2978 | .3270 |
| 2(RS)-chlorobutane | .0046 | .0048 | .1234 | .2934 | .3610 | .3731 | .3789 | .3825 | .3826 |
| 1-chloro-2-methylpropane | .0012 | .0012 | .0488 | .1346 | .1745 | .1821 | .1854 | .1860 | .1833 |
| 2-chloro-2-methylpropane | .9942 | .9938 | .8079 | .4677 | .2718 | .2178 | .1802 | .1336 | .1072 |
| C5H11Cl | | | | | | | | | |
| 1-chloropentane | .0001 | .0001 | .0127 | .0551 | .1008 | .1199 | .1363 | .1620 | .1804 |
| 2(RS)-chloropentane | .0057 | .0060 | .0788 | .1550 | .1888 | .1969 | .2022 | .2080 | .2111 |
| 3-chloropentane | .0057 | .0060 | .0788 | .1550 | .1888 | .1969 | .2022 | .2080 | .2111 |
| 1-chloro-2(RS)-methylbutane | .0004 | .0004 | .0139 | .0400 | .0584 | .0643 | .0686 | .0742 | .0773 |
| 2-chloro-2-methylbutane | .9637 | .9624 | .6920 | .4170 | .2727 | .2306 | .2000 | .1599 | .1356 |
| 2(RS)-chloro-3-methylbutane | .0168 | .0173 | .0865 | .1125 | .1093 | .1056 | .1018 | .0953 | .0904 |
| 1-chloro-3-methylbutane | .0004 | .0004 | .0139 | .0400 | .0584 | .0643 | .0686 | .0742 | .0773 |
| 1-chloro-2,2-dimethylpropane | .0073 | .0075 | .0233 | .0256 | .0230 | .0216 | .0203 | .0183 | .0168 |
| C6H13Cl | | | | | | | | | |
| 1-chlorohexane | .0000 | .0000 | .0047 | .0264 | .0550 | .0681 | .0797 | .0988 | .1130 |
| 2(RS)-chlorohexane | .0012 | .0012 | .0293 | .0744 | .1030 | .1118 | .1183 | .1268 | .1322 |
| 3(RS)-chlorohexane | .0012 | .0012 | .0293 | .0744 | .1030 | .1118 | .1183 | .1268 | .1322 |
| 1-chloro-2(RS)-methylpentane | .0001 | .0001 | .0052 | .0192 | .0319 | .0365 | .0401 | .0452 | .0484 |
| 2-chloro-2-methylpentane | .1985 | .2002 | .2571 | .2002 | .1488 | .1309 | .1170 | .0975 | .0849 |
| 3(RS)-chloro-2-methylpentane | .0035 | .0036 | .0321 | .0540 | .0597 | .0599 | .0595 | .0581 | .0567 |
| 2(RS)-chloro-4-methylpentane | .0035 | .0036 | .0321 | .0540 | .0597 | .0599 | .0595 | .0581 | .0567 |
| 1-chloro-4-methylpentane | .0001 | .0001 | .0052 | .0192 | .0319 | .0365 | .0401 | .0452 | .0484 |
| 1-chloro-3(RS)-methylpentane | .0001 | .0001 | .0052 | .0192 | .0319 | .0365 | .0401 | .0452 | .0484 |
| 2(RS)-chloro-3(RS)-methylpentane | .0035 | .0036 | .0321 | .0540 | .0597 | .0599 | .0595 | .0581 | .0567 |
| 3-chloro-3-methylpentane | .1985 | .2002 | .2571 | .2002 | .1488 | .1309 | .1170 | .0975 | .0849 |
| 1-chloro-2(RS),3-dimethylbutane | .0002 | .0002 | .0057 | .0139 | .0185 | .0196 | .0202 | .0207 | .0208 |
| 2-chloro-2,3-dimethylbutane | .5847 | .5808 | .2821 | .1453 | .0862 | .0702 | .0589 | .0447 | .0364 |
| 1-chloro-2-ethylbutane | .0001 | .0001 | .0052 | .0192 | .0319 | .0365 | .0401 | .0452 | .0484 |
| 1-chloro-2,2-dimethylbutane | .0003 | .0003 | .0052 | .0117 | .0154 | .0164 | .0172 | .0180 | .0185 |
| 2(RS)-chloro-3,3-dimethylbutane | .0045 | .0046 | .0108 | .0109 | .0096 | .0090 | .0085 | .0077 | .0072 |
| 1-chloro-3,3-dimethylbutane | .0001 | .0001 | .0017 | .0039 | .0051 | .0055 | .0057 | .0060 | .0062 |
| C7H15Cl | | | | | | | | | |
| 1-chloroheptane | .0000 | .0000 | .0022 | .0130 | .0284 | .0358 | .0425 | .0539 | .0627 |
| 2(RS)-chloroheptane | .0004 | .0005 | .0135 | .0367 | .0532 | .0588 | .0631 | .0693 | .0734 |
| 3(RS)-chloroheptane | .0004 | .0005 | .0135 | .0367 | .0532 | .0588 | .0631 | .0693 | .0734 |
| 4-chloroheptane | .0004 | .0005 | .0135 | .0367 | .0532 | .0588 | .0631 | .0693 | .0734 |
| 1-chloro-5-methylhexane | .0000 | .0000 | .0024 | .0095 | .0164 | .0192 | .0214 | .0247 | .0269 |
| 2(RS)-chloro-5-methylhexane | .0013 | .0014 | .0148 | .0266 | .0308 | .0315 | .0318 | .0317 | .0314 |
| 3(RS)-chloro-5-methylhexane | .0013 | .0014 | .0148 | .0266 | .0308 | .0315 | .0318 | .0317 | .0314 |
| 3(RS)-chloro-2-methylhexane | .0013 | .0014 | .0148 | .0266 | .0308 | .0315 | .0318 | .0317 | .0314 |

Table 9. Equilibrium mole fractions within isomer groups of monochloroalkanes -- continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 2-chloro-2-methylhexane | .0757 | .0766 | .1181 | .0986 | .0768 | .0688 | .0624 | .0532 | .0472 |
| 1-chloro-2(RS)-methylhexane | .0000 | .0000 | .0024 | .0095 | .0164 | .0192 | .0214 | .0247 | .0269 |
| 1-chloro-4(RS)-methylhexane | .0000 | .0000 | .0024 | .0095 | .0164 | .0192 | .0214 | .0247 | .0269 |
| 2(RS)-chloro-4(RS)-methylhexane | .0013 | .0014 | .0148 | .0266 | .0308 | .0315 | .0318 | .0317 | .0314 |
| 3(RS)-chloro-4(RS)-methylhexane | .0013 | .0014 | .0148 | .0266 | .0308 | .0315 | .0318 | .0317 | .0314 |
| 3-chloro-3(RS)-methylhexane | .0757 | .0766 | .1181 | .0986 | .0768 | .0688 | .0624 | .0532 | .0472 |
| 2(RS)-chloro-3(RS)-methylhexane | .0013 | .0014 | .0148 | .0266 | .0308 | .0315 | .0318 | .0317 | .0314 |
| 1-chloro-3(RS)-methylhexane | .0000 | .0000 | .0024 | .0095 | .0164 | .0192 | .0214 | .0247 | .0269 |
| 1-chloro-4,4-dimethylpentane | .0000 | .0000 | .0008 | .0019 | .0026 | .0029 | .0031 | .0033 | .0034 |
| 2(RS)-chloro-4,4-dimethylpentane | .0017 | .0018 | .0049 | .0054 | .0050 | .0047 | .0045 | .0042 | .0040 |
| 3(RS)-chloro-2,2-dimethylpentane | .0017 | .0018 | .0049 | .0054 | .0050 | .0047 | .0045 | .0042 | .0040 |
| 1-chloro-2,2-dimethylpentane | .0001 | .0001 | .0024 | .0058 | .0079 | .0086 | .0092 | .0099 | .0103 |
| 1-chloro-3,3-dimethylpentane | .0001 | .0001 | .0024 | .0058 | .0079 | .0086 | .0092 | .0099 | .0103 |
| 2(RS)-chloro-3,3-dimethylpentane | .0052 | .0053 | .0148 | .0162 | .0149 | .0142 | .0136 | .0127 | .0120 |
| 1-chloro-3(RS),4-dimethylpentane | .0001 | .0001 | .0026 | .0069 | .0095 | .0103 | .0108 | .0113 | .0115 |
| 2(RS)-chloro-3(RS),4-dimethylpentane | .0039 | .0040 | .0162 | .0193 | .0178 | .0169 | .0160 | .0145 | .0135 |
| 1-chloro-2(RS),3(RS)-dimethylpentane | .0001 | .0001 | .0026 | .0069 | .0095 | .0103 | .0108 | .0113 | .0115 |
| 2-chloro-2,3(RS)-dimethylpentane | .2230 | .2223 | .1296 | .0716 | .0445 | .0369 | .0314 | .0244 | .0202 |
| 3-chloro-2,3(RS)-dimethylpentane | .2230 | .2223 | .1296 | .0716 | .0445 | .0369 | .0314 | .0244 | .0202 |
| 1-chloro-2(RS),4-dimethylpentane | .0001 | .0001 | .0026 | .0069 | .0095 | .0103 | .0108 | .0113 | .0115 |
| 2-chloro-2,4-dimethylpentane | .2230 | .2223 | .1296 | .0716 | .0445 | .0369 | .0314 | .0244 | .0202 |
| 3-chloro-2,4-dimethylpentane | .0039 | .0040 | .0162 | .0193 | .0178 | .0169 | .0160 | .0145 | .0135 |
| 1-chloro-2(RS)-ethylpentane | .0000 | .0000 | .0024 | .0095 | .0164 | .0192 | .0214 | .0247 | .0269 |
| 1-chloro-3-ethylpentane | .0000 | .0000 | .0024 | .0095 | .0164 | .0192 | .0214 | .0247 | .0269 |
| 2(RS)-chloro-3-ethylpentane | .0013 | .0014 | .0148 | .0266 | .0308 | .0315 | .0318 | .0317 | .0314 |
| 3-chloro-3-ethylpentane | .0757 | .0766 | .1181 | .0986 | .0768 | .0688 | .0624 | .0532 | .0472 |
| 1-chloro-2-ethyl-2-methylbutane | .0001 | .0001 | .0024 | .0058 | .0079 | .0086 | .0092 | .0099 | .0103 |
| 1-chloro-2(RS)-ethyl-3-methylbutane | .0001 | .0001 | .0026 | .0069 | .0095 | .0103 | .0108 | .0113 | .0115 |
| 1-chloro-2(RS),3,3-trimethylbutane | .0000 | .0000 | .0004 | .0008 | .0010 | .0010 | .0011 | .0011 | .0011 |
| 2-chloro-2,3,3-trimethylbutane | .0757 | .0745 | .0194 | .0082 | .0046 | .0037 | .0031 | .0024 | .0020 |
| 1-chloro-2,2,3-trimethylbutane | .0001 | .0001 | .0012 | .0023 | .0029 | .0031 | .0032 | .0033 | .0034 |
| C8H17Cl | | | | | | | | | |
| 1-chlorooctane | .0000 | .0000 | .0010 | .0066 | .0154 | .0199 | .0241 | .0314 | .0372 |
| 2(RS)-chlorooctane | .0002 | .0002 | .0060 | .0185 | .0288 | .0326 | .0357 | .0403 | .0435 |
| 3(RS)-chlorooctane | .0002 | .0002 | .0060 | .0185 | .0288 | .0326 | .0357 | .0403 | .0435 |
| 4(RS)-chlorooctane | .0002 | .0002 | .0060 | .0185 | .0288 | .0326 | .0357 | .0403 | .0435 |
| 1-chloro-2(RS)-methylheptane | .0000 | .0000 | .0011 | .0048 | .0089 | .0106 | .0121 | .0144 | .0159 |
| 2-chloro-2-methylheptane | .0262 | .0266 | .0527 | .0498 | .0417 | .0382 | .0353 | .0310 | .0279 |
| 3(RS)-chloro-2-methylheptane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 4(RS)-chloro-2-methylheptane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 3(RS)-chloro-6-methylheptane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 2(RS)-chloro-6-methylheptane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 1-chloro-6-methylheptane | .0000 | .0000 | .0011 | .0048 | .0089 | .0106 | .0121 | .0144 | .0159 |
| 1-chloro-3(RS)-methylheptane | .0000 | .0000 | .0011 | .0048 | .0089 | .0106 | .0121 | .0144 | .0159 |
| 2(RS)-chloro-3(RS)-methylheptane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 3-chloro-3(RS)-methylheptane | .0262 | .0266 | .0527 | .0498 | .0417 | .0382 | .0353 | .0310 | .0279 |
| 4(RS)-chloro-3(RS)-methylheptane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 3(RS)-chloro-5(RS)-methylheptane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 2(RS)-chloro-5(RS)-methylheptane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 1-chloro-5(RS)-methylheptane | .0000 | .0000 | .0011 | .0048 | .0089 | .0106 | .0121 | .0144 | .0159 |
| 1-chloro-4(RS)-methylheptane | .0000 | .0000 | .0011 | .0048 | .0089 | .0106 | .0121 | .0144 | .0159 |
| 2(RS)-chloro-4(RS)-methylheptane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 3(RS)-chloro-4(RS)-methylheptane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 4-chloro-4-methylheptane | .0262 | .0266 | .0527 | .0498 | .0417 | .0382 | .0353 | .0310 | .0279 |
| 1-chloro-2,2-dimethylhexane | .0000 | .0000 | .0011 | .0029 | .0043 | .0048 | .0052 | .0057 | .0061 |

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 3(RS)-chloro-2,2-dimethylhexane | .0006 | .0006 | .0022 | .0027 | .0027 | .0026 | .0026 | .0025 | .0024 |
| 3(RS)-chloro-5,5-dimethylhexane | .0006 | .0006 | .0022 | .0027 | .0027 | .0026 | .0026 | .0025 | .0024 |
| 2(RS)-chloro-5,5-dimethylhexane | .0006 | .0006 | .0022 | .0027 | .0027 | .0026 | .0026 | .0025 | .0024 |
| 1-chloro-5,5-dimethylhexane | .0000 | .0000 | .0004 | .0010 | .0014 | .0016 | .0017 | .0019 | .0020 |
| 1-chloro-3,3-dimethylhexane | .0000 | .0000 | .0011 | .0029 | .0043 | .0048 | .0052 | .0057 | .0061 |
| 2(RS)-chloro-3,3-dimethylhexane | .0018 | .0018 | .0066 | .0082 | .0081 | .0079 | .0077 | .0074 | .0071 |
| 3(RS)-chloro-4,4-dimethylhexane | .0018 | .0018 | .0066 | .0082 | .0081 | .0079 | .0077 | .0074 | .0071 |
| 2(RS)-chloro-4,4-dimethylhexane | .0018 | .0018 | .0066 | .0082 | .0081 | .0079 | .0077 | .0074 | .0071 |
| 1-chloro-4,4-dimethylhexane | .0000 | .0000 | .0011 | .0029 | .0043 | .0048 | .0052 | .0057 | .0061 |
| 1-chloro-4(RS),5-dimethylhexane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |
| 2(RS)-chloro-4(RS),5-dimethylhexane | .0013 | .0014 | .0072 | .0098 | .0097 | .0094 | .0090 | .0085 | .0080 |
| 3(RS)-chloro-4(RS),5-dimethylhexane | .0013 | .0014 | .0072 | .0098 | .0097 | .0094 | .0090 | .0085 | .0080 |
| 3(RS)-chloro-2,3-dimethylhexane | .0773 | .0773 | .0578 | .0362 | .0241 | .0205 | .0178 | .0142 | .0120 |
| 2-chloro-2,3(RS)-dimethylhexane | .0773 | .0773 | .0578 | .0362 | .0241 | .0205 | .0178 | .0142 | .0120 |
| 1-chloro-2(RS),3(RS)-dimethylhexane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |
| 1-chloro-3(RS),5-dimethylhexane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |
| 2(RS)-chloro-3(RS),5-dimethylhexane | .0013 | .0014 | .0072 | .0098 | .0097 | .0094 | .0090 | .0085 | .0080 |
| 3-chloro-3(RS),5-dimethylhexane | .0773 | .0773 | .0578 | .0362 | .0241 | .0205 | .0178 | .0142 | .0120 |
| 3(RS)-chloro-2,4(RS)-dimethylhexane | .0013 | .0014 | .0072 | .0098 | .0097 | .0094 | .0090 | .0085 | .0080 |
| 2-chloro-2,4(RS)-dimethylhexane | .0773 | .0773 | .0578 | .0362 | .0241 | .0205 | .0178 | .0142 | .0120 |
| 1-chloro-2(RS),4(RS)-dimethylhexane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |
| 1-chloro-2(RS),5-dimethylhexane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |
| 2-chloro-2,5-dimethylhexane | .0773 | .0773 | .0578 | .0362 | .0241 | .0205 | .0178 | .0142 | .0120 |
| 3(RS)-chloro-2,5-dimethylhexane | .0013 | .0014 | .0072 | .0098 | .0097 | .0094 | .0090 | .0085 | .0080 |
| 1-chloro-3(RS),4(RS)-dimethylhexane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |
| 2(RS)-chloro-3(RS),4(RS)-dimethylhexane | .0013 | .0014 | .0072 | .0098 | .0097 | .0094 | .0090 | .0085 | .0080 |
| 3-chloro-3(RS),4(RS)-dimethylhexane | .0773 | .0773 | .0578 | .0362 | .0241 | .0205 | .0178 | .0142 | .0120 |
| 1-chloro-2(RS)-ethylhexane | .0000 | .0000 | .0011 | .0048 | .0089 | .0106 | .0121 | .0144 | .0159 |
| 1-chloro-3(RS)-ethylhexane | .0000 | .0000 | .0011 | .0048 | .0089 | .0106 | .0121 | .0144 | .0159 |
| 2(RS)-chloro-3(RS)-ethylhexane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 3-chloro-3-ethylhexane | .0262 | .0266 | .0527 | .0498 | .0417 | .0382 | .0353 | .0310 | .0279 |
| 3(RS)-chloro-4-ethylhexane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 2(RS)-chloro-4-ethylhexane | .0005 | .0005 | .0066 | .0134 | .0167 | .0175 | .0180 | .0185 | .0186 |
| 1-chloro-4-ethylhexane | .0000 | .0000 | .0011 | .0048 | .0089 | .0106 | .0121 | .0144 | .0159 |
| 1-chloro-2(RS)-ethyl-2-methylpentane | .0000 | .0000 | .0011 | .0029 | .0043 | .0048 | .0052 | .0057 | .0061 |
| 1-chloro-2(RS)-isopropylpentane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |
| 1-chloro-2(RS)-ethyl-4-methylpentane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |
| 1-chloro-3(RS),4,4-trimethylpentane | .0000 | .0000 | .0002 | .0004 | .0005 | .0006 | .0006 | .0006 | .0007 |
| 2(RS)-chloro-3(RS),4,4-trimethylpentane | .0005 | .0005 | .0011 | .0011 | .0010 | .0009 | .0009 | .0008 | .0008 |
| 3-chloro-2,2,3(RS)-trimethylpentane | .0262 | .0259 | .0087 | .0041 | .0025 | .0021 | .0018 | .0014 | .0012 |
| 1-chloro-2,2,3(RS)-trimethylpentane | .0000 | .0000 | .0005 | .0012 | .0016 | .0017 | .0018 | .0019 | .0020 |
| 1-chloro-2(RS),4,4-trimethylpentane | .0000 | .0000 | .0002 | .0004 | .0005 | .0006 | .0006 | .0006 | .0007 |
| 2-chloro-2,4,4-trimethylpentane | .0262 | .0259 | .0087 | .0041 | .0025 | .0021 | .0018 | .0014 | .0012 |
| 3(RS)-chloro-2,2,4-trimethylpentane | .0005 | .0005 | .0011 | .0011 | .0010 | .0009 | .0009 | .0008 | .0008 |
| 1-chloro-2,2,3-trimethylpentane | .0000 | .0000 | .0005 | .0012 | .0016 | .0017 | .0018 | .0019 | .0020 |
| 1-chloro-3,3,4-trimethylpentane | .0000 | .0000 | .0005 | .0012 | .0016 | .0017 | .0018 | .0019 | .0020 |
| 2(RS)-chloro-3,3,4-trimethylpentane | .0014 | .0014 | .0032 | .0033 | .0030 | .0028 | .0027 | .0025 | .0023 |
| 2-chloro-2,3,3-trimethylpentane | .0787 | .0777 | .0260 | .0124 | .0074 | .0062 | .0053 | .0041 | .0035 |
| 1-chloro-2(RS),3,3-trimethylpentane | .0000 | .0000 | .0005 | .0012 | .0016 | .0017 | .0018 | .0019 | .0020 |
| 1-chloro-3-ethyl-3-methylpentane | .0000 | .0000 | .0011 | .0029 | .0043 | .0048 | .0052 | .0057 | .0061 |
| 2(RS)-chloro-3-ethyl-3-methylpentane | .0018 | .0018 | .0066 | .0082 | .0081 | .0079 | .0077 | .0074 | .0071 |
| 1-chloro-2(RS)-ethyl-3(RS)-methylpentane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |
| 1-chloro-2(RS),3(RS),4-trimethylpentane | .0000 | .0000 | .0006 | .0014 | .0019 | .0020 | .0021 | .0022 | .0022 |
| 2-chloro-2,3(RS),4-trimethylpentane | .0590 | .0586 | .0284 | .0148 | .0089 | .0073 | .0062 | .0048 | .0039 |
| 3-chloro-2,3,4-trimethylpentane | .0590 | .0586 | .0284 | .0148 | .0089 | .0073 | .0062 | .0048 | .0039 |
| 1-chloro-2-propylpentane | .0000 | .0000 | .0011 | .0048 | .0089 | .0106 | .0121 | .0144 | .0159 |
| 1-chloro-3(RS)-ethyl-4-methylpentane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |

Table 9. Equilibrium mole fractions within isomer groups of monochloroalkanes -- continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 2(RS)-chloro-3(RS)-ethyl-4-methylpentane | .0013 | .0014 | .0072 | .0098 | .0097 | .0094 | .0090 | .0085 | .0080 |
| 3-chloro-3-ethyl-2-methylpentane | .0773 | .0773 | .0578 | .0362 | .0241 | .0205 | .0178 | .0142 | .0120 |
| 2-chloro-3-ethyl-2-methylpentane | .0773 | .0773 | .0578 | .0362 | .0241 | .0205 | .0178 | .0142 | .0120 |
| 1-chloro-3-ethyl-2(RS)-methylpentane | .0000 | .0000 | .0012 | .0035 | .0052 | .0057 | .0061 | .0066 | .0068 |
| 1-chloro-2(RS)-ethyl-3,3-dimethylbutane | .0000 | .0000 | .0002 | .0004 | .0005 | .0006 | .0006 | .0006 | .0007 |
| 1-chloro-2(RS)-ethyl-2,3-dimethylbutane | .0000 | .0000 | .0005 | .0012 | .0016 | .0017 | .0018 | .0019 | .0020 |
| 1-chloro-2,2-diethylbutane | .0000 | .0000 | .0011 | .0029 | .0043 | .0048 | .0052 | .0057 | .0061 |
| 1-chloro-2,2,3,3-tetramethylbutane | .0000 | .0000 | .0001 | .0001 | .0002 | .0002 | .0002 | .0002 | .0002 |
| 1-chloro-2-isopropyl-3-methylbutane | .0000 | .0000 | .0006 | .0014 | .0019 | .0020 | .0021 | .0022 | .0022 |

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| CH3Cl | | | | | | | | | |
| chloromethane | 40.73 | 40.86 | 55.15 | 66.61 | 75.29 | 78.85 | 81.95 | 87.04 | 90.94 |
| C2H5Cl | | | | | | | | | |
| chloroethane | 61.84 | 62.10 | 89.83 | 110.22 | 124.73 | 130.52 | 135.58 | 144.03 | 150.83 |
| C3H7Cl | | | | | | | | | |
| 1-chloropropane | 84.76 | 85.11 | 124.33 | 153.35 | 173.91 | 182.06 | 189.17 | 200.99 | 210.48 |
| 2-chloropropane | 86.94 | 87.25 | 127.38 | 157.91 | 179.05 | 187.27 | 194.36 | 205.97 | 215.09 |
| C4H9Cl | | | | | | | | | |
| 1-chlorobutane | 107.68 | 108.12 | 158.82 | 196.49 | 223.08 | 233.60 | 242.75 | 257.96 | 270.12 |
| 2(RS)-chlorobutane | 109.86 | 110.27 | 161.87 | 201.04 | 228.22 | 238.81 | 247.95 | 262.93 | 274.73 |
| 1-chloro-2-methylpropane | 106.51 | 106.99 | 159.15 | 197.06 | 223.77 | 234.34 | 243.55 | 258.86 | 271.13 |
| 2-chloro-2-methylpropane | 111.03 | 111.55 | 166.90 | 205.50 | 231.79 | 241.98 | 250.76 | 265.11 | 276.40 |
| C5H11Cl | | | | | | | | | |
| 1-chloropentane | 130.6 | 131.1 | 193.3 | 239.6 | 272.2 | 285.1 | 296.3 | 314.9 | 329.8 |
| 2(RS)-chloropentane | 132.8 | 133.3 | 196.4 | 244.2 | 277.4 | 290.4 | 301.5 | 319.9 | 334.4 |
| 3-chloropentane | 132.8 | 133.3 | 196.4 | 244.2 | 277.4 | 290.4 | 301.5 | 319.9 | 334.4 |
| 1-chloro-2(RS)-methylbutane | 129.4 | 130.0 | 193.7 | 240.2 | 272.9 | 285.9 | 297.1 | 315.8 | 330.8 |
| 2-chloro-2-methylbutane | 133.9 | 134.6 | 201.4 | 248.6 | 281.0 | 293.5 | 304.3 | 322.1 | 336.0 |
| 2(RS)-chloro-3-methylbutane | 131.6 | 132.1 | 196.7 | 244.8 | 278.1 | 291.1 | 302.3 | 320.8 | 335.4 |
| 1-chloro-3-methylbutane | 129.4 | 130.0 | 193.7 | 240.2 | 272.9 | 285.9 | 297.1 | 315.8 | 330.8 |
| 1-chloro-2,2-dimethylpropane | 131.6 | 132.2 | 199.3 | 246.4 | 278.3 | 290.7 | 301.2 | 318.5 | 331.9 |
| C6H13Cl | | | | | | | | | |
| 1-chlorohexane | 153.5 | 154.2 | 227.8 | 282.8 | 321.4 | 336.7 | 349.9 | 371.9 | 389.4 |
| 2(RS)-chlorohexane | 155.7 | 156.3 | 230.9 | 287.3 | 326.6 | 341.9 | 355.1 | 376.9 | 394.0 |
| 3(RS)-chlorohexane | 155.7 | 156.3 | 230.9 | 287.3 | 326.6 | 341.9 | 355.1 | 376.9 | 394.0 |
| 1-chloro-2(RS)-methylpentane | 152.4 | 153.0 | 228.1 | 283.3 | 322.1 | 337.4 | 350.7 | 372.8 | 390.4 |
| 2-chloro-2-methylpentane | 156.9 | 157.6 | 235.9 | 291.8 | 330.1 | 345.1 | 357.9 | 379.0 | 395.7 |
| 3(RS)-chloro-2-methylpentane | 154.5 | 155.2 | 231.2 | 287.9 | 327.3 | 342.6 | 355.9 | 377.8 | 395.0 |
| 2(RS)-chloro-4-methylpentane | 154.5 | 155.2 | 231.2 | 287.9 | 327.3 | 342.6 | 355.9 | 377.8 | 395.0 |
| 1-chloro-4-methylpentane | 152.4 | 153.0 | 228.1 | 283.3 | 322.1 | 337.4 | 350.7 | 372.8 | 390.4 |
| 1-chloro-3(RS)-methylpentane | 152.4 | 153.0 | 228.1 | 283.3 | 322.1 | 337.4 | 350.7 | 372.8 | 390.4 |
| 2(RS)-chloro-3(RS)-methylpentane | 154.5 | 155.2 | 231.2 | 287.9 | 327.3 | 342.6 | 355.9 | 377.8 | 395.0 |
| 3-chloro-3-methylpentane | 156.9 | 157.6 | 235.9 | 291.8 | 330.1 | 345.1 | 357.9 | 379.0 | 395.7 |
| 1-chloro-2(RS),3-dimethylbutane | 151.2 | 151.9 | 228.5 | 283.9 | 322.8 | 338.2 | 351.5 | 373.7 | 391.4 |
| 2-chloro-2,3-dimethylbutane | 155.7 | 156.4 | 236.2 | 292.3 | 330.8 | 345.8 | 358.7 | 379.9 | 396.7 |
| 1-chloro-2-ethylbutane | 152.4 | 153.0 | 228.1 | 283.3 | 322.1 | 337.4 | 350.7 | 372.8 | 390.4 |
| 1-chloro-2,2-dimethylbutane | 154.5 | 155.2 | 233.8 | 289.5 | 327.5 | 342.2 | 354.8 | 375.4 | 391.6 |
| 2(RS)-chloro-3,3-dimethylbutane | 156.7 | 157.3 | 236.8 | 294.1 | 332.7 | 347.4 | 360.0 | 380.4 | 396.2 |
| 1-chloro-3,3-dimethylbutane | 154.5 | 155.2 | 233.8 | 289.5 | 327.5 | 342.2 | 354.8 | 375.4 | 391.6 |
| C7H15Cl | | | | | | | | | |
| 1-chloroheptane | 176.4 | 177.2 | 262.3 | 325.9 | 370.6 | 388.2 | 403.5 | 428.9 | 449.1 |
| 2(RS)-chloroheptane | 178.6 | 179.3 | 265.4 | 330.5 | 375.7 | 393.4 | 408.7 | 433.8 | 453.7 |
| 3(RS)-chloroheptane | 178.6 | 179.3 | 265.4 | 330.5 | 375.7 | 393.4 | 408.7 | 433.8 | 453.7 |
| 4-chloroheptane | 178.6 | 179.3 | 265.4 | 330.5 | 375.7 | 393.4 | 408.7 | 433.8 | 453.7 |
| 1-chloro-5-methylhexane | 175.3 | 176.0 | 262.6 | 326.5 | 371.3 | 389.0 | 404.3 | 429.8 | 450.1 |
| 2(RS)-chloro-5-methylhexane | 177.5 | 178.2 | 265.7 | 331.0 | 376.4 | 394.2 | 409.5 | 434.7 | 454.7 |

Table 10. Standard heat capacity at constant pressure for monochloroalkanes in J/K mol -- continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 3(RS)-chloro-5-methylhexane | 177.5 | 178.2 | 265.7 | 331.0 | 376.4 | 394.2 | 409.5 | 434.7 | 454.7 |
| 3(RS)-chloro-2-methylhexane | 177.5 | 178.2 | 265.7 | 331.0 | 376.4 | 394.2 | 409.5 | 434.7 | 454.7 |
| 2-chloro-2-methylhexane | 179.8 | 180.6 | 270.4 | 334.9 | 379.3 | 396.6 | 411.5 | 436.0 | 455.3 |
| 1-chloro-2(RS)-methylhexane | 175.3 | 176.0 | 262.6 | 326.5 | 371.3 | 389.0 | 404.3 | 429.8 | 450.1 |
| 1-chloro-4(RS)-methylhexane | 175.3 | 176.0 | 262.6 | 326.5 | 371.3 | 389.0 | 404.3 | 429.8 | 450.1 |
| 2(RS)-chloro-4(RS)-methylhexane | 177.5 | 178.2 | 265.7 | 331.0 | 376.4 | 394.2 | 409.5 | 434.7 | 454.7 |
| 3(RS)-chloro-4(RS)-methylhexane | 177.5 | 178.2 | 265.7 | 331.0 | 376.4 | 394.2 | 409.5 | 434.7 | 454.7 |
| 3-chloro-3(RS)-methylhexane | 179.8 | 180.6 | 270.4 | 334.9 | 379.3 | 396.6 | 411.5 | 436.0 | 455.3 |
| 2(RS)-chloro-3(RS)-methylhexane | 177.5 | 178.2 | 265.7 | 331.0 | 376.4 | 394.2 | 409.5 | 434.7 | 454.7 |
| 1-chloro-3(RS)-methylhexane | 175.3 | 176.0 | 262.6 | 326.5 | 371.3 | 389.0 | 404.3 | 429.8 | 450.1 |
| 1-chloro-4,4-dimethylpentane | 177.4 | 178.2 | 268.3 | 332.7 | 376.7 | 393.7 | 408.4 | 432.4 | 451.2 |
| 2(RS)-chloro-4,4-dimethylpentane | 179.6 | 180.4 | 271.3 | 337.2 | 381.8 | 399.0 | 413.6 | 437.4 | 455.8 |
| 3(RS)-chloro-2,2-dimethylpentane | 179.6 | 180.4 | 271.3 | 337.2 | 381.8 | 399.0 | 413.6 | 437.4 | 455.8 |
| 1-chloro-2,2-dimethylpentane | 177.4 | 178.2 | 268.3 | 332.7 | 376.7 | 393.7 | 408.4 | 432.4 | 451.2 |
| 1-chloro-3,3-dimethylpentane | 177.4 | 178.2 | 268.3 | 332.7 | 376.7 | 393.7 | 408.4 | 432.4 | 451.2 |
| 2(RS)-chloro-3,3-dimethylpentane | 179.6 | 180.4 | 271.3 | 337.2 | 381.8 | 399.0 | 413.6 | 437.4 | 455.8 |
| 1-chloro-3(RS),4-dimethylpentane | 174.1 | 174.9 | 263.0 | 327.0 | 372.0 | 389.7 | 405.1 | 430.7 | 451.1 |
| 2(RS)-chloro-3(RS),4-dimethylpentane | 176.3 | 177.0 | 266.0 | 331.6 | 377.1 | 394.9 | 410.3 | 435.6 | 455.7 |
| 1-chloro-2(RS),3(RS)-dimethylpentane | 174.1 | 174.9 | 263.0 | 327.0 | 372.0 | 389.7 | 405.1 | 430.7 | 451.1 |
| 2-chloro-2,3(RS)-dimethylpentane | 178.6 | 179.5 | 270.7 | 335.5 | 380.0 | 397.3 | 412.3 | 436.9 | 456.3 |
| 3-chloro-2,3(RS)-dimethylpentane | 178.6 | 179.5 | 270.7 | 335.5 | 380.0 | 397.3 | 412.3 | 436.9 | 456.3 |
| 1-chloro-2(RS),4-dimethylpentane | 174.1 | 174.9 | 263.0 | 327.0 | 372.0 | 389.7 | 405.1 | 430.7 | 451.1 |
| 2-chloro-2,4-dimethylpentane | 178.6 | 179.5 | 270.7 | 335.5 | 380.0 | 397.3 | 412.3 | 436.9 | 456.3 |
| 3-chloro-2,4-dimethylpentane | 176.3 | 177.0 | 266.0 | 331.6 | 377.1 | 394.9 | 410.3 | 435.6 | 455.7 |
| 1-chloro-2(RS)-ethylpentane | 175.3 | 176.0 | 262.6 | 326.5 | 371.3 | 389.0 | 404.3 | 429.8 | 450.1 |
| 1-chloro-3-ethylpentane | 175.3 | 176.0 | 262.6 | 326.5 | 371.3 | 389.0 | 404.3 | 429.8 | 450.1 |
| 2(RS)-chloro-3-ethylpentane | 177.5 | 178.2 | 265.7 | 331.0 | 376.4 | 394.2 | 409.5 | 434.7 | 454.7 |
| 3-chloro-3-ethylpentane | 179.8 | 180.6 | 270.4 | 334.9 | 379.3 | 396.6 | 411.5 | 436.0 | 455.3 |
| 1-chloro-2-ethyl-2-methylbutane | 177.4 | 178.2 | 268.3 | 332.7 | 376.7 | 393.7 | 408.4 | 432.4 | 451.2 |
| 1-chloro-2(RS)-ethyl-3-methylbutane | 174.1 | 174.9 | 263.0 | 327.0 | 372.0 | 389.7 | 405.1 | 430.7 | 451.1 |
| 1-chloro-2(RS),3,3-trimethylbutane | 176.2 | 177.1 | 268.6 | 333.2 | 377.4 | 394.5 | 409.2 | 433.3 | 452.2 |
| 2-chloro-2,3,3-trimethylbutane | 180.8 | 181.6 | 276.3 | 341.7 | 385.4 | 402.1 | 416.4 | 439.5 | 457.5 |
| 1-chloro-2,2,3-trimethylbutane | 176.2 | 177.1 | 268.6 | 333.2 | 377.4 | 394.5 | 409.2 | 433.3 | 452.2 |
| C8H17Cl | | | | | | | | | |
| 1-chlorooctane | 199.4 | 200.2 | 296.8 | 369.0 | 419.8 | 439.7 | 457.1 | 485.8 | 508.7 |
| 2(RS)-chlorooctane | 201.5 | 202.3 | 299.9 | 373.6 | 424.9 | 445.0 | 462.3 | 490.8 | 513.3 |
| 3(RS)-chlorooctane | 201.5 | 202.3 | 299.9 | 373.6 | 424.9 | 445.0 | 462.3 | 490.8 | 513.3 |
| 4(RS)-chlorooctane | 201.5 | 202.3 | 299.9 | 373.6 | 424.9 | 445.0 | 462.3 | 490.8 | 513.3 |
| 1-chloro-2(RS)-methylheptane | 198.2 | 199.0 | 297.1 | 369.6 | 420.5 | 440.5 | 457.9 | 486.7 | 509.7 |
| 2-chloro-2-methylheptane | 202.7 | 203.6 | 304.9 | 378.0 | 428.5 | 448.1 | 465.1 | 493.0 | 515.0 |
| 3(RS)-chloro-2-methylheptane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 4(RS)-chloro-2-methylheptane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 3(RS)-chloro-6-methylheptane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 2(RS)-chloro-6-methylheptane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 1-chloro-6-methylheptane | 198.2 | 199.0 | 297.1 | 369.6 | 420.5 | 440.5 | 457.9 | 486.7 | 509.7 |
| 1-chloro-3(RS)-methylheptane | 198.2 | 199.0 | 297.1 | 369.6 | 420.5 | 440.5 | 457.9 | 486.7 | 509.7 |
| 2(RS)-chloro-3(RS)-methylheptane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 3-chloro-3(RS)-methylheptane | 202.7 | 203.6 | 304.9 | 378.0 | 428.5 | 448.1 | 465.1 | 493.0 | 515.0 |
| 4(RS)-chloro-3(RS)-methylheptane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 3(RS)-chloro-5(RS)-methylheptane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 2(RS)-chloro-5(RS)-methylheptane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 1-chloro-5(RS)-methylheptane | 198.2 | 199.0 | 297.1 | 369.6 | 420.5 | 440.5 | 457.9 | 486.7 | 509.7 |
| 1-chloro-4(RS)-methylheptane | 198.2 | 199.0 | 297.1 | 369.6 | 420.5 | 440.5 | 457.9 | 486.7 | 509.7 |
| 2(RS)-chloro-4(RS)-methylheptane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 3(RS)-chloro-4(RS)-methylheptane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 4-chloro-4-methylheptane | 202.7 | 203.6 | 304.9 | 378.0 | 428.5 | 448.1 | 465.1 | 493.0 | 515.0 |

Table 10. Standard heat capacity at constant pressure for monochloroalkanes in J/K mol — Continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 1-chloro-2,2-dimethylhexane | 200.3 | 201.2 | 302.7 | 375.8 | 425.9 | 445.3 | 462.0 | 489.4 | 510.9 |
| 3(RS)-chloro-2,2-dimethylhexane | 202.5 | 203.4 | 305.8 | 380.4 | 431.0 | 450.5 | 467.2 | 494.3 | 515.5 |
| 3(RS)-chloro-5,5-dimethylhexane | 202.5 | 203.4 | 305.8 | 380.4 | 431.0 | 450.5 | 467.2 | 494.3 | 515.5 |
| 2(RS)-chloro-5,5-dimethylhexane | 202.5 | 203.4 | 305.8 | 380.4 | 431.0 | 450.5 | 467.2 | 494.3 | 515.5 |
| 1-chloro-5,5-dimethylhexane | 200.3 | 201.2 | 302.7 | 375.8 | 425.9 | 445.3 | 462.0 | 489.4 | 510.9 |
| 1-chloro-3,3-dimethylhexane | 200.3 | 201.2 | 302.7 | 375.8 | 425.9 | 445.3 | 462.0 | 489.4 | 510.9 |
| 2(RS)-chloro-3,3-dimethylhexane | 202.5 | 203.4 | 305.8 | 380.4 | 431.0 | 450.5 | 467.2 | 494.3 | 515.5 |
| 3(RS)-chloro-4,4-dimethylhexane | 202.5 | 203.4 | 305.8 | 380.4 | 431.0 | 450.5 | 467.2 | 494.3 | 515.5 |
| 2(RS)-chloro-4,4-dimethylhexane | 202.5 | 203.4 | 305.8 | 380.4 | 431.0 | 450.5 | 467.2 | 494.3 | 515.5 |
| 1-chloro-4,4-dimethylhexane | 200.3 | 201.2 | 302.7 | 375.8 | 425.9 | 445.3 | 462.0 | 489.4 | 510.9 |
| 1-chloro-4(RS),5-dimethylhexane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 2(RS)-chloro-4(RS),5-dimethylhexane | 199.2 | 200.1 | 300.5 | 374.7 | 426.3 | 446.5 | 463.9 | 492.6 | 515.3 |
| 3(RS)-chloro-4(RS),5-dimethylhexane | 199.2 | 200.1 | 300.5 | 374.7 | 426.3 | 446.5 | 463.9 | 492.6 | 515.3 |
| 3(RS)-chloro-2,3-dimethylhexane | 201.5 | 202.5 | 305.2 | 378.6 | 429.2 | 448.9 | 465.9 | 493.9 | 516.0 |
| 2-chloro-2,3(RS)-dimethylhexane | 201.5 | 202.5 | 305.2 | 378.6 | 429.2 | 448.9 | 465.9 | 493.9 | 516.0 |
| 1-chloro-2(RS),3(RS)-dimethylhexane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 1-chloro-3(RS),5-dimethylhexane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 2(RS)-chloro-3(RS),5-dimethylhexane | 199.2 | 200.1 | 300.5 | 374.7 | 426.3 | 446.5 | 463.9 | 492.6 | 515.3 |
| 3-chloro-3(RS),5-dimethylhexane | 201.5 | 202.5 | 305.2 | 378.6 | 429.2 | 448.9 | 465.9 | 493.9 | 516.0 |
| 3(RS)-chloro-2,4(RS)-dimethylhexane | 199.2 | 200.1 | 300.5 | 374.7 | 426.3 | 446.5 | 463.9 | 492.6 | 515.3 |
| 2-chloro-2,4(RS)-dimethylhexane | 201.5 | 202.5 | 305.2 | 378.6 | 429.2 | 448.9 | 465.9 | 493.9 | 516.0 |
| 1-chloro-2(RS),4(RS)-dimethylhexane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 1-chloro-2(RS),5-dimethylhexane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 2-chloro-2,5-dimethylhexane | 201.5 | 202.5 | 305.2 | 378.6 | 429.2 | 448.9 | 465.9 | 493.9 | 516.0 |
| 3(RS)-chloro-2,5-dimethylhexane | 199.2 | 200.1 | 300.5 | 374.7 | 426.3 | 446.5 | 463.9 | 492.6 | 515.3 |
| 1-chloro-3(RS),4(RS)-dimethylhexane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 2(RS)-chloro-3(RS),4(RS)-dimethylhexane | 199.2 | 200.1 | 300.5 | 374.7 | 426.3 | 446.5 | 463.9 | 492.6 | 515.3 |
| 3-chloro-3(RS),4(RS)-dimethylhexane | 201.5 | 202.5 | 305.2 | 378.6 | 429.2 | 448.9 | 465.9 | 493.9 | 516.0 |
| 1-chloro-2(RS)-ethylhexane | 198.2 | 199.0 | 297.1 | 369.6 | 420.5 | 440.5 | 457.9 | 486.7 | 509.7 |
| 1-chloro-3(RS)-ethylhexane | 198.2 | 199.0 | 297.1 | 369.6 | 420.5 | 440.5 | 457.9 | 486.7 | 509.7 |
| 2(RS)-chloro-3(RS)-ethylhexane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 3-chloro-3-ethylhexane | 202.7 | 203.6 | 304.9 | 378.0 | 428.5 | 448.1 | 465.1 | 493.0 | 515.0 |
| 3(RS)-chloro-4-ethylhexane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 2(RS)-chloro-4-ethylhexane | 200.4 | 201.2 | 300.2 | 374.2 | 425.6 | 445.7 | 463.1 | 491.7 | 514.3 |
| 1-chloro-4-ethylhexane | 198.2 | 199.0 | 297.1 | 369.6 | 420.5 | 440.5 | 457.9 | 486.7 | 509.7 |
| 1-chloro-2(RS)-ethyl-2-methylpentane | 200.3 | 201.2 | 302.7 | 375.8 | 425.9 | 445.3 | 462.0 | 489.4 | 510.9 |
| 1-chloro-2(RS)-isopropylpentane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 1-chloro-2(RS)-ethyl-4-methylpentane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 1-chloro-3(RS),4,4-trimethylpentane | 199.2 | 200.1 | 303.1 | 376.4 | 426.5 | 446.0 | 462.8 | 490.3 | 511.9 |
| 2(RS)-chloro-3(RS),4,4-trimethylpentane | 201.3 | 202.2 | 306.1 | 380.9 | 431.7 | 451.2 | 468.0 | 495.2 | 516.5 |
| 3-chloro-2,2,3(RS)-trimethylpentane | 203.7 | 204.6 | 310.8 | 384.8 | 434.6 | 453.7 | 470.0 | 496.5 | 517.2 |
| 1-chloro-2,2,3(RS)-trimethylpentane | 199.2 | 200.1 | 303.1 | 376.4 | 426.5 | 446.0 | 462.8 | 490.3 | 511.9 |
| 1-chloro-2(RS),4,4-trimethylpentane | 199.2 | 200.1 | 303.1 | 376.4 | 426.5 | 446.0 | 462.8 | 490.3 | 511.9 |
| 2-chloro-2,4,4-trimethylpentane | 203.7 | 204.6 | 310.8 | 384.8 | 434.6 | 453.7 | 470.0 | 496.5 | 517.2 |
| 3(RS)-chloro-2,2,4-trimethylpentane | 201.3 | 202.2 | 306.1 | 380.9 | 431.7 | 451.2 | 468.0 | 495.2 | 516.5 |
| 1-chloro-2,2,3-trimethylpentane | 199.2 | 200.1 | 303.1 | 376.4 | 426.5 | 446.0 | 462.8 | 490.3 | 511.9 |
| 1-chloro-3,3,4-trimethylpentane | 199.2 | 200.1 | 303.1 | 376.4 | 426.5 | 446.0 | 462.8 | 490.3 | 511.9 |
| 2(RS)-chloro-3,3,4-trimethylpentane | 201.3 | 202.2 | 306.1 | 380.9 | 431.7 | 451.2 | 468.0 | 495.2 | 516.5 |
| 2-chloro-2,3,3-trimethylpentane | 203.7 | 204.6 | 310.8 | 384.8 | 434.6 | 453.7 | 470.0 | 496.5 | 517.2 |
| 1-chloro-2(RS),3,3-trimethylpentane | 199.2 | 200.1 | 303.1 | 376.4 | 426.5 | 446.0 | 462.8 | 490.3 | 511.9 |
| 1-chloro-3-ethyl-3-methylpentane | 200.3 | 201.2 | 302.7 | 375.8 | 425.9 | 445.3 | 462.0 | 489.4 | 510.9 |
| 2(RS)-chloro-3-ethyl-3-methylpentane | 202.5 | 203.4 | 305.8 | 380.4 | 431.0 | 450.5 | 467.2 | 494.3 | 515.5 |
| 1-chloro-2(RS)-ethyl-3(RS)-methylpentane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 1-chloro-2(RS),3(RS),4-trimethylpentane | 195.9 | 196.8 | 297.8 | 370.8 | 421.8 | 442.0 | 459.5 | 488.5 | 511.7 |
| 2-chloro-2,3(RS),4-trimethylpentane | 200.4 | 201.3 | 305.5 | 379.2 | 429.9 | 449.6 | 466.7 | 494.8 | 517.0 |
| 3-chloro-2,3,4-trimethylpentane | 200.4 | 201.3 | 305.5 | 379.2 | 429.9 | 449.6 | 466.7 | 494.8 | 517.0 |
| 1-chloro-2-propylpentane | 198.2 | 199.0 | 297.1 | 369.6 | 420.5 | 440.5 | 457.9 | 486.7 | 509.7 |

Table 10. Standard heat capacity at constant pressure for monochloroalkanes in J/K mol -- continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 1-chloro-3(RS)-ethyl-4-methylpentane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 2(RS)-chloro-3(RS)-ethyl-4-methylpentane | 199.2 | 200.1 | 300.5 | 374.7 | 426.3 | 446.5 | 463.9 | 492.6 | 515.3 |
| 3-chloro-3-ethyl-2-methylpentane | 201.5 | 202.5 | 305.2 | 378.6 | 429.2 | 448.9 | 465.9 | 493.9 | 516.0 |
| 2-chloro-3-ethyl-2-methylpentane | 201.5 | 202.5 | 305.2 | 378.6 | 429.2 | 448.9 | 465.9 | 493.9 | 516.0 |
| 1-chloro-3-ethyl-2(RS)-methylpentane | 197.0 | 197.9 | 297.5 | 370.2 | 421.2 | 441.2 | 458.7 | 487.6 | 510.7 |
| 1-chloro-2(RS)-ethyl-3,3-dimethylbutane | 199.2 | 200.1 | 303.1 | 376.4 | 426.5 | 446.0 | 462.8 | 490.3 | 511.9 |
| 1-chloro-2(RS)-ethyl-2,3-dimethylbutane | 199.2 | 200.1 | 303.1 | 376.4 | 426.5 | 446.0 | 462.8 | 490.3 | 511.9 |
| 1-chloro-2,2-diethylbutane | 200.3 | 201.2 | 302.7 | 375.8 | 425.9 | 445.3 | 462.0 | 489.4 | 510.9 |
| 1-chloro-2,2,3,3-tetramethylbutane | 201.3 | 202.3 | 308.7 | 382.6 | 431.9 | 450.8 | 466.9 | 492.9 | 513.1 |
| 1-chloro-2-isopropyl-3-methylbutane | 195.9 | 196.8 | 297.8 | 370.8 | 421.8 | 442.0 | 459.5 | 488.5 | 511.7 |

Entropy of monochloroalkanes in J/K mol

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| CH3Cl | | | | | | | | | |
| chloromethane | 234.37 | 234.62 | 258.88 | 279.34 | 297.18 | 305.30 | 312.96 | 327.08 | 339.82 |
| C2H5Cl | | | | | | | | | |
| chloroethane | 276.62 | 277.00 | 315.40 | 349.07 | 378.61 | 392.06 | 404.74 | 428.10 | 449.21 |
| C3H7Cl | | | | | | | | | |
| 1-chloropropane | 316.03 | 316.56 | 369.43 | 416.16 | 457.32 | 476.07 | 493.76 | 526.37 | 555.81 |
| 2-chloropropane | 306.39 | 306.93 | 360.91 | 408.94 | 451.32 | 470.62 | 488.81 | 522.26 | 552.40 |
| C4H9Cl | | | | | | | | | |
| 1-chlorobutane | 355.44 | 356.11 | 423.45 | 483.26 | 536.02 | 560.08 | 582.79 | 624.63 | 662.42 |
| 2(RS)-chlorobutane | 345.81 | 346.49 | 414.93 | 476.03 | 530.03 | 554.63 | 577.83 | 620.53 | 659.01 |
| 1-chloro-2-methylpropane | 344.22 | 344.88 | 412.11 | 472.08 | 525.00 | 549.14 | 571.91 | 613.89 | 651.83 |
| 2-chloro-2-methylpropane | 317.46 | 318.14 | 388.58 | 451.30 | 506.31 | 531.27 | 554.76 | 597.86 | 636.62 |
| C5H11Cl | | | | | | | | | |
| 1-chloropentane | 394.9 | 395.7 | 477.5 | 550.4 | 614.7 | 644.1 | 671.8 | 722.9 | 769.0 |
| 2(RS)-chloropentane | 385.2 | 386.0 | 469.0 | 543.1 | 608.7 | 638.6 | 666.9 | 718.8 | 765.6 |
| 3-chloropentane | 385.2 | 386.0 | 469.0 | 543.1 | 608.7 | 638.6 | 666.9 | 718.8 | 765.6 |
| 1-chloro-2(RS)-methylbutane | 383.6 | 384.4 | 466.1 | 539.2 | 603.7 | 633.2 | 660.9 | 712.2 | 758.4 |
| 2-chloro-2-methylbutane | 366.0 | 366.8 | 451.7 | 527.5 | 594.1 | 624.4 | 652.9 | 705.3 | 752.4 |
| 2(RS)-chloro-3-methylbutane | 374.0 | 374.8 | 457.6 | 531.9 | 597.7 | 627.7 | 656.0 | 708.1 | 755.0 |
| 1-chloro-3-methylbutane | 383.6 | 384.4 | 466.1 | 539.2 | 603.7 | 633.2 | 660.9 | 712.2 | 758.4 |
| 1-chloro-2,2-dimethylpropane | 356.8 | 357.6 | 441.4 | 516.5 | 582.5 | 612.4 | 640.7 | 692.4 | 739.0 |
| C6H13Cl | | | | | | | | | |
| 1-chlorohexane | 434.3 | 435.2 | 531.5 | 617.5 | 693.4 | 728.1 | 760.8 | 821.1 | 875.6 |
| 2(RS)-chlorohexane | 424.6 | 425.6 | 523.0 | 610.2 | 687.4 | 722.7 | 755.9 | 817.0 | 872.2 |
| 3(RS)-chlorohexane | 424.6 | 425.6 | 523.0 | 610.2 | 687.4 | 722.7 | 755.9 | 817.0 | 872.2 |
| 1-chloro-2(RS)-methylpentane | 423.0 | 424.0 | 520.2 | 606.3 | 682.4 | 717.2 | 750.0 | 810.4 | 865.0 |
| 2-chloro-2-methylpentane | 405.4 | 406.4 | 505.8 | 594.6 | 672.9 | 708.4 | 741.9 | 803.5 | 859.0 |
| 3(RS)-chloro-2-methylpentane | 413.4 | 414.4 | 511.6 | 599.0 | 676.4 | 711.7 | 745.0 | 806.3 | 861.6 |
| 2(RS)-chloro-4-methylpentane | 413.4 | 414.4 | 511.6 | 599.0 | 676.4 | 711.7 | 745.0 | 806.3 | 861.6 |
| 1-chloro-4-methylpentane | 423.0 | 424.0 | 520.2 | 606.3 | 682.4 | 717.2 | 750.0 | 810.4 | 865.0 |
| 1-chloro-3(RS)-methylpentane | 423.0 | 424.0 | 520.2 | 606.3 | 682.4 | 717.2 | 750.0 | 810.4 | 865.0 |
| 2(RS)-chloro-3(RS)-methylpentane | 413.4 | 414.4 | 511.6 | 599.0 | 676.4 | 711.7 | 745.0 | 806.3 | 861.6 |
| 3-chloro-3-methylpentane | 405.4 | 406.4 | 505.8 | 594.6 | 672.9 | 708.4 | 741.9 | 803.5 | 859.0 |
| 1-chloro-2(RS),3-dimethylbutane | 411.8 | 412.8 | 508.8 | 595.1 | 671.4 | 706.2 | 739.1 | 799.7 | 854.4 |
| 2-chloro-2,3-dimethylbutane | 394.2 | 395.2 | 494.4 | 583.4 | 661.8 | 697.5 | 731.1 | 792.8 | 848.4 |
| 1-chloro-2-ethylbutane | 423.0 | 424.0 | 520.2 | 606.3 | 682.4 | 717.2 | 750.0 | 810.4 | 865.0 |
| 1-chloro-2,2-dimethylbutane | 405.4 | 406.3 | 504.5 | 592.7 | 670.3 | 705.6 | 738.8 | 799.8 | 854.7 |
| 2(RS)-chloro-3,3-dimethylbutane | 386.6 | 387.6 | 486.9 | 576.3 | 655.2 | 691.0 | 724.7 | 786.6 | 842.2 |
| 1-chloro-3,3-dimethylbutane | 396.2 | 397.2 | 495.4 | 583.6 | 661.2 | 696.5 | 729.7 | 790.7 | 845.6 |
| C7H15Cl | | | | | | | | | |
| 1-chloroheptane | 473.7 | 474.8 | 585.5 | 684.6 | 772.1 | 812.1 | 849.9 | 919.4 | 982.2 |
| 2(RS)-chloroheptane | 464.0 | 465.2 | 577.0 | 677.3 | 766.1 | 806.7 | 844.9 | 915.3 | 978.8 |
| 3(RS)-chloroheptane | 464.0 | 465.2 | 577.0 | 677.3 | 766.1 | 806.7 | 844.9 | 915.3 | 978.8 |
| 4-chloroheptane | 464.0 | 465.2 | 577.0 | 677.3 | 766.1 | 806.7 | 844.9 | 915.3 | 978.8 |
| 1-chloro-5-methylhexane | 462.5 | 463.5 | 574.2 | 673.4 | 761.1 | 801.2 | 839.0 | 908.7 | 971.6 |
| 2(RS)-chloro-5-methylhexane | 452.8 | 453.9 | 565.7 | 666.1 | 755.1 | 795.7 | 834.0 | 904.6 | 968.2 |

Table 11. Standard entropy of monochloroalkanes in J/K mol -- continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 3(RS)-chloro-5-methylhexane | 452.8 | 453.9 | 565.7 | 666.1 | 755.1 | 795.7 | 834.0 | 904.6 | 968.2 |
| 3(RS)-chloro-2-methylhexane | 452.8 | 453.9 | 565.7 | 666.1 | 755.1 | 795.7 | 834.0 | 904.6 | 968.2 |
| 2-chloro-2-methylhexane | 444.8 | 445.9 | 559.8 | 661.7 | 751.6 | 792.4 | 831.0 | 901.8 | 965.6 |
| 1-chloro-2(RS)-methylhexane | 462.5 | 463.5 | 574.2 | 673.4 | 761.1 | 801.2 | 839.0 | 908.7 | 971.6 |
| 1-chloro-4(RS)-methylhexane | 462.5 | 463.5 | 574.2 | 673.4 | 761.1 | 801.2 | 839.0 | 908.7 | 971.6 |
| 2(RS)-chloro-4(RS)-methylhexane | 452.8 | 453.9 | 565.7 | 666.1 | 755.1 | 795.7 | 834.0 | 904.6 | 968.2 |
| 3(RS)-chloro-4(RS)-methylhexane | 452.8 | 453.9 | 565.7 | 666.1 | 755.1 | 795.7 | 834.0 | 904.6 | 968.2 |
| 3-chloro-3(RS)-methylhexane | 444.8 | 445.9 | 559.8 | 661.7 | 751.6 | 792.4 | 831.0 | 901.8 | 965.6 |
| 2(RS)-chloro-3(RS)-methylhexane | 452.8 | 453.9 | 565.7 | 666.1 | 755.1 | 795.7 | 834.0 | 904.6 | 968.2 |
| 1-chloro-3(RS)-methylhexane | 462.5 | 463.5 | 574.2 | 673.4 | 761.1 | 801.2 | 839.0 | 908.7 | 971.6 |
| 1-chloro-4,4-dimethylpentane | 435.7 | 436.8 | 549.4 | 650.6 | 739.9 | 780.5 | 818.7 | 889.0 | 952.2 |
| 2(RS)-chloro-4,4-dimethylpentane | 426.0 | 427.1 | 540.9 | 643.4 | 733.9 | 775.0 | 813.7 | 884.9 | 948.8 |
| 3(RS)-chloro-2,2-dimethylpentane | 426.0 | 427.1 | 540.9 | 643.4 | 733.9 | 775.0 | 813.7 | 884.9 | 948.8 |
| 1-chloro-2,2-dimethylpentane | 444.8 | 445.9 | 558.6 | 659.8 | 749.0 | 789.6 | 827.8 | 898.1 | 961.3 |
| 1-chloro-3,3-dimethylpentane | 444.8 | 445.9 | 558.6 | 659.8 | 749.0 | 789.6 | 827.8 | 898.1 | 961.3 |
| 2(RS)-chloro-3,3-dimethylpentane | 435.2 | 436.3 | 550.0 | 652.6 | 743.0 | 784.2 | 822.9 | 894.0 | 957.9 |
| 1-chloro-3(RS),4-dimethylpentane | 451.2 | 452.3 | 562.9 | 662.2 | 750.1 | 790.2 | 828.1 | 897.9 | 961.1 |
| 2(RS)-chloro-3(RS),4-dimethylpentane | 441.6 | 442.7 | 554.3 | 655.0 | 744.1 | 784.8 | 823.2 | 893.8 | 957.6 |
| 1-chloro-2(RS),3(RS)-dimethylpentane | 451.2 | 452.3 | 562.9 | 662.2 | 750.1 | 790.2 | 828.1 | 897.9 | 961.1 |
| 2-chloro-2,3(RS)-dimethylpentane | 433.6 | 434.7 | 548.5 | 650.5 | 740.5 | 781.5 | 820.1 | 891.0 | 955.0 |
| 3-chloro-2,3(RS)-dimethylpentane | 433.6 | 434.7 | 548.5 | 650.5 | 740.5 | 781.5 | 820.1 | 891.0 | 955.0 |
| 1-chloro-2(RS),4-dimethylpentane | 451.2 | 452.3 | 562.9 | 662.2 | 750.1 | 790.2 | 828.1 | 897.9 | 961.1 |
| 2-chloro-2,4-dimethylpentane | 433.6 | 434.7 | 548.5 | 650.5 | 740.5 | 781.5 | 820.1 | 891.0 | 955.0 |
| 3-chloro-2,4-dimethylpentane | 441.6 | 442.7 | 554.3 | 655.0 | 744.1 | 784.8 | 823.2 | 893.8 | 957.6 |
| 1-chloro-2(RS)-ethylpentane | 462.5 | 463.5 | 574.2 | 673.4 | 761.1 | 801.2 | 839.0 | 908.7 | 971.6 |
| 1-chloro-3-ethylpentane | 462.5 | 463.5 | 574.2 | 673.4 | 761.1 | 801.2 | 839.0 | 908.7 | 971.6 |
| 2(RS)-chloro-3-ethylpentane | 452.8 | 453.9 | 565.7 | 666.1 | 755.1 | 795.7 | 834.0 | 904.6 | 968.2 |
| 3-chloro-3-ethylpentane | 444.8 | 445.9 | 559.8 | 661.7 | 751.6 | 792.4 | 831.0 | 901.8 | 965.6 |
| 1-chloro-2-ethyl-2-methylbutane | 444.8 | 445.9 | 558.6 | 659.8 | 749.0 | 789.6 | 827.8 | 898.1 | 961.3 |
| 1-chloro-2(RS)-ethyl-3-methylbutane | 451.2 | 452.3 | 562.9 | 662.2 | 750.1 | 790.2 | 828.1 | 897.9 | 961.1 |
| 1-chloro-2(RS),3,3-trimethylbutane | 424.4 | 425.5 | 538.1 | 639.5 | 728.9 | 769.5 | 807.8 | 878.2 | 941.6 |
| 2-chloro-2,3,3-trimethylbutane | 406.8 | 407.9 | 523.7 | 627.8 | 719.3 | 760.8 | 799.8 | 871.3 | 935.5 |
| 1-chloro-2,2,3-trimethylbutane | 433.6 | 434.7 | 547.2 | 648.6 | 738.0 | 778.7 | 817.0 | 887.4 | 950.7 |
| C8H17Cl | | | | | | | | | |
| 1-chlorooctane | 513.1 | 514.3 | 639.6 | 751.6 | 850.8 | 896.1 | 938.9 | 1017.7 | 1088.8 |
| 2(RS)-chlorooctane | 503.5 | 504.7 | 631.0 | 744.4 | 844.9 | 890.7 | 933.9 | 1013.6 | 1085.4 |
| 3(RS)-chlorooctane | 503.5 | 504.7 | 631.0 | 744.4 | 844.9 | 890.7 | 933.9 | 1013.6 | 1085.4 |
| 4(RS)-chlorooctane | 503.5 | 504.7 | 631.0 | 744.4 | 844.9 | 890.7 | 933.9 | 1013.6 | 1085.4 |
| 1-chloro-2(RS)-methylheptane | 501.9 | 503.1 | 628.2 | 740.5 | 839.8 | 885.2 | 928.0 | 1006.9 | 1078.3 |
| 2-chloro-2-methylheptane | 484.2 | 485.5 | 613.8 | 728.8 | 830.3 | 876.5 | 920.0 | 1000.0 | 1072.2 |
| 3(RS)-chloro-2-methylheptane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 4(RS)-chloro-2-methylheptane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 3(RS)-chloro-6-methylheptane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 2(RS)-chloro-6-methylheptane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 1-chloro-6-methylheptane | 501.9 | 503.1 | 628.2 | 740.5 | 839.8 | 885.2 | 928.0 | 1006.9 | 1078.3 |
| 1-chloro-3(RS)-methylheptane | 501.9 | 503.1 | 628.2 | 740.5 | 839.8 | 885.2 | 928.0 | 1006.9 | 1078.3 |
| 2(RS)-chloro-3(RS)-methylheptane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 3-chloro-3(RS)-methylheptane | 484.2 | 485.5 | 613.8 | 728.8 | 830.3 | 876.5 | 920.0 | 1000.0 | 1072.2 |
| 4(RS)-chloro-3(RS)-methylheptane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 3(RS)-chloro-5(RS)-methylheptane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 2(RS)-chloro-5(RS)-methylheptane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 1-chloro-5(RS)-methylheptane | 501.9 | 503.1 | 628.2 | 740.5 | 839.8 | 885.2 | 928.0 | 1006.9 | 1078.3 |
| 1-chloro-4(RS)-methylheptane | 501.9 | 503.1 | 628.2 | 740.5 | 839.8 | 885.2 | 928.0 | 1006.9 | 1078.3 |
| 2(RS)-chloro-4(RS)-methylheptane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 3(RS)-chloro-4(RS)-methylheptane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 4-chloro-4-methylheptane | 484.2 | 485.5 | 613.8 | 728.8 | 830.3 | 876.5 | 920.0 | 1000.0 | 1072.2 |

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 1-chloro-2,2-dimethylhexane | 484.2 | 485.4 | 612.6 | 726.9 | 827.7 | 873.6 | 916.9 | 996.4 | 1067.9 |
| 3(RS)-chloro-2,2-dimethylhexane | 465.4 | 466.7 | 594.9 | 710.5 | 812.6 | 859.0 | 902.8 | 983.1 | 1055.4 |
| 3(RS)-chloro-5,5-dimethylhexane | 465.4 | 466.7 | 594.9 | 710.5 | 812.6 | 859.0 | 902.8 | 983.1 | 1055.4 |
| 2(RS)-chloro-5,5-dimethylhexane | 465.4 | 466.7 | 594.9 | 710.5 | 812.6 | 859.0 | 902.8 | 983.1 | 1055.4 |
| 1-chloro-5,5-dimethylhexane | 475.1 | 476.3 | 603.5 | 717.7 | 818.6 | 864.5 | 907.7 | 987.2 | 1058.8 |
| 1-chloro-3,3-dimethylhexane | 484.2 | 485.4 | 612.6 | 726.9 | 827.7 | 873.6 | 916.9 | 996.4 | 1067.9 |
| 2(RS)-chloro-3,3-dimethylhexane | 474.6 | 475.8 | 604.1 | 719.7 | 821.7 | 868.2 | 911.9 | 992.3 | 1064.5 |
| 3(RS)-chloro-4,4-dimethylhexane | 474.6 | 475.8 | 604.1 | 719.7 | 821.7 | 868.2 | 911.9 | 992.3 | 1064.5 |
| 2(RS)-chloro-4,4-dimethylhexane | 474.6 | 475.8 | 604.1 | 719.7 | 821.7 | 868.2 | 911.9 | 992.3 | 1064.5 |
| 1-chloro-4,4-dimethylhexane | 484.2 | 485.4 | 612.6 | 726.9 | 827.7 | 873.6 | 916.9 | 996.4 | 1067.9 |
| 1-chloro-4(RS),5-dimethylhexane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 2(RS)-chloro-4(RS),5-dimethylhexane | 481.0 | 482.2 | 608.4 | 722.1 | 822.8 | 868.8 | 912.2 | 992.1 | 1064.2 |
| 3(RS)-chloro-4(RS),5-dimethylhexane | 481.0 | 482.2 | 608.4 | 722.1 | 822.8 | 868.8 | 912.2 | 992.1 | 1064.2 |
| 3(RS)-chloro-2,3-dimethylhexane | 473.0 | 474.3 | 602.5 | 717.6 | 819.2 | 865.5 | 909.1 | 989.3 | 1061.6 |
| 2-chloro-2,3(RS)-dimethylhexane | 473.0 | 474.3 | 602.5 | 717.6 | 819.2 | 865.5 | 909.1 | 989.3 | 1061.6 |
| 1-chloro-2(RS),3(RS)-dimethylhexane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 1-chloro-3(RS),5-dimethylhexane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 2(RS)-chloro-3(RS),5-dimethylhexane | 481.0 | 482.2 | 608.4 | 722.1 | 822.8 | 868.8 | 912.2 | 992.1 | 1064.2 |
| 3-chloro-3(RS),5-dimethylhexane | 473.0 | 474.3 | 602.5 | 717.6 | 819.2 | 865.5 | 909.1 | 989.3 | 1061.6 |
| 3(RS)-chloro-2,4(RS)-dimethylhexane | 481.0 | 482.2 | 608.4 | 722.1 | 822.8 | 868.8 | 912.2 | 992.1 | 1064.2 |
| 2-chloro-2,4(RS)-dimethylhexane | 473.0 | 474.3 | 602.5 | 717.6 | 819.2 | 865.5 | 909.1 | 989.3 | 1061.6 |
| 1-chloro-2(RS),4(RS)-dimethylhexane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 1-chloro-2(RS),5-dimethylhexane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 2-chloro-2,5-dimethylhexane | 473.0 | 474.3 | 602.5 | 717.6 | 819.2 | 865.5 | 909.1 | 989.3 | 1061.6 |
| 3(RS)-chloro-2,5-dimethylhexane | 481.0 | 482.2 | 608.4 | 722.1 | 822.8 | 868.8 | 912.2 | 992.1 | 1064.2 |
| 1-chloro-3(RS),4(RS)-dimethylhexane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 2(RS)-chloro-3(RS),4(RS)-dimethylhexane | 481.0 | 482.2 | 608.4 | 722.1 | 822.8 | 868.8 | 912.2 | 992.1 | 1064.2 |
| 3-chloro-3(RS),4(RS)-dimethylhexane | 473.0 | 474.3 | 602.5 | 717.6 | 819.2 | 865.5 | 909.1 | 989.3 | 1061.6 |
| 1-chloro-2(RS)-ethylhexane | 501.9 | 503.1 | 628.2 | 740.5 | 839.8 | 885.2 | 928.0 | 1006.9 | 1078.3 |
| 1-chloro-3(RS)-ethylhexane | 501.9 | 503.1 | 628.2 | 740.5 | 839.8 | 885.2 | 928.0 | 1006.9 | 1078.3 |
| 2(RS)-chloro-3(RS)-ethylhexane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 3-chloro-3-ethylhexane | 484.2 | 485.5 | 613.8 | 728.8 | 830.3 | 876.5 | 920.0 | 1000.0 | 1072.2 |
| 3(RS)-chloro-4-ethylhexane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 2(RS)-chloro-4-ethylhexane | 492.2 | 493.5 | 619.7 | 733.2 | 833.8 | 879.7 | 923.1 | 1002.8 | 1074.8 |
| 1-chloro-4-ethylhexane | 501.9 | 503.1 | 628.2 | 740.5 | 839.8 | 885.2 | 928.0 | 1006.9 | 1078.3 |
| 1-chloro-2(RS)-ethyl-2-methylpentane | 484.2 | 485.4 | 612.6 | 726.9 | 827.7 | 873.6 | 916.9 | 996.4 | 1067.9 |
| 1-chloro-2(RS)-isopropylpentane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 1-chloro-2(RS)-ethyl-4-methylpentane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 1-chloro-3(RS),4,4-trimethylpentane | 463.8 | 465.1 | 592.1 | 706.6 | 807.6 | 853.5 | 896.9 | 976.5 | 1048.2 |
| 2(RS)-chloro-3(RS),4,4-trimethylpentane | 454.2 | 455.5 | 583.6 | 699.3 | 801.6 | 848.1 | 891.9 | 972.4 | 1044.8 |
| 3-chloro-2,2,3(RS)-trimethylpentane | 446.2 | 447.5 | 577.7 | 694.9 | 798.0 | 844.8 | 888.8 | 969.6 | 1042.1 |
| 1-chloro-2,2,3(RS)-trimethylpentane | 473.0 | 474.2 | 601.3 | 715.7 | 816.7 | 862.7 | 906.0 | 985.6 | 1057.4 |
| 1-chloro-2(RS),4,4-trimethylpentane | 463.8 | 465.1 | 592.1 | 706.6 | 807.6 | 853.5 | 896.9 | 976.5 | 1048.2 |
| 2-chloro-2,4,4-trimethylpentane | 446.2 | 447.5 | 577.7 | 694.9 | 798.0 | 844.8 | 888.8 | 969.6 | 1042.1 |
| 3(RS)-chloro-2,2,4-trimethylpentane | 454.2 | 455.5 | 583.6 | 699.3 | 801.6 | 848.1 | 891.9 | 972.4 | 1044.8 |
| 1-chloro-2,2,3-trimethylpentane | 473.0 | 474.2 | 601.3 | 715.7 | 816.7 | 862.7 | 906.0 | 985.6 | 1057.4 |
| 1-chloro-3,3,4-trimethylpentane | 473.0 | 474.2 | 601.3 | 715.7 | 816.7 | 862.7 | 906.0 | 985.6 | 1057.4 |
| 2(RS)-chloro-3,3,4-trimethylpentane | 463.3 | 464.6 | 592.7 | 708.5 | 810.7 | 857.2 | 901.0 | 981.5 | 1053.9 |
| 2-chloro-2,3,3-trimethylpentane | 455.3 | 456.6 | 586.9 | 704.1 | 807.1 | 853.9 | 898.0 | 978.7 | 1051.3 |
| 1-chloro-2(RS),3,3-trimethylpentane | 473.0 | 474.2 | 601.3 | 715.7 | 816.7 | 862.7 | 906.0 | 985.6 | 1057.4 |
| 1-chloro-3-ethyl-3-methylpentane | 484.2 | 485.4 | 612.6 | 726.9 | 827.7 | 873.6 | 916.9 | 996.4 | 1067.9 |
| 2(RS)-chloro-3-ethyl-3-methylpentane | 474.6 | 475.8 | 604.1 | 719.7 | 821.7 | 868.2 | 911.9 | 992.3 | 1064.5 |
| 1-chloro-2(RS)-ethyl-3(RS)-methylpentane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 1-chloro-2(RS),3(RS),4-trimethylpentane | 479.4 | 480.6 | 605.5 | 718.1 | 817.8 | 863.3 | 906.3 | 985.5 | 1057.1 |
| 2-chloro-2,3(RS),4-trimethylpentane | 461.8 | 463.0 | 591.1 | 706.5 | 808.2 | 854.6 | 898.2 | 978.6 | 1051.0 |
| 3-chloro-2,3,4-trimethylpentane | 461.8 | 463.0 | 591.1 | 706.5 | 808.2 | 854.6 | 898.2 | 978.6 | 1051.0 |
| 1-chloro-2-propylpentane | 501.9 | 503.1 | 628.2 | 740.5 | 839.8 | 885.2 | 928.0 | 1006.9 | 1078.3 |

Table 11. Standard entropy of monochloroalkanes in J/K mol -- continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 1-chloro-3(RS)-ethyl-4-methylpentane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 2(RS)-chloro-3(RS)-ethyl-4-methylpentane | 481.0 | 482.2 | 608.4 | 722.1 | 822.8 | 868.8 | 912.2 | 992.1 | 1064.2 |
| 3-chloro-3-ethyl-2-methylpentane | 473.0 | 474.3 | 602.5 | 717.6 | 819.2 | 865.5 | 909.1 | 989.3 | 1061.6 |
| 2-chloro-3-ethyl-2-methylpentane | 473.0 | 474.3 | 602.5 | 717.6 | 819.2 | 865.5 | 909.1 | 989.3 | 1061.6 |
| 1-chloro-3-ethyl-2(RS)-methylpentane | 490.6 | 491.9 | 616.9 | 729.3 | 828.8 | 874.2 | 917.1 | 996.2 | 1067.7 |
| 1-chloro-2(RS)-ethyl-3,3-dimethylbutane | 463.8 | 465.1 | 592.1 | 706.6 | 807.6 | 853.5 | 896.9 | 976.5 | 1048.2 |
| 1-chloro-2(RS)-ethyl-2,3-dimethylbutane | 473.0 | 474.2 | 601.3 | 715.7 | 816.7 | 862.7 | 906.0 | 985.6 | 1057.4 |
| 1-chloro-2,2-diethylbutane | 484.2 | 485.4 | 612.6 | 726.9 | 827.7 | 873.6 | 916.9 | 996.4 | 1067.9 |
| 1-chloro-2,2,3,3-tetramethylbutane | 446.2 | 447.4 | 576.5 | 693.0 | 795.5 | 842.0 | 885.7 | 965.9 | 1037.9 |
| 1-chloro-2-isopropyl-3-methylbutane | 479.4 | 480.6 | 605.5 | 718.1 | 817.8 | 863.3 | 906.3 | 985.5 | 1057.1 |

Table 12. Standard enthalpy of formation for monochloroalkanes in kJ/mol

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| CH3Cl | | | | | | | | | |
| chloromethane | -83.68 | -83.73 | -88.73 | -92.30 | -94.63 | -95.41 | -96.00 | -96.69 | -96.94 |
| C2H5Cl | | | | | | | | | |
| chloroethane | -112.97 | -113.05 | -120.57 | -125.46 | -128.33 | -129.19 | -129.74 | -130.11 | -129.74 |
| C3H7Cl | | | | | | | | | |
| 1-chloropropane | -133.60 | -133.70 | -143.63 | -149.93 | -153.42 | -154.36 | -154.89 | -154.94 | -153.98 |
| 2-chloropropane | -145.90 | -146.00 | -155.49 | -161.01 | -163.51 | -163.94 | -163.94 | -162.98 | -161.05 |
| C4H9Cl | | | | | | | | | |
| 1-chlorobutane | -154.22 | -154.36 | -166.70 | -174.40 | -178.50 | -179.53 | -180.04 | -179.77 | -178.22 |
| 2(RS)-chlorobutane | -166.52 | -166.65 | -178.56 | -185.47 | -188.60 | -189.11 | -189.09 | -187.81 | -185.29 |
| 1-chloro-2-methylpropane | -163.59 | -163.73 | -176.10 | -183.71 | -187.68 | -188.64 | -189.07 | -188.64 | -186.89 |
| 2-chloro-2-methylpropane | -188.32 | -188.45 | -199.54 | -205.50 | -207.82 | -208.00 | -207.68 | -205.90 | -203.00 |
| C5H11Cl | | | | | | | | | |
| 1-chloropentane | -174.8 | -175.0 | -189.8 | -198.9 | -203.6 | -204.7 | -205.2 | -204.6 | -202.5 |
| 2(RS)-chloropentane | -187.2 | -187.3 | -201.6 | -209.9 | -213.7 | -214.3 | -214.2 | -212.6 | -209.5 |
| 3-chloropentane | -187.2 | -187.3 | -201.6 | -209.9 | -213.7 | -214.3 | -214.2 | -212.6 | -209.5 |
| 1-chloro-2(RS)-methylbutane | -180.9 | -181.0 | -195.8 | -204.8 | -209.4 | -210.5 | -210.9 | -210.1 | -207.8 |
| 2-chloro-2-methylbutane | -205.6 | -205.8 | -219.3 | -226.6 | -229.6 | -229.8 | -229.5 | -227.4 | -223.9 |
| 2(RS)-chloro-3-methylbutane | -193.2 | -193.3 | -207.7 | -215.9 | -219.5 | -220.0 | -219.9 | -218.2 | -214.9 |
| 1-chloro-3-methylbutane | -180.9 | -181.0 | -195.8 | -204.8 | -209.4 | -210.5 | -210.9 | -210.1 | -207.8 |
| 1-chloro-2,2-dimethylpropane | -196.2 | -196.4 | -210.3 | -218.1 | -221.6 | -222.1 | -222.1 | -220.6 | -217.9 |
| C6H13Cl | | | | | | | | | |
| 1-chlorohexane | -195.5 | -195.7 | -212.8 | -223.3 | -228.7 | -229.9 | -230.3 | -229.4 | -226.7 |
| 2(RS)-chlorohexane | -207.8 | -208.0 | -224.7 | -234.4 | -238.8 | -239.5 | -239.4 | -237.5 | -233.8 |
| 3(RS)-chlorohexane | -207.8 | -208.0 | -224.7 | -234.4 | -238.8 | -239.5 | -239.4 | -237.5 | -233.8 |
| 1-chloro-2(RS)-methylpentane | -201.5 | -201.7 | -218.9 | -229.3 | -234.5 | -235.6 | -236.0 | -234.9 | -232.0 |
| 2-chloro-2-methylpentane | -226.2 | -226.4 | -242.3 | -251.1 | -254.6 | -255.0 | -254.6 | -252.2 | -248.1 |
| 3(RS)-chloro-2-methylpentane | -213.8 | -214.0 | -230.7 | -240.4 | -244.6 | -245.2 | -245.1 | -243.0 | -239.1 |
| 2(RS)-chloro-4-methylpentane | -213.8 | -214.0 | -230.7 | -240.4 | -244.6 | -245.2 | -245.1 | -243.0 | -239.1 |
| 1-chloro-4-methylpentane | -201.5 | -201.7 | -218.9 | -229.3 | -234.5 | -235.6 | -236.0 | -234.9 | -232.0 |
| 1-chloro-3(RS)-methylpentane | -201.5 | -201.7 | -218.9 | -229.3 | -234.5 | -235.6 | -236.0 | -234.9 | -232.0 |
| 2(RS)-chloro-3(RS)-methylpentane | -213.8 | -214.0 | -230.7 | -240.4 | -244.6 | -245.2 | -245.1 | -243.0 | -239.1 |
| 3-chloro-3-methylpentane | -226.2 | -226.4 | -242.3 | -251.1 | -254.6 | -255.0 | -254.6 | -252.2 | -248.1 |
| 1-chloro-2(RS),3-dimethylbutane | -207.5 | -207.7 | -224.9 | -235.3 | -240.3 | -241.4 | -241.7 | -240.5 | -237.3 |
| 2-chloro-2,3-dimethylbutane | -232.3 | -232.4 | -248.4 | -257.0 | -260.5 | -260.8 | -260.3 | -257.7 | -253.5 |
| 1-chloro-2-ethylbutane | -201.5 | -201.7 | -218.9 | -229.3 | -234.5 | -235.6 | -236.0 | -234.9 | -232.0 |
| 1-chloro-2,2-dimethylbutane | -210.2 | -210.3 | -226.7 | -235.9 | -240.0 | -240.6 | -240.5 | -238.8 | -235.5 |
| 2(RS)-chloro-3,3-dimethylbutane | -222.5 | -222.6 | -238.6 | -247.0 | -250.0 | -250.2 | -249.6 | -246.8 | -242.5 |
| 1-chloro-3,3-dimethylbutane | -210.2 | -210.3 | -226.7 | -235.9 | -240.0 | -240.6 | -240.5 | -238.8 | -235.5 |
| C7H15Cl | | | | | | | | | |
| 1-chloroheptane | -216.1 | -216.3 | -235.9 | -247.8 | -253.8 | -255.1 | -255.5 | -254.3 | -250.9 |
| 2(RS)-chloroheptane | -228.4 | -228.6 | -247.8 | -258.9 | -263.9 | -264.6 | -264.5 | -262.3 | -258.0 |
| 3(RS)-chloroheptane | -228.4 | -228.6 | -247.8 | -258.9 | -263.9 | -264.6 | -264.5 | -262.3 | -258.0 |
| 4-chloroheptane | -228.4 | -228.6 | -247.8 | -258.9 | -263.9 | -264.6 | -264.5 | -262.3 | -258.0 |
| 1-chloro-5-methylhexane | -222.1 | -222.3 | -242.0 | -253.8 | -259.6 | -260.8 | -261.2 | -259.8 | -256.3 |
| 2(RS)-chloro-5-methylhexane | -234.4 | -234.6 | -253.8 | -264.8 | -269.7 | -270.4 | -270.2 | -267.8 | -263.3 |

Table 12. Standard enthalpy of formation for monochloroalkanes in kJ/mol -- continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 3(RS)-chloro-5-methylhexane | -234.4 | -234.6 | -253.8 | -264.8 | -269.7 | -270.4 | -270.2 | -267.8 | -263.3 |
| 3(RS)-chloro-2-methylhexane | -234.4 | -234.6 | -253.8 | -264.8 | -269.7 | -270.4 | -270.2 | -267.8 | -263.3 |
| 2-chloro-2-methylhexane | -246.9 | -247.1 | -265.4 | -275.6 | -279.7 | -280.2 | -279.8 | -277.0 | -272.4 |
| 1-chloro-2(RS)-methylhexane | -222.1 | -222.3 | -242.0 | -253.8 | -259.6 | -260.8 | -261.2 | -259.8 | -256.3 |
| 1-chloro-4(RS)-methylhexane | -222.1 | -222.3 | -242.0 | -253.8 | -259.6 | -260.8 | -261.2 | -259.8 | -256.3 |
| 2(RS)-chloro-4(RS)-methylhexane | -234.4 | -234.6 | -253.8 | -264.8 | -269.7 | -270.4 | -270.2 | -267.8 | -263.3 |
| 3(RS)-chloro-4(RS)-methylhexane | -234.4 | -234.6 | -253.8 | -264.8 | -269.7 | -270.4 | -270.2 | -267.8 | -263.3 |
| 3-chloro-3(RS)-methylhexane | -246.9 | -247.1 | -265.4 | -275.6 | -279.7 | -280.2 | -279.8 | -277.0 | -272.4 |
| 2(RS)-chloro-3(RS)-methylhexane | -234.4 | -234.6 | -253.8 | -264.8 | -269.7 | -270.4 | -270.2 | -267.8 | -263.3 |
| 1-chloro-3(RS)-methylhexane | -222.1 | -222.3 | -242.0 | -253.8 | -259.6 | -260.8 | -261.2 | -259.8 | -256.3 |
| 1-chloro-4,4-dimethylpentane | -230.8 | -231.0 | -249.8 | -260.4 | -265.0 | -265.8 | -265.7 | -263.6 | -259.7 |
| 2(RS)-chloro-4,4-dimethylpentane | -243.1 | -243.3 | -261.6 | -271.5 | -275.1 | -275.3 | -274.7 | -271.6 | -266.8 |
| 3(RS)-chloro-2,2-dimethylpentane | -243.1 | -243.3 | -261.6 | -271.5 | -275.1 | -275.3 | -274.7 | -271.6 | -266.8 |
| 1-chloro-2,2-dimethylpentane | -230.8 | -231.0 | -249.8 | -260.4 | -265.0 | -265.8 | -265.7 | -263.6 | -259.7 |
| 1-chloro-3,3-dimethylpentane | -230.8 | -231.0 | -249.8 | -260.4 | -265.0 | -265.8 | -265.7 | -263.6 | -259.7 |
| 2(RS)-chloro-3,3-dimethylpentane | -243.1 | -243.3 | -261.6 | -271.5 | -275.1 | -275.3 | -274.7 | -271.6 | -266.8 |
| 1-chloro-3(RS),4-dimethylpentane | -228.2 | -228.4 | -248.0 | -259.7 | -265.4 | -266.6 | -266.9 | -265.3 | -261.6 |
| 2(RS)-chloro-3(RS),4-dimethylpentane | -240.5 | -240.7 | -259.9 | -270.8 | -275.5 | -276.2 | -275.9 | -273.3 | -268.7 |
| 1-chloro-2(RS),3(RS)-dimethylpentane | -228.2 | -228.4 | -248.0 | -259.7 | -265.4 | -266.6 | -266.9 | -265.3 | -261.6 |
| 2-chloro-2,3(RS)-dimethylpentane | -252.9 | -253.1 | -271.5 | -281.5 | -285.6 | -285.9 | -285.5 | -282.6 | -277.7 |
| 3-chloro-2,3(RS)-dimethylpentane | -252.9 | -253.1 | -271.5 | -281.5 | -285.6 | -285.9 | -285.5 | -282.6 | -277.7 |
| 1-chloro-2(RS),4-dimethylpentane | -228.2 | -228.4 | -248.0 | -259.7 | -265.4 | -266.6 | -266.9 | -265.3 | -261.6 |
| 2-chloro-2,4-dimethylpentane | -252.9 | -253.1 | -271.5 | -281.5 | -285.6 | -285.9 | -285.5 | -282.6 | -277.7 |
| 3-chloro-2,4-dimethylpentane | -240.5 | -240.7 | -259.9 | -270.8 | -275.5 | -276.2 | -275.9 | -273.3 | -268.7 |
| 1-chloro-2(RS)-ethylpentane | -222.1 | -222.3 | -242.0 | -253.8 | -259.6 | -260.8 | -261.2 | -259.8 | -256.3 |
| 1-chloro-3-ethylpentane | -222.1 | -222.3 | -242.0 | -253.8 | -259.6 | -260.8 | -261.2 | -259.8 | -256.3 |
| 2(RS)-chloro-3-ethylpentane | -234.4 | -234.6 | -253.8 | -264.8 | -269.7 | -270.4 | -270.2 | -267.8 | -263.3 |
| 3-chloro-3-ethylpentane | -246.9 | -247.1 | -265.4 | -275.6 | -279.7 | -280.2 | -279.8 | -277.0 | -272.4 |
| 1-chloro-2-ethyl-2-methylbutane | -230.8 | -231.0 | -249.8 | -260.4 | -265.0 | -265.8 | -265.7 | -263.6 | -259.7 |
| 1-chloro-2(RS)-ethyl-3-methylbutane | -228.2 | -228.4 | -248.0 | -259.7 | -265.4 | -266.6 | -266.9 | -265.3 | -261.6 |
| 1-chloro-2(RS),3,3-trimethylbutane | -233.5 | -233.7 | -252.5 | -263.0 | -267.5 | -268.2 | -268.0 | -265.8 | -261.7 |
| 2-chloro-2,3,3-trimethylbutane | -258.2 | -258.4 | -275.9 | -284.8 | -287.7 | -287.5 | -286.6 | -283.0 | -277.8 |
| 1-chloro-2,2,3-trimethylbutane | -233.5 | -233.7 | -252.5 | -263.0 | -267.5 | -268.2 | -268.0 | -265.8 | -261.7 |
| C8H17Cl | | | | | | | | | |
| 1-chlorooctane | -236.7 | -237.0 | -259.0 | -272.3 | -278.8 | -280.2 | -280.6 | -279.1 | -275.2 |
| 2(RS)-chlorooctane | -249.0 | -249.3 | -270.8 | -283.3 | -288.9 | -289.8 | -289.7 | -287.1 | -282.3 |
| 3(RS)-chlorooctane | -249.0 | -249.3 | -270.8 | -283.3 | -288.9 | -289.8 | -289.7 | -287.1 | -282.3 |
| 4(RS)-chlorooctane | -249.0 | -249.3 | -270.8 | -283.3 | -288.9 | -289.8 | -289.7 | -287.1 | -282.3 |
| 1-chloro-2(RS)-methylheptane | -242.8 | -243.0 | -265.0 | -278.2 | -284.7 | -286.0 | -286.3 | -284.6 | -280.5 |
| 2-chloro-2-methylheptane | -267.5 | -267.7 | -288.5 | -300.0 | -304.8 | -305.3 | -304.9 | -301.9 | -296.6 |
| 3(RS)-chloro-2-methylheptane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 4(RS)-chloro-2-methylheptane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 3(RS)-chloro-6-methylheptane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 2(RS)-chloro-6-methylheptane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 1-chloro-6-methylheptane | -242.8 | -243.0 | -265.0 | -278.2 | -284.7 | -286.0 | -286.3 | -284.6 | -280.5 |
| 1-chloro-3(RS)-methylheptane | -242.8 | -243.0 | -265.0 | -278.2 | -284.7 | -286.0 | -286.3 | -284.6 | -280.5 |
| 2(RS)-chloro-3(RS)-methylheptane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 3-chloro-3(RS)-methylheptane | -267.5 | -267.7 | -288.5 | -300.0 | -304.8 | -305.3 | -304.9 | -301.9 | -296.6 |
| 4(RS)-chloro-3(RS)-methylheptane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 3(RS)-chloro-5(RS)-methylheptane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 2(RS)-chloro-5(RS)-methylheptane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 1-chloro-5(RS)-methylheptane | -242.8 | -243.0 | -265.0 | -278.2 | -284.7 | -286.0 | -286.3 | -284.6 | -280.5 |
| 1-chloro-4(RS)-methylheptane | -242.8 | -243.0 | -265.0 | -278.2 | -284.7 | -286.0 | -286.3 | -284.6 | -280.5 |
| 2(RS)-chloro-4(RS)-methylheptane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 3(RS)-chloro-4(RS)-methylheptane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 4-chloro-4-methylheptane | -267.5 | -267.7 | -288.5 | -300.0 | -304.8 | -305.3 | -304.9 | -301.9 | -296.6 |

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 1-chloro-2,2-dimethylhexane | -251.4 | -251.7 | -272.9 | -284.8 | -290.1 | -290.9 | -290.8 | -288.4 | -283.9 |
| 3(RS)-chloro-2,2-dimethylhexane | -263.7 | -264.0 | -284.7 | -295.9 | -300.2 | -300.5 | -299.9 | -296.5 | -291.0 |
| 3(RS)-chloro-5,5-dimethylhexane | -263.7 | -264.0 | -284.7 | -295.9 | -300.2 | -300.5 | -299.9 | -296.5 | -291.0 |
| 2(RS)-chloro-5,5-dimethylhexane | -263.7 | -264.0 | -284.7 | -295.9 | -300.2 | -300.5 | -299.9 | -296.5 | -291.0 |
| 1-chloro-5,5-dimethylhexane | -251.4 | -251.7 | -272.9 | -284.8 | -290.1 | -290.9 | -290.8 | -288.4 | -283.9 |
| 1-chloro-3,3-dimethylhexane | -251.4 | -251.7 | -272.9 | -284.8 | -290.1 | -290.9 | -290.8 | -288.4 | -283.9 |
| 2(RS)-chloro-3,3-dimethylhexane | -263.7 | -264.0 | -284.7 | -295.9 | -300.2 | -300.5 | -299.9 | -296.5 | -291.0 |
| 3(RS)-chloro-4,4-dimethylhexane | -263.7 | -264.0 | -284.7 | -295.9 | -300.2 | -300.5 | -299.9 | -296.5 | -291.0 |
| 2(RS)-chloro-4,4-dimethylhexane | -263.7 | -264.0 | -284.7 | -295.9 | -300.2 | -300.5 | -299.9 | -296.5 | -291.0 |
| 1-chloro-4,4-dimethylhexane | -251.4 | -251.7 | -272.9 | -284.8 | -290.1 | -290.9 | -290.8 | -288.4 | -283.9 |
| 1-chloro-4(RS),5-dimethylhexane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 2(RS)-chloro-4(RS),5-dimethylhexane | -261.1 | -261.3 | -282.9 | -295.3 | -300.6 | -301.3 | -301.1 | -298.2 | -292.9 |
| 3(RS)-chloro-4(RS),5-dimethylhexane | -261.1 | -261.3 | -282.9 | -295.3 | -300.6 | -301.3 | -301.1 | -298.2 | -292.9 |
| 3(RS)-chloro-2,3-dimethylhexane | -273.5 | -273.7 | -294.5 | -306.0 | -310.7 | -311.1 | -310.6 | -307.4 | -301.9 |
| 2-chloro-2,3(RS)-dimethylhexane | -273.5 | -273.7 | -294.5 | -306.0 | -310.7 | -311.1 | -310.6 | -307.4 | -301.9 |
| 1-chloro-2(RS),3(RS)-dimethylhexane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 1-chloro-3(RS),5-dimethylhexane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 2(RS)-chloro-3(RS),5-dimethylhexane | -261.1 | -261.3 | -282.9 | -295.3 | -300.6 | -301.3 | -301.1 | -298.2 | -292.9 |
| 3-chloro-3(RS),5-dimethylhexane | -273.5 | -273.7 | -294.5 | -306.0 | -310.7 | -311.1 | -310.6 | -307.4 | -301.9 |
| 3(RS)-chloro-2,4(RS)-dimethylhexane | -261.1 | -261.3 | -282.9 | -295.3 | -300.6 | -301.3 | -301.1 | -298.2 | -292.9 |
| 2-chloro-2,4(RS)-dimethylhexane | -273.5 | -273.7 | -294.5 | -306.0 | -310.7 | -311.1 | -310.6 | -307.4 | -301.9 |
| 1-chloro-2(RS),4(RS)-dimethylhexane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 1-chloro-2(RS),5-dimethylhexane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 2-chloro-2,5-dimethylhexane | -273.5 | -273.7 | -294.5 | -306.0 | -310.7 | -311.1 | -310.6 | -307.4 | -301.9 |
| 3(RS)-chloro-2,5-dimethylhexane | -261.1 | -261.3 | -282.9 | -295.3 | -300.6 | -301.3 | -301.1 | -298.2 | -292.9 |
| 1-chloro-3(RS),4(RS)-dimethylhexane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 2(RS)-chloro-3(RS),4(RS)-dimethylhexane | -261.1 | -261.3 | -282.9 | -295.3 | -300.6 | -301.3 | -301.1 | -298.2 | -292.9 |
| 3-chloro-3(RS),4(RS)-dimethylhexane | -273.5 | -273.7 | -294.5 | -306.0 | -310.7 | -311.1 | -310.6 | -307.4 | -301.9 |
| 1-chloro-2(RS)-ethylhexane | -242.8 | -243.0 | -265.0 | -278.2 | -284.7 | -286.0 | -286.3 | -284.6 | -280.5 |
| 1-chloro-3(RS)-ethylhexane | -242.8 | -243.0 | -265.0 | -278.2 | -284.7 | -286.0 | -286.3 | -284.6 | -280.5 |
| 2(RS)-chloro-3(RS)-ethylhexane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 3-chloro-3-ethylhexane | -267.5 | -267.7 | -288.5 | -300.0 | -304.8 | -305.3 | -304.9 | -301.9 | -296.6 |
| 3(RS)-chloro-4-ethylhexane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 2(RS)-chloro-4-ethylhexane | -255.1 | -255.3 | -276.9 | -289.3 | -294.8 | -295.6 | -295.4 | -292.6 | -287.6 |
| 1-chloro-4-ethylhexane | -242.8 | -243.0 | -265.0 | -278.2 | -284.7 | -286.0 | -286.3 | -284.6 | -280.5 |
| 1-chloro-2(RS)-ethyl-2-methylpentane | -251.4 | -251.7 | -272.9 | -284.8 | -290.1 | -290.9 | -290.8 | -288.4 | -283.9 |
| 1-chloro-2(RS)-isopropylpentane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 1-chloro-2(RS)-ethyl-4-methylpentane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 1-chloro-3(RS),4,4-trimethylpentane | -254.1 | -254.3 | -275.6 | -287.5 | -292.6 | -293.3 | -293.2 | -290.6 | -285.9 |
| 2(RS)-chloro-3(RS),4,4-trimethylpentane | -266.4 | -266.6 | -287.4 | -298.5 | -302.7 | -302.9 | -302.2 | -298.6 | -293.0 |
| 3-chloro-2,2,3(RS)-trimethylpentane | -278.8 | -279.1 | -299.0 | -309.3 | -312.7 | -312.7 | -311.8 | -307.9 | -302.0 |
| 1-chloro-2,2,3(RS)-trimethylpentane | -254.1 | -254.3 | -275.6 | -287.5 | -292.6 | -293.3 | -293.2 | -290.6 | -285.9 |
| 1-chloro-2(RS),4,4-trimethylpentane | -254.1 | -254.3 | -275.6 | -287.5 | -292.6 | -293.3 | -293.2 | -290.6 | -285.9 |
| 2-chloro-2,4,4-trimethylpentane | -278.8 | -279.1 | -299.0 | -309.3 | -312.7 | -312.7 | -311.8 | -307.9 | -302.0 |
| 3(RS)-chloro-2,2,4-trimethylpentane | -266.4 | -266.6 | -287.4 | -298.5 | -302.7 | -302.9 | -302.2 | -298.6 | -293.0 |
| 1-chloro-2,2,3-trimethylpentane | -254.1 | -254.3 | -275.6 | -287.5 | -292.6 | -293.3 | -293.2 | -290.6 | -285.9 |
| 1-chloro-3,3,4-trimethylpentane | -254.1 | -254.3 | -275.6 | -287.5 | -292.6 | -293.3 | -293.2 | -290.6 | -285.9 |
| 2(RS)-chloro-3,3,4-trimethylpentane | -266.4 | -266.6 | -287.4 | -298.5 | -302.7 | -302.9 | -302.2 | -298.6 | -293.0 |
| 2-chloro-2,3,3-trimethylpentane | -278.8 | -279.1 | -299.0 | -309.3 | -312.7 | -312.7 | -311.8 | -307.9 | -302.0 |
| 1-chloro-2(RS),3,3-trimethylpentane | -254.1 | -254.3 | -275.6 | -287.5 | -292.6 | -293.3 | -293.2 | -290.6 | -285.9 |
| 1-chloro-3-ethyl-3-methylpentane | -251.4 | -251.7 | -272.9 | -284.8 | -290.1 | -290.9 | -290.8 | -288.4 | -283.9 |
| 2(RS)-chloro-3-ethyl-3-methylpentane | -263.7 | -264.0 | -284.7 | -295.9 | -300.2 | -300.5 | -299.9 | -296.5 | -291.0 |
| 1-chloro-2(RS)-ethyl-3(RS)-methylpentane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 1-chloro-2(RS),3(RS),4-trimethylpentane | -251.5 | -251.7 | -273.8 | -286.8 | -293.0 | -294.2 | -294.3 | -292.3 | -287.8 |
| 2-chloro-2,3(RS),4-trimethylpentane | -276.2 | -276.4 | -297.2 | -308.6 | -313.1 | -313.5 | -313.0 | -309.6 | -303.9 |
| 3-chloro-2,3,4-trimethylpentane | -276.2 | -276.4 | -297.2 | -308.6 | -313.1 | -313.5 | -313.0 | -309.6 | -303.9 |
| 1-chloro-2-propylpentane | -242.8 | -243.0 | -265.0 | -278.2 | -284.7 | -286.0 | -286.3 | -284.6 | -280.5 |

Table 12. Standard enthalpy of formation for monochloroalkanes in kJ/mol -- continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 1-chloro-3(RS)-ethyl-4-methylpentane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 2(RS)-chloro-3(RS)-ethyl-4-methylpentane | -261.1 | -261.3 | -282.9 | -295.3 | -300.6 | -301.3 | -301.1 | -298.2 | -292.9 |
| 3-chloro-3-ethyl-2-methylpentane | -273.5 | -273.7 | -294.5 | -306.0 | -310.7 | -311.1 | -310.6 | -307.4 | -301.9 |
| 2-chloro-3-ethyl-2-methylpentane | -273.5 | -273.7 | -294.5 | -306.0 | -310.7 | -311.1 | -310.6 | -307.4 | -301.9 |
| 1-chloro-3-ethyl-2(RS)-methylpentane | -248.8 | -249.0 | -271.1 | -284.2 | -290.5 | -291.8 | -292.0 | -290.1 | -285.8 |
| 1-chloro-2(RS)-ethyl-3,3-dimethylbutane | -254.1 | -254.3 | -275.6 | -287.5 | -292.6 | -293.3 | -293.2 | -290.6 | -285.9 |
| 1-chloro-2(RS)-ethyl-2,3-dimethylbutane | -254.1 | -254.3 | -275.6 | -287.5 | -292.6 | -293.3 | -293.2 | -290.6 | -285.9 |
| 1-chloro-2,2-diethylbutane | -251.4 | -251.7 | -272.9 | -284.8 | -290.1 | -290.9 | -290.8 | -288.4 | -283.9 |
| 1-chloro-2,2,3,3-tetramethylbutane | -259.4 | -259.6 | -280.0 | -290.7 | -294.7 | -294.9 | -294.3 | -291.1 | -286.0 |
| 1-chloro-2-isopropyl-3-methylbutane | -251.5 | -251.7 | -273.8 | -286.8 | -293.0 | -294.2 | -294.3 | -292.3 | -287.8 |

Table 13. Standard Gibbs energy of formation for monochloroalkanes in kJ/mol

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| CH3Cl | | | | | | | | | |
| chloromethane | -60.15 | -60.00 | -42.72 | -23.64 | -3.69 | 6.46 | 16.67 | 37.23 | 57.85 |
| C2H5Cl | | | | | | | | | |
| chloroethane | -61.36 | -61.04 | -24.13 | 15.40 | 56.05 | 84.61 | 97.20 | 138.51 | 179.84 |
| C3H7Cl | | | | | | | | | |
| 1-chloropropane | -53.06 | -52.56 | 4.50 | 64.97 | 126.87 | 170.10 | 189.35 | 251.98 | 314.54 |
| 2-chloropropane | -62.49 | -61.97 | -3.10 | 58.96 | 122.17 | 165.98 | 185.74 | 249.27 | 312.59 |
| C4H9Cl | | | | | | | | | |
| 1-chlorobutane | -44.77 | -44.09 | 33.12 | 114.55 | 197.69 | 255.60 | 281.50 | 365.44 | 449.25 |
| 2(RS)-chlorobutane | -54.19 | -53.50 | 25.52 | 108.53 | 193.00 | 251.47 | 277.89 | 362.73 | 447.29 |
| 1-chloro-2-methylpropane | -50.79 | -50.09 | 29.38 | 113.07 | 198.43 | 257.43 | 284.43 | 370.53 | 456.47 |
| 2-chloro-2-methylpropane | -67.54 | -66.79 | 17.71 | 105.81 | 195.12 | 255.94 | 284.69 | 374.10 | 463.16 |
| C5H11Cl | | | | | | | | | |
| 1-chloropentane | -36.5 | -35.6 | 61.7 | 164.1 | 268.5 | 341.1 | 373.6 | 478.9 | 584.0 |
| 2(RS)-chloropentane | -45.9 | -45.0 | 54.1 | 158.1 | 263.8 | 337.0 | 370.0 | 476.2 | 582.0 |
| 3-chloropentane | -45.9 | -45.0 | 54.1 | 158.1 | 263.8 | 337.0 | 370.0 | 476.2 | 582.0 |
| 1-chloro-2(RS)-methylbutane | -39.1 | -38.3 | 61.3 | 166.0 | 272.6 | 346.3 | 379.9 | 487.3 | 594.5 |
| 2-chloro-2-methylbutane | -58.6 | -57.7 | 45.1 | 152.3 | 261.1 | 335.7 | 370.1 | 479.0 | 587.5 |
| 2(RS)-chloro-3-methylbutane | -48.6 | -47.7 | 53.8 | 160.0 | 267.9 | 342.1 | 376.3 | 484.6 | 592.6 |
| 1-chloro-3-methylbutane | -39.1 | -38.3 | 61.3 | 166.0 | 272.6 | 346.3 | 379.9 | 487.3 | 594.5 |
| 1-chloro-2,2-dimethylpropane | -46.5 | -45.6 | 59.2 | 168.6 | 279.6 | 355.3 | 391.0 | 502.5 | 613.5 |
| C6H13Cl | | | | | | | | | |
| 1-chlorohexane | -28.2 | -27.1 | 90.4 | 213.7 | 339.3 | 426.6 | 465.8 | 592.4 | 718.7 |
| 2(RS)-chlorohexane | -37.6 | -36.5 | 82.8 | 207.7 | 334.6 | 422.5 | 462.2 | 589.7 | 716.7 |
| 3(RS)-chlorohexane | -37.6 | -36.5 | 82.8 | 207.7 | 334.6 | 422.5 | 462.2 | 589.7 | 716.7 |
| 1-chloro-2(RS)-methylpentane | -30.9 | -29.8 | 90.0 | 215.6 | 343.4 | 431.8 | 472.1 | 600.8 | 729.2 |
| 2-chloro-2-methylpentane | -50.3 | -49.2 | 73.7 | 201.9 | 331.9 | 421.1 | 462.3 | 592.5 | 722.2 |
| 3(RS)-chloro-2-methylpentane | -40.3 | -39.2 | 82.4 | 209.5 | 338.7 | 427.6 | 468.5 | 598.1 | 727.3 |
| 2(RS)-chloro-4-methylpentane | -40.3 | -39.2 | 82.4 | 209.5 | 338.7 | 427.6 | 468.5 | 598.1 | 727.3 |
| 1-chloro-4-methylpentane | -30.9 | -29.8 | 90.0 | 215.6 | 343.4 | 431.8 | 472.1 | 600.8 | 729.2 |
| 1-chloro-3(RS)-methylpentane | -30.9 | -29.8 | 90.0 | 215.6 | 343.4 | 431.8 | 472.1 | 600.8 | 729.2 |
| 2(RS)-chloro-3(RS)-methylpentane | -40.3 | -39.2 | 82.4 | 209.5 | 338.7 | 427.6 | 468.5 | 598.1 | 727.3 |
| 3-chloro-3-methylpentane | -50.3 | -49.2 | 73.7 | 201.9 | 331.9 | 421.1 | 462.3 | 592.5 | 722.2 |
| 1-chloro-2(RS),3-dimethylbutane | -33.5 | -32.5 | 89.6 | 217.4 | 347.5 | 437.0 | 478.3 | 609.2 | 739.8 |
| 2-chloro-2,3-dimethylbutane | -53.0 | -51.9 | 73.3 | 203.8 | 336.0 | 426.3 | 468.6 | 600.9 | 732.8 |
| 1-chloro-2-ethylbutane | -30.9 | -29.8 | 90.0 | 215.6 | 343.4 | 431.8 | 472.1 | 600.8 | 729.2 |
| 1-chloro-2,2-dimethylbutane | -34.2 | -33.2 | 89.9 | 218.5 | 348.9 | 438.4 | 479.8 | 610.7 | 741.2 |
| 2(RS)-chloro-3,3-dimethylbutane | -41.0 | -39.8 | 86.9 | 218.8 | 352.4 | 443.4 | 486.3 | 619.9 | 753.0 |
| 1-chloro-3,3-dimethylbutane | -31.5 | -30.4 | 94.5 | 224.8 | 357.1 | 447.5 | 489.9 | 622.6 | 754.9 |
| C7H15Cl | | | | | | | | | |
| 1-chloroheptane | -19.9 | -18.7 | 119.0 | 263.3 | 410.2 | 512.1 | 557.9 | 705.8 | 853.4 |
| 2(RS)-chloroheptane | -29.3 | -28.1 | 111.4 | 257.3 | 405.5 | 507.9 | 554.3 | 703.1 | 851.4 |
| 3(RS)-chloroheptane | -29.3 | -28.1 | 111.4 | 257.3 | 405.5 | 507.9 | 554.3 | 703.1 | 851.4 |
| 4-chloroheptane | -29.3 | -28.1 | 111.4 | 257.3 | 405.5 | 507.9 | 554.3 | 703.1 | 851.4 |
| 1-chloro-5-methylhexane | -22.6 | -21.3 | 118.6 | 265.1 | 414.2 | 517.3 | 564.2 | 714.3 | 863.9 |
| 2(RS)-chloro-5-methylhexane | -32.0 | -30.7 | 111.0 | 259.1 | 409.5 | 513.1 | 560.6 | 711.6 | 862.0 |

Table 13. Standard Gibbs energy of formation for monochloroalkanes in kJ/mol -- continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 3(RS)-chloro-5-methylhexane | -32.0 | -30.7 | 111.0 | 259.1 | 409.5 | 513.1 | 560.6 | 711.6 | 862.0 |
| 3(RS)-chloro-2-methylhexane | -32.0 | -30.7 | 111.0 | 259.1 | 409.5 | 513.1 | 560.6 | 711.6 | 862.0 |
| 2-chloro-2-methylhexane | -42.0 | -40.8 | 102.4 | 251.5 | 402.7 | 506.6 | 554.4 | 706.0 | 856.9 |
| 1-chloro-2(RS)-methylhexane | -22.6 | -21.3 | 118.6 | 265.1 | 414.2 | 517.3 | 564.2 | 714.3 | 863.9 |
| 1-chloro-4(RS)-methylhexane | -22.6 | -21.3 | 118.6 | 265.1 | 414.2 | 517.3 | 564.2 | 714.3 | 863.9 |
| 2(RS)-chloro-4(RS)-methylhexane | -32.0 | -30.7 | 111.0 | 259.1 | 409.5 | 513.1 | 560.6 | 711.6 | 862.0 |
| 3(RS)-chloro-4(RS)-methylhexane | -32.0 | -30.7 | 111.0 | 259.1 | 409.5 | 513.1 | 560.6 | 711.6 | 862.0 |
| 3-chloro-3(RS)-methylhexane | -42.0 | -40.8 | 102.4 | 251.5 | 402.7 | 506.6 | 554.4 | 706.0 | 856.9 |
| 2(RS)-chloro-3(RS)-methylhexane | -32.0 | -30.7 | 111.0 | 259.1 | 409.5 | 513.1 | 560.6 | 711.6 | 862.0 |
| 1-chloro-3(RS)-methylhexane | -22.6 | -21.3 | 118.6 | 265.1 | 414.2 | 517.3 | 564.2 | 714.3 | 863.9 |
| 1-chloro-4,4-dimethylpentane | -23.2 | -21.9 | 123.1 | 274.4 | 427.9 | 533.0 | 582.0 | 736.1 | 889.7 |
| 2(RS)-chloro-4,4-dimethylpentane | -32.7 | -31.3 | 115.5 | 268.4 | 423.2 | 528.9 | 578.4 | 733.4 | 887.7 |
| 3(RS)-chloro-2,2-dimethylpentane | -32.7 | -31.3 | 115.5 | 268.4 | 423.2 | 528.9 | 578.4 | 733.4 | 887.7 |
| 1-chloro-2,2-dimethylpentane | -26.0 | -24.7 | 118.6 | 268.0 | 419.7 | 523.9 | 572.0 | 724.2 | 875.9 |
| 1-chloro-3,3-dimethylpentane | -26.0 | -24.7 | 118.6 | 268.0 | 419.7 | 523.9 | 572.0 | 724.2 | 875.9 |
| 2(RS)-chloro-3,3-dimethylpentane | -35.4 | -34.1 | 111.0 | 262.0 | 415.0 | 519.8 | 568.4 | 721.5 | 874.0 |
| 1-chloro-3(RS),4-dimethylpentane | -25.2 | -24.0 | 118.2 | 267.0 | 418.3 | 522.4 | 570.5 | 722.7 | 874.5 |
| 2(RS)-chloro-3(RS),4-dimethylpentane | -34.7 | -33.4 | 110.6 | 261.0 | 413.6 | 518.3 | 566.9 | 720.0 | 872.5 |
| 1-chloro-2(RS),3(RS)-dimethylpentane | -25.2 | -24.0 | 118.2 | 267.0 | 418.3 | 522.4 | 570.5 | 722.7 | 874.5 |
| 2-chloro-2,3(RS)-dimethylpentane | -44.7 | -43.4 | 102.0 | 253.4 | 406.8 | 511.8 | 560.7 | 714.4 | 867.5 |
| 3-chloro-2,3(RS)-dimethylpentane | -44.7 | -43.4 | 102.0 | 253.4 | 406.8 | 511.8 | 560.7 | 714.4 | 867.5 |
| 1-chloro-2(RS),4-dimethylpentane | -25.2 | -24.0 | 118.2 | 267.0 | 418.3 | 522.4 | 570.5 | 722.7 | 874.5 |
| 2-chloro-2,4-dimethylpentane | -44.7 | -43.4 | 102.0 | 253.4 | 406.8 | 511.8 | 560.7 | 714.4 | 867.5 |
| 3-chloro-2,4-dimethylpentane | -34.7 | -33.4 | 110.6 | 261.0 | 413.6 | 518.3 | 566.9 | 720.0 | 872.5 |
| 1-chloro-2(RS)-ethylpentane | -22.6 | -21.3 | 118.6 | 265.1 | 414.2 | 517.3 | 564.2 | 714.3 | 863.9 |
| 1-chloro-3-ethylpentane | -22.6 | -21.3 | 118.6 | 265.1 | 414.2 | 517.3 | 564.2 | 714.3 | 863.9 |
| 2(RS)-chloro-3-ethylpentane | -32.0 | -30.7 | 111.0 | 259.1 | 409.5 | 513.1 | 560.6 | 711.6 | 862.0 |
| 3-chloro-3-ethylpentane | -42.0 | -40.8 | 102.4 | 251.5 | 402.7 | 506.6 | 554.4 | 706.0 | 856.9 |
| 1-chloro-2-ethyl-2-methylbutane | -26.0 | -24.7 | 118.6 | 268.0 | 419.7 | 523.9 | 572.0 | 724.2 | 875.9 |
| 1-chloro-2(RS)-ethyl-3-methylbutane | -25.2 | -24.0 | 118.2 | 267.0 | 418.3 | 522.4 | 570.5 | 722.7 | 874.5 |
| 1-chloro-2(RS),3,3-trimethylbutane | -22.6 | -21.2 | 126.1 | 279.6 | 435.4 | 541.6 | 591.7 | 747.9 | 903.6 |
| 2-chloro-2,3,3-trimethylbutane | -42.0 | -40.7 | 109.9 | 266.0 | 423.8 | 530.9 | 581.9 | 739.6 | 896.6 |
| 1-chloro-2,2,3-trimethylbutane | -25.3 | -24.0 | 121.5 | 273.2 | 427.1 | 532.4 | 581.6 | 736.0 | 889.9 |
| C8H17Cl | | | | | | | | | |
| 1-chlorooctane | -11.6 | -10.2 | 147.6 | 312.8 | 481.0 | 597.6 | 650.1 | 819.3 | 988.1 |
| 2(RS)-chlorooctane | -21.0 | -19.6 | 140.0 | 306.8 | 476.3 | 593.4 | 646.5 | 816.6 | 986.1 |
| 3(RS)-chlorooctane | -21.0 | -19.6 | 140.0 | 306.8 | 476.3 | 593.4 | 646.5 | 816.6 | 986.1 |
| 4(RS)-chlorooctane | -21.0 | -19.6 | 140.0 | 306.8 | 476.3 | 593.4 | 646.5 | 816.6 | 986.1 |
| 1-chloro-2(RS)-methylheptane | -14.3 | -12.8 | 147.2 | 314.7 | 485.1 | 602.8 | 656.4 | 827.7 | 998.6 |
| 2-chloro-2-methylheptane | -33.7 | -32.3 | 131.0 | 301.1 | 473.5 | 592.1 | 646.6 | 819.4 | 991.6 |
| 3(RS)-chloro-2-methylheptane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 4(RS)-chloro-2-methylheptane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 3(RS)-chloro-6-methylheptane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 2(RS)-chloro-6-methylheptane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 1-chloro-6-methylheptane | -14.3 | -12.8 | 147.2 | 314.7 | 485.1 | 602.8 | 656.4 | 827.7 | 998.6 |
| 1-chloro-3(RS)-methylheptane | -14.3 | -12.8 | 147.2 | 314.7 | 485.1 | 602.8 | 656.4 | 827.7 | 998.6 |
| 2(RS)-chloro-3(RS)-methylheptane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 3-chloro-3(RS)-methylheptane | -33.7 | -32.3 | 131.0 | 301.1 | 473.5 | 592.1 | 646.6 | 819.4 | 991.6 |
| 4(RS)-chloro-3(RS)-methylheptane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 3(RS)-chloro-5(RS)-methylheptane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 2(RS)-chloro-5(RS)-methylheptane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 1-chloro-5(RS)-methylheptane | -14.3 | -12.8 | 147.2 | 314.7 | 485.1 | 602.8 | 656.4 | 827.7 | 998.6 |
| 1-chloro-4(RS)-methylheptane | -14.3 | -12.8 | 147.2 | 314.7 | 485.1 | 602.8 | 656.4 | 827.7 | 998.6 |
| 2(RS)-chloro-4(RS)-methylheptane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 3(RS)-chloro-4(RS)-methylheptane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 4-chloro-4-methylheptane | -33.7 | -32.3 | 131.0 | 301.1 | 473.5 | 592.1 | 646.6 | 819.4 | 991.6 |

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 1-chloro-2,2-dimethylhexane | -17.7 | -16.2 | 147.2 | 317.6 | 490.5 | 609.4 | 664.1 | 837.7 | 1010.7 |
| 3(RS)-chloro-2,2-dimethylhexane | -24.4 | -22.9 | 144.2 | 318.0 | 494.0 | 614.4 | 670.6 | 846.8 | 1022.4 |
| 3(RS)-chloro-5,5-dimethylhexane | -24.4 | -22.9 | 144.2 | 318.0 | 494.0 | 614.4 | 670.6 | 846.8 | 1022.4 |
| 2(RS)-chloro-5,5-dimethylhexane | -24.4 | -22.9 | 144.2 | 318.0 | 494.0 | 614.4 | 670.6 | 846.8 | 1022.4 |
| 1-chloro-5,5-dimethylhexane | -14.9 | -13.5 | 151.8 | 324.0 | 498.7 | 618.5 | 674.2 | 849.5 | 1024.4 |
| 1-chloro-3,3-dimethylhexane | -17.7 | -16.2 | 147.2 | 317.6 | 490.5 | 609.4 | 664.1 | 837.7 | 1010.7 |
| 2(RS)-chloro-3,3-dimethylhexane | -27.1 | -25.6 | 139.6 | 311.6 | 485.8 | 605.3 | 660.5 | 835.0 | 1008.7 |
| 3(RS)-chloro-4,4-dimethylhexane | -27.1 | -25.6 | 139.6 | 311.6 | 485.8 | 605.3 | 660.5 | 835.0 | 1008.7 |
| 2(RS)-chloro-4,4-dimethylhexane | -27.1 | -25.6 | 139.6 | 311.6 | 485.8 | 605.3 | 660.5 | 835.0 | 1008.7 |
| 1-chloro-4,4-dimethylhexane | -17.7 | -16.2 | 147.2 | 317.6 | 490.5 | 609.4 | 664.1 | 837.7 | 1010.7 |
| 1-chloro-4(RS),5-dimethylhexane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 2(RS)-chloro-4(RS),5-dimethylhexane | -26.4 | -24.9 | 139.2 | 310.6 | 484.5 | 603.8 | 659.0 | 833.5 | 1007.2 |
| 3(RS)-chloro-4(RS),5-dimethylhexane | -26.4 | -24.9 | 139.2 | 310.6 | 484.5 | 603.8 | 659.0 | 833.5 | 1007.2 |
| 3(RS)-chloro-2,3-dimethylhexane | -36.4 | -34.9 | 130.6 | 302.9 | 477.6 | 597.3 | 652.9 | 827.9 | 1002.2 |
| 2-chloro-2,3(RS)-dimethylhexane | -36.4 | -34.9 | 130.6 | 302.9 | 477.6 | 597.3 | 652.9 | 827.9 | 1002.2 |
| 1-chloro-2(RS),3(RS)-dimethylhexane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 1-chloro-3(RS),5-dimethylhexane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 2(RS)-chloro-3(RS),5-dimethylhexane | -26.4 | -24.9 | 139.2 | 310.6 | 484.5 | 603.8 | 659.0 | 833.5 | 1007.2 |
| 3-chloro-3(RS),5-dimethylhexane | -36.4 | -34.9 | 130.6 | 302.9 | 477.6 | 597.3 | 652.9 | 827.9 | 1002.2 |
| 3(RS)-chloro-2,4(RS)-dimethylhexane | -26.4 | -24.9 | 139.2 | 310.6 | 484.5 | 603.8 | 659.0 | 833.5 | 1007.2 |
| 2-chloro-2,4(RS)-dimethylhexane | -36.4 | -34.9 | 130.6 | 302.9 | 477.6 | 597.3 | 652.9 | 827.9 | 1002.2 |
| 1-chloro-2(RS),4(RS)-dimethylhexane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 1-chloro-2(RS),5-dimethylhexane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 2-chloro-2,5-dimethylhexane | -36.4 | -34.9 | 130.6 | 302.9 | 477.6 | 597.3 | 652.9 | 827.9 | 1002.2 |
| 3(RS)-chloro-2,5-dimethylhexane | -26.4 | -24.9 | 139.2 | 310.6 | 484.5 | 603.8 | 659.0 | 833.5 | 1007.2 |
| 1-chloro-3(RS),4(RS)-dimethylhexane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 2(RS)-chloro-3(RS),4(RS)-dimethylhexane | -26.4 | -24.9 | 139.2 | 310.6 | 484.5 | 603.8 | 659.0 | 833.5 | 1007.2 |
| 3-chloro-3(RS),4(RS)-dimethylhexane | -36.4 | -34.9 | 130.6 | 302.9 | 477.6 | 597.3 | 652.9 | 827.9 | 1002.2 |
| 1-chloro-2(RS)-ethylhexane | -14.3 | -12.8 | 147.2 | 314.7 | 485.1 | 602.8 | 656.4 | 827.7 | 998.6 |
| 1-chloro-3(RS)-ethylhexane | -14.3 | -12.8 | 147.2 | 314.7 | 485.1 | 602.8 | 656.4 | 827.7 | 998.6 |
| 2(RS)-chloro-3(RS)-ethylhexane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 3-chloro-3-ethylhexane | -33.7 | -32.3 | 131.0 | 301.1 | 473.5 | 592.1 | 646.6 | 819.4 | 991.6 |
| 3(RS)-chloro-4-ethylhexane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 2(RS)-chloro-4-ethylhexane | -23.7 | -22.3 | 139.6 | 308.7 | 480.4 | 598.6 | 652.8 | 825.0 | 996.7 |
| 1-chloro-4-ethylhexane | -14.3 | -12.8 | 147.2 | 314.7 | 485.1 | 602.8 | 656.4 | 827.7 | 998.6 |
| 1-chloro-2(RS)-ethyl-2-methylpentane | -17.7 | -16.2 | 147.2 | 317.6 | 490.5 | 609.4 | 664.1 | 837.7 | 1010.7 |
| 1-chloro-2(RS)-isopropylpentane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 1-chloro-2(RS)-ethyl-4-methylpentane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 1-chloro-3(RS),4,4-trimethylpentane | -14.3 | -12.8 | 154.7 | 329.2 | 506.2 | 627.1 | 683.8 | 861.3 | 1038.3 |
| 2(RS)-chloro-3(RS),4,4-trimethylpentane | -23.7 | -22.2 | 147.1 | 323.2 | 501.5 | 622.9 | 680.2 | 858.6 | 1036.3 |
| 3-chloro-2,2,3(RS)-trimethylpentane | -33.7 | -32.2 | 138.5 | 315.6 | 494.6 | 616.4 | 674.0 | 853.0 | 1031.3 |
| 1-chloro-2,2,3(RS)-trimethylpentane | -17.0 | -15.5 | 150.1 | 322.8 | 498.0 | 617.9 | 673.8 | 849.4 | 1024.6 |
| 1-chloro-2(RS),4,4-trimethylpentane | -14.3 | -12.8 | 154.7 | 329.2 | 506.2 | 627.1 | 683.8 | 861.3 | 1038.3 |
| 2-chloro-2,4,4-trimethylpentane | -33.7 | -32.2 | 138.5 | 315.6 | 494.6 | 616.4 | 674.0 | 853.0 | 1031.3 |
| 3(RS)-chloro-2,2,4-trimethylpentane | -23.7 | -22.2 | 147.1 | 323.2 | 501.5 | 622.9 | 680.2 | 858.6 | 1036.3 |
| 1-chloro-2,2,3-trimethylpentane | -17.0 | -15.5 | 150.1 | 322.8 | 498.0 | 617.9 | 673.8 | 849.4 | 1024.6 |
| 1-chloro-3,3,4-trimethylpentane | -17.0 | -15.5 | 150.1 | 322.8 | 498.0 | 617.9 | 673.8 | 849.4 | 1024.6 |
| 2(RS)-chloro-3,3,4-trimethylpentane | -26.4 | -24.9 | 142.6 | 316.8 | 493.3 | 613.8 | 670.2 | 846.7 | 1022.6 |
| 2-chloro-2,3,3-trimethylpentane | -36.5 | -35.0 | 133.9 | 309.2 | 486.4 | 607.3 | 664.0 | 841.1 | 1017.6 |
| 1-chloro-2(RS),3,3-trimethylpentane | -17.0 | -15.5 | 150.1 | 322.8 | 498.0 | 617.9 | 673.8 | 849.4 | 1024.6 |
| 1-chloro-3-ethyl-3-methylpentane | -17.7 | -16.2 | 147.2 | 317.6 | 490.5 | 609.4 | 664.1 | 837.7 | 1010.7 |
| 2(RS)-chloro-3-ethyl-3-methylpentane | -27.1 | -25.6 | 139.6 | 311.6 | 485.8 | 605.3 | 660.5 | 835.0 | 1008.7 |
| 1-chloro-2(RS)-ethyl-3(RS)-methylpentane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 1-chloro-2(RS),3(RS),4-trimethylpentane | -16.3 | -14.8 | 149.8 | 321.8 | 496.6 | 616.5 | 672.3 | 847.9 | 1023.1 |
| 2-chloro-2,3(RS),4-trimethylpentane | -35.7 | -34.3 | 133.5 | 308.1 | 485.0 | 605.8 | 662.5 | 839.6 | 1016.1 |
| 3-chloro-2,3,4-trimethylpentane | -35.7 | -34.3 | 133.5 | 308.1 | 485.0 | 605.8 | 662.5 | 839.6 | 1016.1 |
| 1-chloro-2-propylpentane | -14.3 | -12.8 | 147.2 | 314.7 | 485.1 | 602.8 | 656.4 | 827.7 | 998.6 |

Table 13. Standard Gibbs energy of formation for monochloroalkanes in kJ/mol -- continued

| T/K | 298.15 | 300 | 500 | 700 | 900 | 1000 | 1100 | 1300 | 1500 |
|---|---|---|---|---|---|---|---|---|---|
| 1-chloro-3(RS)-ethyl-4-methylpentane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 2(RS)-chloro-3(RS)-ethyl-4-methylpentane | -26.4 | -24.9 | 139.2 | 310.6 | 484.5 | 603.8 | 659.0 | 833.5 | 1007.2 |
| 3-chloro-3-ethyl-2-methylpentane | -36.4 | -34.9 | 130.6 | 302.9 | 477.6 | 597.3 | 652.9 | 827.9 | 1002.2 |
| 2-chloro-3-ethyl-2-methylpentane | -36.4 | -34.9 | 130.6 | 302.9 | 477.6 | 597.3 | 652.9 | 827.9 | 1002.2 |
| 1-chloro-3-ethyl-2(RS)-methylpentane | -16.9 | -15.5 | 146.8 | 316.6 | 489.2 | 607.9 | 662.7 | 836.2 | 1009.2 |
| 1-chloro-2(RS)-ethyl-3,3-dimethylbutane | -14.3 | -12.8 | 154.7 | 329.2 | 506.2 | 627.1 | 683.8 | 861.3 | 1038.3 |
| 1-chloro-2(RS)-ethyl-2,3-dimethylbutane | -17.0 | -15.5 | 150.1 | 322.8 | 498.0 | 617.9 | 673.8 | 849.4 | 1024.6 |
| 1-chloro-2,2-diethylbutane | -17.7 | -16.2 | 147.2 | 317.6 | 490.5 | 609.4 | 664.1 | 837.7 | 1010.7 |
| 1-chloro-2,2,3,3-tetramethylbutane | -14.3 | -12.8 | 158.0 | 335.5 | 515.0 | 637.0 | 694.9 | 874.6 | 1053.6 |
| 1-chloro-2-isopropyl-3-methylbutane | -16.3 | -14.8 | 149.8 | 321.8 | 496.6 | 616.5 | 672.3 | 847.9 | 1023.1 |

Table 14. Log K for the formation of a monochloroalkane isomer group from an alkene isomer group and hydrogen chloride (reaction 4)

| T/K | C2H5Cl | C3H7Cl | C4H9Cl | C5H11Cl | C6H13Cl | C7H15Cl | C8H17Cl |
|---|---|---|---|---|---|---|---|
| 298.15 | 5.992 | 5.261 | 5.256 | 4.017 | 3.702 | 3.939 | 3.833 |
| 300.00 | 5.919 | 5.179 | 5.169 | 3.940 | 3.623 | 3.861 | 3.755 |
| 500.00 | .789 | .062 | -.393 | -.938 | -1.256 | -1.056 | -1.160 |
| 700.00 | -1.431 | -2.071 | -2.590 | -2.883 | -3.210 | -3.041 | -3.146 |
| 900.00 | -2.661 | -3.211 | -3.680 | -3.888 | -4.209 | -4.065 | -4.171 |
| 1000.00 | -3.505 | -4.225 | -4.876 | -5.272 | -5.796 | -5.875 | -6.189 |

## 7. Discussion

The increments in isomer group values per $CH_2$ were found to be sufficiently constant so that the thermodynamic properties of isomer group $C_9H_{19}Cl$ and above may be estimated by linear extrapolation.

The values of standard thermodynamic properties of isomer groups given here may be used in predicting equilibrium compositions of organic systems at temperature-catalyst conditions where species in an isomer group are in equilibrium. This is illustrated by Table 14 which gives log $K$ for the gas reaction.

$$C_nH_{2n}\ \text{(alkene isomer group)} + HCl = C_nH_{2n+1}Cl\ \text{(monochloroalkane isomer group)} \quad (4)$$

where the reference pressure is 1 bar and ideality is assumed. There is significant dependence of the equilibrium constant for this reaction on carbon number. The values of $\Delta_f G°(I)$ for the alkene isomer groups are from Alberty and Gehrig[4], and the values of $\Delta_f G°$ for HCl(g) are from Chase, et al.[23]

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## 9. Nomenclature and Units

$C_{pi}°$ = standard heat capacity at constant pressure of isomer $i$, J $K^{-1}$ $mol^{-1}$

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

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

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

$H°(I,T)-H°(I,298.15\ K)$ = standard enthalpy for isomer groups relative to isomer groups at 298.15 K, kJ $mol^{-1}$

$H°(I,T)-H°(I,298.15\ K)+\Delta_f H°(I,298.15\ K)$ = standard enthalpy of formation for isomer groups relative to elements at 298.15 K, kJ $mol^{-1}$

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

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

$n$ = number of carbon atoms in a molecule

$N_I$ = number of isomers in an isomer group

OPT = number of optical isomers

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

$S_i°$ = standard entropy of isomer $i$, J $K^{-1}$ $mol^{-1}$

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

TSN = total symmetry number

$y_i$ = mole fraction of isomer $i$ within the isomer group

$y_I$ = mole fraction of isomer group I in a mixture

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