

Standard Chemical Thermodynamic Properties of Alkylcyclopentane Isomer Groups, Alkylcyclohexane Isomer Groups, and Combined Isomer Groups

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The standard chemical thermodynamic properties of the alkylcyclopentane isomer groups have been calculated through C_9H_{18} in the ideal gas phase from 298.15 to 1000 K, and the properties of the alkylcyclohexane isomer groups have been calculated through $C_{10}H_{20}$. The properties of individual species for which literature data are not available have been estimated using the Benson method. The increments per carbon atom in the isomer group properties have been calculated to determine the extent to which extrapolations may be made to higher carbon numbers. Since alkylcyclopentanes and alkylcyclohexanes of the same carbon number are isomers, the chemical thermodynamic properties of these combined isomer groups have also been calculated. Values of C_p° , S° , $\Delta_f H^\circ$, and $\Delta_f G^\circ$ are given for the individual cyclopentane species through C_9H_{18} and for the individual cyclohexane species through $C_{10}H_{20}$ for a standard state pressure of 1 bar.

Key words: alkylcyclopentanes; alkylcyclohexanes; 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

In making equilibrium calculations on organic systems involving many isomers, it is advantageous to reduce the number of components by dealing with the recommendation of B. D. Smith.¹ Then in a second step of the calculation the equilibrium mole fraction of each isomer group may be distributed to the individual molecular species, if their standard Gibbs energies of formation are known. As the carbon number in a homologous series increases, the number of isomers increases so rapidly that it is useful to have tables of standard thermodynamic properties of isomer groups.

Earlier papers in this series have provided tables of isomer group properties of alkanes² through C₁₀H₂₂, alkylbenzenes³ through C₁₂H₁₈, and alkenes⁴ through C₈H₁₆. This article provides tables for alkylcyclopentanes through C₉H₁₈, alkylcyclohexanes through C₁₀H₂₀, and tables for combined alkylcyclopentane-alkylcyclohexane isomer groups. Table 1 gives the numbers of isomers and indicates the numbers of these isomers for which thermodynamic properties are known.

The properties for the cyclopentanes through C₇H₁₄

and the properties of the cyclohexanes through C₈H₁₆ were published by Rossini *et al.*,⁶ and small changes were made by Stull, Westrum, and Sinke.⁵ Values for some of the higher cyclopentanes and cyclohexanes had been calculated by Kilpatrick *et al.*,⁷ but calculations were not made for all members of these higher isomer groups. Therefore, we have used the Benson group method⁸ to estimate the thermodynamic properties of C₈H₁₆ and C₉H₁₈ cyclopentanes and C₉H₁₈ and C₁₀H₂₀ cyclohexanes. Since the numbers of isomers increase geometrically with carbon number, considerable work would be required to extend these calculations to higher carbon numbers. However, the calculations described here indicate that linear extrapolations may be used to obtain estimates of standard thermodynamic properties of isomer groups at higher carbon numbers.

2. Calculation of Standard Thermodynamic Properties of Alkylcyclopentane and Alkylcyclohexane Isomer Groups

The derivations of the equations for the standard Gibbs energy of formation $\Delta_f G^\circ(\text{I})$ for an isomer group and the equilibrium mole fraction r_i of various isomers in the group have been reviewed by Smith and Missen.⁹ These equations are

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

$$r_i = \frac{y_i}{y_I} = \exp \left\{ \left[\Delta_f G^\circ(\text{I}) - \Delta_f G_i^\circ \right] / RT \right\}, \quad (2)$$

where $\Delta_f G_i^\circ$ is the standard Gibbs energy of formation of an individual isomer, N_I is the number of isomers in the group, including stereoisomers, y_i is the equilibrium mole fraction of isomer i in a reaction mixture, and y_I is the equilibrium mole fraction of the isomer group. The expressions for $\Delta_f H^\circ(\text{I})$, $S^\circ(\text{I})$, and $C_p^\circ(\text{I})$ were derived by Alberty.¹⁰ For the

TABLE 1. Numbers of isomers

	Alkylcyclopentanes		Alkylcyclohexanes	
	Structures ^a	Stereoisomers	Structures ^a	Stereoisomers
C ₅ H ₁₀	1(1)	1		
C ₆ H ₁₂	1(1)	1	1(1)	1
C ₇ H ₁₄	6(6)	8	1(1)	1
C ₈ H ₁₆	13(1)	19	8(8)	10
C ₉ H ₁₈	44(1) ^b	75	19(3)	31
C ₁₀ H ₂₀			89(1) ^c	148

^aThe number of tables in Stull, Westrum, and Sinke (Ref. 5) is given in parentheses.

^bData on 1-cyclopentyl-*n*-alkanes are given up to C₂₁H₄₂.

^cData on 1-cyclohexyl-*n*-alkanes are given up to C₂₂H₄₄.

alkylcyclopentanes and alkylcyclohexanes the standard chemical thermodynamic properties for an isomer group are interrelated by

$$\Delta_f G^\circ(\text{I}) = \Delta_f H^\circ(\text{I}) - T [S^\circ(\text{I}) - nS_{\text{graphite}}^\circ - nS_{\text{H}_2}^\circ(\text{g})], \quad (3)$$

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. Rather than having a line in a thermodynamic table for each stereoisomer, this article follows the standard practice of giving properties of racemates. Thus $R \ln 2$ is added to the calculated standard entropy and $RT \ln 2$ is subtracted from the standard Gibbs energy of formation of one of the chiral forms at each temperature.

Since the International Union of Pure and Applied Chemistry has recommended that thermodynamic data be given in SI units for a standard state pressure of 1 bar (10^5 Pa), this has been done for the tables in this article. The change in standard state pressure from 1 atm to 1 bar does not affect C_p° and $\Delta_f H^\circ$, but the standard entropy of an ideal gas is increased by $R \ln(1.01325) = 0.109 \text{ J K}^{-1} \text{ mol}^{-1}$ at any temperature and the standard Gibbs energy of formation is reduced by $[RT \ln(1.01325)]\delta$, where δ is the net increase ($1 - n$) in moles of gas in the formation reaction.¹¹

3. Estimation of Thermodynamic Properties of Alkylcyclopentanes and Alkylcyclohexanes Using the Benson Group Method

The alkylcyclopentanes and alkylcyclohexanes involve the C-(H)₃(C), C-(H)₂(C)₂, C-(H)(C)₃, and C-(C)₄ groups, ring corrections, *cis* corrections, and alkane *gauche* corrections.^{8,12,13} *Cis* corrections were applied to cyclopentanes because the rings were assumed to be planar, but they were not applied to the alkylcyclohexanes because the rings were assumed to have the chair conformation.

The calculation of alkane *gauche* corrections for alkylcyclohexanes has been discussed by O'Neal and Benson.¹³ They point out that in *trans*-1,4-dimethylcyclohexane the methyl groups can both be equatorial (the low-energy form) or both axial, when the ring is in the chair form; therefore, the methyl groups are both assumed to be axial. However, in *cis*-1,4-dimethylcyclohexane there must always be one axial methyl group. The difference between $\Delta_f H^\circ(298)$ for *cis* and *trans*-1,4-dimethylcyclohexane confirms the value of the alkane *gauche* correction of 3.35 kJ mol^{-1} determined from other homologous series. Since an axial methyl group has a *gauche* interaction with each of the two next nearest ring carbon atoms, *cis*-1,4-dimethylcyclohexane is expected to be $2 \times 3.35 = 6.70 \text{ kJ mol}^{-1}$ less stable than the *trans* isomer; the difference in $\Delta_f H^\circ$ obtained experimentally is 7.95 kJ mol^{-1} . The numbers of alkane *gauche* interactions for the C₈H₁₆, C₉H₁₈, and C₁₀H₂₀ alkylcyclohexanes were determined by examining each structure.

Total symmetry numbers were determined following procedures described by Davies, Syverud, and Steiner,¹⁴ assuming the cyclopentane ring is flat, and the cyclohexane

ring is in the chair form. Thus the total symmetry numbers of the alkylcyclohexanes are determined entirely by the number of methyl groups. Chiral substances were identified by ascertaining that they are not superimposable on their mirror images. The computer programs used in making the Benson calculations are described in the first paper in this series.²

The numbers of various groups, non-next-nearest neighbor corrections, ring corrections, total symmetry numbers, and numbers of optical isomers for all molecular species in an isomer group were arranged in a matrix. As a check this matrix was multiplied by a matrix with columns giving the numbers of carbon atoms and hydrogen atoms associated with the Benson groups. Since this multiplication yields the numbers of carbon and hydrogen atoms in each molecule, it provides a check of the self-consistency of the assignments.

Table 2 provides a comparison between the chemical thermodynamic properties of the alkylcyclopentanes calculated using the Benson method⁸ and those in Stull, Westrum, and Sinke.⁵ The differences between the literature and estimated values at each temperature were squared, divided by the number of pairs of values, and the square root was taken. The root-mean-square deviations are less than about $1 \text{ J K}^{-1} \text{ mol}^{-1}$ for the heat capacity, $5 \text{ J K}^{-1} \text{ mol}^{-1}$ for the entropy, 1 kJ mol^{-1} for the enthalpy, and 3 kJ mol^{-1} for the Gibbs energy. This is a little better fit than for the alkenes⁴ and not quite as good as for the alkylbenzenes.³ Table 10 provides the same comparison for the alkylcyclohexanes. The root-mean-square deviations are less than about $1.5 \text{ J K}^{-1} \text{ mol}^{-1}$ for the heat capacity, $1 \text{ J K}^{-1} \text{ mol}^{-1}$ for the entropy, 0.6 kJ mol^{-1} for the enthalpy, and 0.7 kJ mol^{-1} for the Gibbs energy. Thus the fit is better than for the alkylcyclopentanes.

4. Calculation of Standard Thermodynamic Properties for Alkylcyclopentane and Alkylcyclohexane Isomer Groups

The equations and procedures for calculating the various standard thermodynamic properties of isomer groups are described in the first paper in this series. The standard thermodynamic properties of the alkylcyclopentane isomer groups through C₉H₁₈ are given in Tables 3–8 in joules for a standard state pressure of 1 bar in the ideal gas state. The values calculated using the Benson method have been used to calculate the isomer group properties because of the excellent fit of the literature data. The increments in the isomer group properties per carbon atom have been included in these tables to guide extrapolations to higher carbon numbers.

Table 9 gives the equilibrium mole fractions r_i of the individual species within the alkylcyclopentane isomer groups. The names of the substances follow IUPAC recommendations,¹⁵ except that the RS designations have not been used since they are very complicated to determine for these molecules. Instead chiral molecules are indicated with asterisks. Some of the calculated equilibrium mole fractions are given to more significant figures than warranted by the accu-

racy of the $\Delta_f G_i^\circ$ values, but the tables are easier to read when they are printed this way, rather than in exponential notation.

Tables 11–16 give the isomer group properties for the alkylcyclohexanes through $C_{10}H_{20}$. The values calculated using the Benson method have been used to calculate the isomer group properties because of the excellent fit of the literature data. The fact that the increments approach constant values as the carbon number increases indicates that they are useful for extrapolations.

Table 17 gives the calculated equilibrium mole fractions r_i of the individual species within the alkylcyclohexane isomer groups.

5. Calculation of Standard Thermodynamic Properties for Combined Isomer Groups of Alkylcyclopentanes and Alkylcyclohexanes

Since alkylcyclopentanes and alkylcyclohexanes of the same carbon number are isomers, the equilibrium mole fractions of individual species in this combined group are a function only of temperature for the ideal gas state. Therefore, the standard Gibbs energy of formation of the combined isomer group can be calculated by extending the summation in Eq. (1) over species in both isomer groups if the standard Gibbs energy of formation of all the species are known. This method also allows the calculation of combined isomer group thermodynamic properties through C_9H_{18} by using appropriate equations for $C_p^\circ(I)$, $S^\circ(I)$, and $\Delta_f H^\circ(I)$. In order to calculate the thermodynamic properties of the $C_{10}H_{20}$ combined isomer group it was necessary to estimate the properties of the $C_{10}H_{20}$ alkylcyclopentane isomer group by adding the C_9 – C_8 increment to the values of the C_9H_{18} isomer group. The standard Gibbs energy of the $C_{10}H_{20}$ combined isomer group was calculated using

$$\Delta_f G^\circ(I) = -RT \ln \{ \exp [-\Delta_f G^\circ(C_{10}H_{20}, \text{cyclopent})] / RT + \sum_{i=1}^{N_i} \exp [-\Delta_f G_i^\circ(C_{10}H_{20}, \text{cyclohex}) / RT] \}, \quad (4)$$

where $\Delta_f G^\circ(C_{10}H_{20}, \text{cyclopent})$ is the estimated value for the $C_{10}H_{20}$ cyclopentane isomer group. Tables 18–23 give the standard thermodynamic properties of the combined isomer groups.

The calculated equilibrium mole fractions within the combined isomer groups are given in Table 24. Note that under the $C_{10}H_{20}$ combined isomer group mole fractions, the alkylcyclopentanes are grouped together as one isomer group because $\Delta_f G_i^\circ$ of individual species are not known. These are the equilibrium mole fractions that would be expected using a catalyst that equilibrates alkylcyclopentanes with alkylcyclohexanes of the same carbon number.

In the combined isomer group, the cyclohexanes predominate at high temperatures.

6. Standard Thermodynamic Properties of Individual Alkylcyclopentanes and Alkylcyclohexanes

The values of C_p° , S° , $\Delta_f H^\circ$, and $\Delta_f G^\circ$ in the ideal gas state for all the alkylcyclopentane species through C_9H_{18} are given in Tables 25–28 in joules for a standard state pressure of 1 bar. The values for all the alkylcyclohexane species through $C_{10}H_{20}$ are given in Tables 29–32. The values for chiral forms, indicated by asterisks, are for the racemates.

7. Discussion

For both the alkylcyclopentanes and alkylcyclohexanes the differences in enthalpy between isomers is greater than the differences in entropy so that the equilibrium mole fractions are more nearly equal at high temperatures.

The tables for the combined alkylcyclopentane and alkylcyclohexane isomer group are of interest under conditions where these isomer groups are equilibrated. To a first approximation this seems to be the case in the zeolite ZSM-5 conversion of methanol to gasoline.^{16,17} The alkenes are also isomers of the cyclopentanes and cyclohexanes of the same carbon number and could be included in combined tables.

8. Nomenclature

C_{Pi}°	= standard heat capacity at constant pressure of isomer i , $J K^{-1} mol^{-1}$
$C_p^\circ(I)$	= standard heat capacity at constant pressure of isomer group I, $J K^{-1} mol^{-1}$
$\Delta_f G_i^\circ$	= standard Gibbs energy of formation of isomer i , $kJ mol^{-1}$
$\Delta_f G^\circ(I)$	= standard Gibbs energy of formation of isomer group I, $kJ mol^{-1}$
$H^\circ(I, T) - H^\circ(I, 298.15 K)$	= standard enthalpy for isomer groups relative to isomer groups at 298.15 K, $kJ mol^{-1}$
$H^\circ(I, T) - H^\circ(I, 298.15 K) + \Delta_f H^\circ(I, 298.15 K)$	= standard enthalpy for isomer groups relative to elements at 298.15 K, $kJ mol^{-1}$
$\Delta_f H_i^\circ$	= standard enthalpy of formation of isomer i , $kJ mol^{-1}$
$\Delta_f H^\circ(I)$	= standard enthalpy of formation of isomer group I, $kJ mol^{-1}$
n	= 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 , $J K^{-1} mol^{-1}$
$S^\circ(I)$	= 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

Table 2. Root mean square deviations between alkylcyclopentane thermodynamic properties from Stull, Westrum, and Sinke and from the Benson method

T/K	298	300	400	500	600	700	800	900	1000
Standard heat capacity at constant pressure in J/K mol									
C5H10	1.15	1.36	.94	1.16	1.39	.98	.87	1.07	.97
C6H12	.41	1.02	1.05	.27	.74	.89	.32	.32	.63
C7H14	.36	.07	.45	.22	.12	.50	.24	.66	.93
Standard entropy in J/K mol									
C5H10	2.22	.10	.43	4.33	6.67	.45	1.71	1.27	.33
C6H12	.47	2.88	.41	.53	3.05	.53	1.60	5.31	.62
C7H14	.75	4.53	.66	.66	3.16	.69	.66	3.20	.74
Standard enthalpy of formation in kJ/mol									
C5H10	.11	.98	.54	.11	.97	.54	.22	.85	.60
C6H12	.27	.75	.67	.31	.66	.75	.34	.61	.81
C7H14	.37	.59	.85	.40	.59	.89	.41	.55	.92
Standard Gibbs energy of formation in kJ/mol									
C5H10	.55	1.01	.57	1.41	2.98	.57	.47	1.36	.57
C6H12	.04	2.19	.56	.01	2.49	.54	1.46	4.32	.51
C7H14	.97	4.22	.48	.19	3.43	.45	.26	3.75	.43

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

T/K	C5H10	C6H12	C7H14	C8H16	C9H18
298.15	87.81	104.09	135.99	163.13	230.43
300.00	88.47	104.90	136.90	164.21	231.61
400.00	122.36	146.63	183.95	219.93	281.81
500.00	152.62	183.75	226.09	268.47	320.18
600.00	179.24	216.27	262.80	309.39	356.74
700.00	202.23	244.19	294.09	343.61	390.66
800.00	221.58	267.50	320.04	371.77	420.23
900.00	237.30	286.22	340.76	394.16	444.45
1000.00	249.38	300.33	356.28	410.88	462.82

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8
298.15	16.28	31.90	27.14	67.29
300.00	16.43	31.99	27.31	67.40
400.00	24.26	37.32	35.99	61.88
500.00	31.13	42.34	42.37	51.72
600.00	37.03	46.53	46.59	47.35
700.00	41.96	49.90	49.53	47.05
800.00	45.92	52.54	51.73	48.46
900.00	48.92	54.54	53.41	50.29
1000.00	50.95	55.95	54.59	51.95

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

T/K	C5H10	C6H12	C7H14	C8H16	C9H18
298.15	292.25	339.59	378.43	413.20	438.13
300.00	292.80	340.23	379.28	414.21	439.56
400.00	322.98	376.24	425.21	469.22	513.62
500.00	353.60	413.03	470.88	523.66	580.69
600.00	383.84	449.47	515.43	576.33	642.32
700.00	413.24	484.97	558.36	626.68	699.91
800.00	441.55	519.15	599.38	674.46	754.06
900.00	468.59	551.78	638.32	719.60	805.01
1000.00	494.25	582.71	675.07	762.05	852.84

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8
298.15	47.33	38.85	34.77	24.93
300.00	47.43	39.05	34.94	25.34
400.00	53.26	48.97	44.02	41.40
500.00	59.43	57.85	52.78	57.03
600.00	65.64	65.95	60.91	65.99
700.00	71.73	73.39	68.32	73.23
800.00	77.60	80.23	75.08	79.59
900.00	83.19	86.54	81.28	85.40
1000.00	88.46	92.37	86.97	90.79

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

T/K	C5H10	C6H12	C7H14	C8H16	C9H18
298.15	-76.78	-102.59	-136.95	-164.14	-195.31
300.00	-76.97	-102.83	-137.20	-164.41	-195.52
400.00	-86.08	-113.83	-148.68	-176.65	-205.09
500.00	-93.58	-122.81	-157.92	-186.21	-213.26
600.00	-99.51	-129.83	-165.00	-193.34	-219.99
700.00	-103.94	-135.01	-170.06	-198.29	-224.96
800.00	-107.11	-138.66	-173.46	-201.50	-228.28
900.00	-109.20	-141.01	-175.47	-203.26	-230.11
1000.00	-110.42	-142.35	-176.39	-203.89	-230.75

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8
298.15	-25.82	-34.36	-27.19	-31.17
300.00	-25.86	-34.37	-27.21	-31.11
400.00	-27.75	-34.85	-27.97	-28.44
500.00	-29.23	-35.11	-28.29	-27.05
600.00	-30.32	-35.17	-28.33	-26.66
700.00	-31.07	-35.05	-28.23	-26.67
800.00	-31.55	-34.80	-28.04	-26.78
900.00	-31.81	-34.46	-27.79	-26.85
1000.00	-31.93	-34.05	-27.50	-26.86

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

T/K	C5H10	C6H12	C7H14	C8H16	C9H18
298.15	39.41	40.15	34.87	37.98	40.05
300.00	40.12	41.02	35.92	39.21	41.49
400.00	80.59	90.71	95.45	109.05	122.02
500.00	123.16	142.92	157.59	181.62	204.76
600.00	167.06	196.73	221.36	255.86	288.98
700.00	211.89	251.62	286.21	331.18	374.27
800.00	257.19	307.07	351.59	406.99	460.05
900.00	302.89	362.97	417.39	483.21	546.26
1000.00	348.78	419.09	483.37	559.58	632.63

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8
298.15	.74	-5.28	3.11	2.07
300.00	.90	-5.10	3.29	2.27
400.00	10.12	4.74	13.60	12.97
500.00	19.77	14.67	24.03	23.14
600.00	29.67	24.63	34.50	33.13
700.00	39.74	34.59	44.97	43.09
800.00	49.88	44.52	55.40	53.06
900.00	60.08	54.42	65.82	63.05
1000.00	70.30	64.28	76.22	73.04

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

T/K	C5H10	C6H12	C7H14	C8H16	C9H18
298.15	.00	.00	.00	.00	.00
300.00	.16	.19	.25	.30	.43
400.00	10.67	12.73	16.24	19.46	26.18
500.00	24.43	29.27	36.76	43.91	56.27
600.00	41.03	49.28	61.22	72.83	90.09
700.00	60.16	72.37	89.14	105.57	127.53
800.00	81.36	97.97	119.86	141.35	168.08
900.00	104.33	125.68	152.94	179.69	211.35
1000.00	128.74	155.11	187.90	220.07	256.85

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8
298.15	.00	.00	.00	.00
300.00	.03	.06	.05	.12
400.00	2.06	3.51	3.22	6.72
500.00	4.83	7.49	7.15	12.36
600.00	8.25	11.94	11.61	17.26
700.00	12.21	16.77	16.43	21.96
800.00	16.61	21.90	21.49	26.73
900.00	21.36	27.25	26.75	31.66
1000.00	26.37	32.79	32.16	36.79

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

T/K	C5H10	C6H12	C7H14	C8H16	C9H18
298.15	-76.78	-102.59	-136.95	-164.14	-195.31
300.00	-76.61	-102.40	-136.70	-163.84	-194.88
400.00	-66.10	-89.86	-120.71	-144.68	-169.13
500.00	-52.34	-73.32	-100.19	-120.23	-139.04
600.00	-35.74	-53.31	-75.73	-91.31	-105.22
700.00	-16.62	-30.23	-47.82	-58.58	-67.78
800.00	-4.58	-4.62	-17.09	-22.79	-27.23
900.00	27.55	23.09	15.98	15.54	16.04
1000.00	51.97	52.52	50.95	55.92	61.54

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8
298.15	-25.82	-34.36	-27.19	-31.17
300.00	-25.79	-34.30	-27.14	-31.11
400.00	-23.75	-30.85	-23.97	-24.44
500.00	-20.98	-26.87	-20.04	-18.05
600.00	-17.57	-22.42	-15.58	-13.00
700.00	-13.61	-17.59	-10.76	-8.00
800.00	-9.21	-12.47	-5.70	-4.00
900.00	-4.46	-7.11	-4.44	5.00
1000.00	1.55	-1.57	4.97	11.62

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Table 9. Equilibrium mole fractions within alkylcyclopentane isomer groups

T/K		298.15	300	400	500	600	700	800	900	1000
C5H10	cyclopentane	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
C6H12	methylcyclopentane	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
C7H14	ethyl	.0059	.0061	.0218	.0458	.0739	.1024	.1296	.1545	.1768
	1,2-dimethyl, trans*	.2581	.2582	.2577	.2511	.2425	.2337	.2253	.2178	.2110
	1,2-dimethyl, cis	.0477	.0482	.0715	.0858	.0939	.0983	.1003	.1011	.1011
	1,3-dimethyl, trans*	.2581	.2582	.2577	.2511	.2425	.2337	.2253	.2178	.2110
	1,3-dimethyl, cis	.2581	.2582	.2577	.2511	.2425	.2337	.2253	.2178	.2110
	1,1-dimethyl	.1722	.1711	.1335	.1152	.1048	.0983	.0941	.0912	.0891
C8H16	1,1,2-trimethyl*	.1793	.1788	.1519	.1286	.1103	.0966	.0863	.0786	.0726
	1-ethyl-2-methyl*	.0031	.0032	.0124	.0256	.0389	.0503	.0595	.0666	.0720
	1-ethyl-3-methyl, cis*	.0166	.0170	.0447	.0748	.1004	.1197	.1336	.1434	.1503
	1-ethyl-3-methyl, trans*	.0166	.0170	.0447	.0748	.1004	.1197	.1336	.1434	.1503
	1-ethyl-1-methyl	.0029	.0029	.0085	.0153	.0222	.0283	.0337	.0384	.0424
	isopropyl	.0021	.0022	.0082	.0167	.0257	.0337	.0404	.0458	.0502
	n-propyl	.0007	.0008	.0052	.0153	.0299	.0466	.0635	.0795	.0942
	1-2-3-trimethyl, cis cis	.0124	.0126	.0203	.0239	.0247	.0241	.0230	.0218	.0206
	1-2-3-trimethyl, trans trans*	.1344	.1349	.1466	.1401	.1276	.1148	.1034	.0938	.0859
	1,2,3-trimethyl, cis cis	.3633	.3609	.2644	.2049	.1647	.1365	.1161	.1011	.0897
	1,2,4-trimethyl, cis cis	.0672	.0674	.0733	.0700	.0638	.0574	.0517	.0469	.0430
	1,2,4-trimethyl, cis trans	.0672	.0674	.0733	.0700	.0638	.0574	.0517	.0469	.0430
	1,2,4-trimethyl, trans trans*	.1344	.1349	.1466	.1401	.1276	.1148	.1034	.0938	.0859
C9H18	n-butyl	.0001	.0001	.0010	.0041	.0092	.0154	.0219	.0283	.0342
	1-propyl-2-methyl, cis*	.0002	.0003	.0024	.0069	.0120	.0166	.0205	.0236	.0262
	1-propyl-2-methyl, trans*	.0013	.0014	.0088	.0201	.0309	.0395	.0460	.0509	.0546
	1-propyl-3-methyl, cis*	.0013	.0014	.0088	.0201	.0309	.0395	.0460	.0509	.0546
	1-propyl-3-methyl, trans*	.0013	.0014	.0088	.0201	.0309	.0395	.0460	.0509	.0546
	1-propyl-1-methyl	.0002	.0002	.0017	.0041	.0068	.0093	.0116	.0136	.0154
	1,2-diethyl, cis	.0000	.0000	.0004	.0015	.0031	.0047	.0062	.0076	.0088
	1,2-diethyl, trans*	.0002	.0002	.0016	.0045	.0079	.0111	.0139	.0163	.0183
	1,3-diethyl, cis*	.0003	.0004	.0032	.0090	.0158	.0222	.0278	.0326	.0365
	1,3-diethyl, trans*	.0002	.0002	.0016	.0045	.0079	.0111	.0139	.0163	.0183
	1,1-diethyl	.0000	.0000	.0001	.0004	.0009	.0015	.0021	.0028	.0034
	1-ethyl-1,2-dimethyl, cis*	.0010	.0010	.0040	.0069	.0089	.0101	.0109	.0114	.0118
	1-ethyl-1,2-dimethyl, trans*	.0010	.0010	.0040	.0069	.0089	.0101	.0109	.0114	.0118
	1-ethyl-2,2-dimethyl*	.0038	.0039	.0109	.0155	.0173	.0179	.0180	.0178	.0176
	1-ethyl-2,3-dimethyl, cis cis*	.0005	.0006	.0029	.0058	.0078	.0090	.0096	.0099	.0100
	1-ethyl-2,3-dimethyl, trans trans*	.0028	.0029	.0105	.0168	.0201	.0213	.0215	.0213	.0209
	1-ethyl-2,3-dimethyl, trans cis*	.0153	.0158	.0380	.0493	.0518	.0507	.0484	.0459	.0436
	1-ethyl-2,3-dimethyl, cis trans*	.0028	.0029	.0105	.0168	.0201	.0213	.0215	.0213	.0209
	1-ethyl-2,4-dimethyl, cis cis*	.0028	.0029	.0105	.0168	.0201	.0213	.0215	.0213	.0209
	1-ethyl-2,4-dimethyl, trans cis*	.0153	.0158	.0380	.0493	.0518	.0507	.0484	.0459	.0436
	1-ethyl-2,4-dimethyl, cis trans*	.0028	.0029	.0105	.0168	.0201	.0213	.0215	.0213	.0209
	1-ethyl-2,4-dimethyl, trans trans*	.0153	.0158	.0380	.0493	.0518	.0507	.0484	.0459	.0436
	1-ethyl-1,5-dimethyl, cis cis	.0003	.0003	.0015	.0029	.0039	.0045	.0048	.0049	.0050
	1-ethyl-1,5-dimethyl, cis trans*	.0028	.0029	.0105	.0168	.0201	.0213	.0215	.0213	.0209
	1-ethyl-1,5-dimethyl, trans trans*	.0153	.0158	.0380	.0493	.0518	.0507	.0484	.0459	.0436
	1-ethyl-3,3-dimethyl*	.0204	.0209	.0394	.0452	.0448	.0426	.0404	.0384	.0368
	1-ethyl-3,4-dimethyl, cis cis	.0014	.0015	.0053	.0084	.0100	.0107	.0108	.0107	.0104
	1-ethyl-3,4-dimethyl, trans cis*	.0153	.0158	.0380	.0493	.0518	.0507	.0484	.0459	.0436
	1-ethyl-3,4-dimethyl, trans trans*	.0028	.0029	.0105	.0168	.0201	.0213	.0215	.0213	.0209
	1,2,3,4-tetramethyl, cis cis cis	.0021	.0022	.0048	.0054	.0049	.0043	.0037	.0032	.0029
	1,2,3,4-tetramethyl, trans trans trans*	.0230	.0234	.0346	.0315	.0255	.0204	.0167	.0139	.0119
	1,2,3,4-tetramethyl, trans cis cis*	.1242	.1251	.1247	.0922	.0659	.0486	.0374	.0300	.0249
	1,2,3,4-tetramethyl, cis trans trans*	.0115	.0117	.0173	.0158	.0128	.0102	.0083	.0070	.0060
	1,2,3,4-tetramethyl, trans trans cis	.0621	.0625	.0624	.0461	.0329	.0243	.0187	.0150	.0125
	1,1,2-tetramethyl	.0019	.0019	.0026	.0023	.0018	.0015	.0013	.0011	.0010
	1,1,3,3-tetramethyl	.2990	.2940	.1207	.0568	.0318	.0205	.0147	.0113	.0093
	1,2,3,4-tetramethyl, trans cis trans*	.3359	.3347	.2249	.1349	.0850	.0578	.0421	.0324	.0260
	isobutyl	.0002	.0002	.0016	.0045	.0079	.0111	.0139	.0163	.0183
	1-methylpropyl	.0000	.0000	.0006	.0020	.0040	.0062	.0084	.0104	.0122
	1,1-dimethylethyl	.0001	.0001	.0003	.0007	.0010	.0013	.0015	.0017	.0018
	1-isopropyl-2-methyl, cis*	.0007	.0008	.0039	.0075	.0103	.0120	.0130	.0136	.0140
	1-isopropyl-2-methyl, trans*	.0040	.0041	.0139	.0220	.0265	.0285	.0293	.0294	.0291
	1-isopropyl-3-methyl, cis*	.0040	.0041	.0139	.0220	.0265	.0285	.0293	.0294	.0291
	1-isopropyl-3-methyl, trans*	.0040	.0041	.0139	.0220	.0265	.0285	.0293	.0294	.0291

Table 10. Root mean square deviations between alkylcyclohexane thermodynamic properties from Stull, Westrum, and Sinke and from the Benson method

T/K	298	300	400	500	600	700	800	900	1000
Standard heat capacity at constant pressure in J/K mol									
C6H12	1.67	.04	.55	1.69	.03	.55	1.68	.01	.64
C7H14	1.18	.29	.69	.89	.26	.64	.84	.01	.47
C8H16	.86	.22	.44	.77	.24	.38	.40	.14	.51
Standard entropy in J/K mol									
C6H12	.90	.00	.79	.89	.01	.79	.40	.01	.69
C7H14	.08	.04	.66	.11	.08	.68	.24	.11	.69
C8H16	.35	.09	.67	.45	.06	.65	.52	.05	.64
Standard enthalpy of formation in kJ/mol									
C6H12	.15	.24	.45	.15	.24	.45	.03	.24	.46
C7H14	.16	.23	.48	.26	.20	.51	.35	.18	.54
C8H16	.44	.20	.56	.53	.22	.57	.58	.23	.58
Standard Gibbs energy of formation in kJ/mol									
C6H12	.11	.24	.45	.12	.24	.45	.19	.24	.47
C7H14	.21	.24	.50	.20	.25	.52	.19	.26	.55
C8H16	.15	.27	.58	.11	.28	.62	.06	.27	.66

Table 11. Standard heat capacity at constant pressure for alkylcyclohexane isomer groups in J/K mol

T/K	C6H12	C7H14	C8H16	C9H18	C10H20
298.15	113.24	135.17	165.21	205.20	234.76
300.00	114.08	136.14	166.31	206.41	236.21
400.00	156.89	185.61	222.23	265.24	303.79
500.00	195.19	229.78	271.26	315.26	357.69
600.00	228.96	268.62	314.02	359.57	404.64
700.00	258.21	302.16	350.78	398.39	445.95
800.00	282.93	330.38	381.62	431.39	481.27
900.00	303.14	353.29	406.55	458.26	510.11
1000.00	318.82	370.89	425.55	478.79	532.12

Table 12. Standard entropy for alkylcyclohexane isomer groups in J/K mol

T/K	C6H12	C7H14	C8H16	C9H18	C10H20
298.15	294.59	343.44	381.51	416.86	454.19
300.00	295.29	344.27	382.53	418.13	455.64
400.00	334.08	390.34	438.21	485.86	533.31
500.00	373.29	436.60	493.19	550.54	607.05
600.00	411.93	482.01	546.52	612.02	676.50
700.00	449.48	526.01	597.76	670.43	742.06
800.00	485.62	568.26	646.68	725.85	803.98
900.00	520.16	608.54	693.13	778.28	862.40
1000.00	552.95	646.72	737.00	827.68	917.34

Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9
298.15	21.93	30.03	39.99	29.57
300.00	22.06	30.17	40.10	29.79
400.00	28.72	36.62	43.01	30.55
500.00	34.59	41.49	43.99	42.44
600.00	39.67	45.40	45.54	45.07
700.00	43.95	48.62	47.61	47.56
800.00	47.45	51.24	49.77	49.88
900.00	50.16	53.26	51.71	51.85
1000.00	52.07	54.66	53.24	53.33

Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9
298.15	48.85	38.07	35.35	37.32
300.00	48.98	38.26	35.60	37.51
400.00	56.26	47.87	47.65	47.44
500.00	63.31	56.58	57.35	56.51
600.00	70.08	64.51	65.50	64.49
700.00	76.53	71.75	72.67	71.62
800.00	82.63	78.42	79.17	78.13
900.00	88.39	84.58	85.15	84.12
1000.00	93.78	90.27	90.68	89.66

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Table 13. Standard enthalpy of formation for alkylcyclohexane isomer groups in kJ/mol

T/K	C6H12	C7H14	C8H16	C9H18	C10H20
298.15	-123.76	-153.76	-182.53	-209.20	-234.98
300.00	-123.98	-154.01	-182.79	-209.46	-235.26
400.00	-134.02	-165.44	-194.80	-221.21	-247.47
500.00	-141.90	-174.41	-204.11	-230.43	-256.88
600.00	-147.72	-181.02	-210.88	-237.23	-263.81
700.00	-151.57	-185.38	-215.24	-241.65	-268.31
800.00	-153.74	-187.86	-217.60	-244.02	-270.68
900.00	-154.48	-188.72	-218.24	-244.60	-271.18
1000.00	-154.04	-188.29	-217.53	-243.74	-270.18

Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9
298.15	-30.00	-28.76	-26.67	-25.79
300.00	-30.03	-28.78	-26.67	-25.80
400.00	-31.42	-29.36	-26.41	-26.26
500.00	-32.50	-29.70	-26.32	-26.45
600.00	-33.30	-29.86	-26.36	-26.58
700.00	-33.82	-29.86	-26.41	-26.66
800.00	-34.12	-29.74	-26.42	-26.66
900.00	-34.24	-29.52	-26.35	-26.58
1000.00	-34.24	-29.24	-26.22	-26.44

Table 14. Standard Gibbs energy of formation for alkylcyclohexane isomer groups in kJ/mol

T/K	C6H12	C7H14	C8H16	C9H18	C10H20
298.15	32.39	28.50	29.05	32.50	36.25
300.00	33.35	29.61	30.34	33.98	37.91
400.00	87.39	92.64	103.31	117.01	130.94
500.00	143.70	158.24	178.96	202.67	226.67
600.00	201.37	225.40	256.21	289.92	324.03
700.00	259.91	293.54	334.47	378.21	422.44
800.00	318.81	362.09	413.12	466.87	521.22
900.00	377.96	430.94	492.05	555.83	620.30
1000.00	437.15	499.82	571.00	644.79	719.38

Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9
298.15	-3.90	.55	3.45	3.75
300.00	-3.74	.73	3.64	3.93
400.00	5.25	10.67	13.70	13.93
500.00	14.55	20.71	23.71	24.00
600.00	24.03	30.81	33.72	34.10
700.00	33.63	40.93	43.74	44.23
800.00	43.28	51.03	53.75	54.35
900.00	52.97	61.12	63.78	64.47
1000.00	62.67	71.18	73.79	74.59

Table 15. Standard enthalpy for alkylcyclohexane isomer groups relative to the isomer group at 298.15 K in kJ/mol

T/K	C6H12	C7H14	C8H16	C9H18	C10H20
298.15	.00	.00	.00	.00	.00
300.00	.21	.25	.31	.38	.43
400.00	13.72	16.30	19.70	23.95	27.47
500.00	31.34	37.08	44.39	53.00	60.58
600.00	52.56	62.02	73.67	86.74	98.70
700.00	76.98	90.63	106.99	124.72	141.32
800.00	104.05	122.27	143.64	166.23	187.69
900.00	133.39	156.49	183.08	210.75	237.31
1000.00	164.58	192.82	224.82	257.75	289.57

Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9
298.15	.00	.00	.00	.00
300.00	.04	.06	.07	.05
400.00	2.57	3.40	4.26	3.52
500.00	5.74	7.31	8.60	7.58
600.00	9.46	11.66	13.07	11.96
700.00	13.65	16.37	17.73	16.59
800.00	18.22	21.36	22.59	21.46
900.00	23.11	26.59	27.67	26.55
1000.00	28.23	32.00	32.93	31.83

Table 16. Standard enthalpy for alkylcyclohexane isomer groups relative to the elements at 298.15 K in kJ/mol

T/K	C6H12	C7H14	C8H16	C9H18	C10H20
298.15	-123.76	-153.76	-182.53	-209.20	-234.98
300.00	-123.55	-153.51	-182.22	-208.82	-234.55
400.00	-110.04	-137.46	-162.83	-185.24	-207.51
500.00	-92.42	-116.68	-138.13	-156.20	-174.41
600.00	-71.20	-91.75	-108.85	-122.46	-136.28
700.00	-46.78	-63.13	-75.53	-84.48	-93.67
800.00	-19.71	-31.49	-38.89	-42.97	-47.29
900.00	9.62	2.73	.56	1.55	2.32
1000.00	40.82	39.05	42.29	48.55	54.59

Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9
298.15	-30.00	-28.76	-26.67	-25.79
300.00	-29.96	-28.71	-26.60	-25.73
400.00	-27.43	-25.36	-22.42	-22.27
500.00	-24.26	-21.45	-18.07	-18.20
600.00	-20.54	-17.11	-13.60	-13.83
700.00	-16.35	-12.40	-8.94	-9.19
800.00	-11.78	-7.40	-4.08	-4.32
900.00	-6.89	-2.17	1.00	.77
1000.00	-1.76	3.24	6.26	6.04

Table 17. Equilibrium mole fractions within alkylcyclohexane isomer groups

T/K		298	300	400	500	600	700	800	900	1000
C6H12	cyclohexane	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
C7H14	methylcyclohexane	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
C8H16	ethyl	.0114	.0118	.0359	.0671	.0988	.1280	.1535	.1755	.1943
	1,1-dimethyl	.0225	.0226	.0294	.0337	.0366	.0389	.0407	.0423	.0438
	1,2-dimethyl, trans*	.1299	.1306	.1553	.1643	.1659	.1642	.1614	.1582	.1550
	1,2-dimethyl, cis	.0337	.0341	.0568	.0734	.0848	.0924	.0976	.1011	.1036
	1,3-dimethyl, cis	.5013	.4998	.4249	.3675	.3244	.2919	.2669	.2474	.2319
	1,3-dimethyl, trans*	.0337	.0341	.0568	.0734	.0848	.0924	.0976	.1011	.1036
	1,4-dimethyl, cis	.0168	.0171	.0284	.0367	.0424	.0462	.0488	.0506	.0518
	1,4-dimethyl, trans	.2507	.2499	.2125	.1838	.1622	.1460	.1335	.1237	.1159
C9H18	n-propyl	.0016	.0017	.0088	.0207	.0342	.0472	.0587	.0687	.0773
	1-ethyl-1-methyl	.0004	.0004	.0019	.0042	.0066	.0091	.0114	.0136	.0156
	1-ethyl-2-methyl, cis*	.0006	.0007	.0037	.0091	.0153	.0216	.0273	.0324	.0369
	1-ethyl-2-methyl, trans*	.0096	.0099	.0278	.0453	.0587	.0681	.0747	.0792	.0825
	1-ethyl-3-methyl, cis*	.0369	.0377	.0761	.1014	.1148	.1211	.1235	.1239	.1233
	1-ethyl-3-methyl, trans*	.0025	.0026	.0102	.0203	.0300	.0383	.0451	.0506	.0551
	1-ethyl-4-methyl, cis*	.0025	.0026	.0102	.0203	.0300	.0383	.0451	.0506	.0551
	1-ethyl-4-methyl, trans*	.0369	.0377	.0761	.1014	.1148	.1211	.1235	.1239	.1233
	1,2,3-trimethyl, cis cis	.0037	.0037	.0080	.0111	.0129	.0138	.0143	.0146	.0147
	1,2,3-trimethyl, trans trans*	.0073	.0075	.0161	.0222	.0257	.0277	.0287	.0292	.0294
	1,2,3-trimethyl, trans cis	.0544	.0547	.0601	.0555	.0493	.0437	.0392	.0357	.0329
	1,2,4-trimethyl, cis cis*	.0282	.0286	.0439	.0496	.0504	.0492	.0474	.0457	.0440
	1,2,4-trimethyl, trans trans*	.4199	.4186	.3288	.2484	.1927	.1554	.1298	.1117	.0984
	1,2,4-trimethyl, trans cis*	.0282	.0286	.0439	.0496	.0504	.0492	.0474	.0457	.0440
	1,2,4-trimethyl, cis trans*	.0282	.0286	.0439	.0496	.0504	.0492	.0474	.0457	.0440
	1,3,5-trimethyl, cis cis	.2700	.2670	.1499	.0926	.0628	.0460	.0358	.0291	.0245
	1,3,5-trimethyl, cis trans	.0544	.0547	.0601	.0555	.0493	.0437	.0392	.0357	.0329
	1,1,2-trimethyl*	.0098	.0099	.0166	.0204	.0223	.0233	.0239	.0244	.0248
	isopropyl	.0048	.0049	.0139	.0227	.0294	.0341	.0373	.0396	.0412
C10H20	n-butyl	.0003	.0003	.0023	.0069	.0128	.0189	.0246	.0295	.0338
	1,1-dimethyl ethyl	.0003	.0003	.0007	.0011	.0014	.0016	.0017	.0018	.0018
	1-methyl propyl*	.0015	.0016	.0073	.0150	.0220	.0273	.0312	.0341	.0361
	isobutyl	.0008	.0008	.0036	.0075	.0110	.0137	.0156	.0170	.0181
	1-propyl-1-methyl	.0001	.0001	.0005	.0014	.0025	.0036	.0048	.0058	.0068
	1-isopropyl-1-methyl	.0008	.0008	.0022	.0034	.0042	.0047	.0050	.0053	.0054
	1,1-diethyl	.0000	.0000	.0000	.0001	.0003	.0006	.0009	.0012	.0015
	1,2-diethyl, trans*	.0002	.0002	.0013	.0034	.0056	.0077	.0094	.0109	.0121
	1,2-diethyl, cis	.0001	.0001	.0005	.0015	.0029	.0043	.0057	.0070	.0081
	1,3-diethyl, trans*	.0001	.0001	.0005	.0015	.0029	.0043	.0057	.0070	.0081
	1,3-diethyl, cis	.0008	.0008	.0036	.0075	.0110	.0137	.0156	.0170	.0181
	1,4-diethyl, trans	.0004	.0004	.0018	.0038	.0055	.0068	.0078	.0085	.0090
	1,1,2-tetramethyl	.0001	.0001	.0002	.0003	.0004	.0004	.0005	.0005	.0005
	1,1,3,3-tetramethyl	.0059	.0059	.0049	.0038	.0030	.0025	.0022	.0020	.0018
	1,1,4,4-tetramethyl	.0030	.0030	.0024	.0019	.0015	.0013	.0011	.0010	.0009
	1-propyl-2-methyl, trans*	.0004	.0004	.0027	.0067	.0112	.0154	.0189	.0218	.0241
	1-propyl-2-methyl, cis*	.0001	.0001	.0010	.0030	.0057	.0086	.0114	.0139	.0161
	1-propyl-3-methyl, trans*	.0004	.0004	.0027	.0067	.0112	.0154	.0189	.0218	.0241
	1-propyl-3-methyl, cis*	.0059	.0061	.0200	.0336	.0429	.0485	.0517	.0533	.0540
	1-propyl-4-methyl, cis	.0002	.0002	.0013	.0034	.0056	.0077	.0094	.0109	.0121
	1-propyl-4-methyl, trans	.0030	.0031	.0100	.0168	.0215	.0243	.0258	.0266	.0270
	1-isopropyl-2-methyl, trans*	.0001	.0001	.0009	.0022	.0037	.0051	.0063	.0073	.0080
	1-isopropyl-2-methyl, cis*	.0000	.0000	.0001	.0004	.0010	.0016	.0023	.0030	.0036
	1-isopropyl-3-methyl, trans*	.0000	.0000	.0003	.0010	.0019	.0029	.0038	.0046	.0054
	1-isopropyl-3-methyl, cis*	.0005	.0005	.0024	.0050	.0073	.0091	.0104	.0114	.0120
	1-isopropyl-4-methyl, trans	.0003	.0003	.0012	.0025	.0037	.0046	.0052	.0057	.0060
	1-isopropyl-4-methyl, cis	.0000	.0000	.0002	.0005	.0010	.0014	.0019	.0023	.0027
	1-ethyl-1,2-dimethyl, trans*	.0001	.0001	.0006	.0013	.0022	.0030	.0037	.0043	.0049
	1-ethyl-1,2-dimethyl, cis*	.0001	.0001	.0006	.0013	.0022	.0030	.0037	.0043	.0049
	1-ethyl-1,3-dimethyl, trans*	.0016	.0016	.0044	.0067	.0083	.0093	.0100	.0105	.0109
	1-ethyl-1,3-dimethyl, cis*	.0016	.0016	.0044	.0067	.0083	.0093	.0100	.0105	.0109
	1-ethyl-1,4-dimethyl, trans	.0008	.0008	.0022	.0034	.0042	.0047	.0050	.0053	.0054
	1-ethyl-1,4-dimethyl, cis	.0008	.0008	.0022	.0034	.0042	.0047	.0050	.0053	.0054
	1-ethyl-2,2-dimethyl*	.0016	.0016	.0044	.0067	.0083	.0093	.0100	.0105	.0109
	1-ethyl-3,3-dimethyl*	.0060	.0062	.0119	.0151	.0163	.0166	.0166	.0164	.0163
	1-ethyl-4,4-dimethyl	.0030	.0031	.0060	.0075	.0081	.0083	.0083	.0082	.0081
	1-ethyl-2,3-dimethyl, cis cis*	.0003	.0003	.0015	.0033	.0049	.0062	.0073	.0080	.0086
	1-ethyl-2,3-dimethyl, cis trans*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-2,3-dimethyl, trans cis*	.0045	.0046	.0115	.0164	.0188	.0197	.0198	.0196	.0193
	1-ethyl-2,3-dimethyl, trans trans*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-3,4-dimethyl, cis cis*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-3,4-dimethyl, trans cis*	.0175	.0178	.0315	.0368	.0368	.0350	.0328	.0307	.0288
	1-ethyl-3,4-dimethyl, cis trans*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-3,4-dimethyl, trans trans*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-3,5-dimethyl, cis cis	.0337	.0340	.0432	.0411	.0360	.0311	.0271	.0240	.0216
	1-ethyl-3,5-dimethyl, trans cis*	.0045	.0046	.0115	.0164	.0188	.0197	.0198	.0196	.0193
	1-ethyl-3,5-dimethyl, trans trans	.0023	.0023	.0058	.0082	.0094	.0099	.0099	.0098	.0096
	1-ethyl-2,4-dimethyl, cis cis*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-2,4-dimethyl, trans trans*	.0175	.0178	.0315	.0368	.0368	.0350	.0328	.0307	.0288
	1-ethyl-2,4-dimethyl, cis trans*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-2,4-dimethyl, trans cis*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-2,5-dimethyl, cis cis*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-2,5-dimethyl, cis trans*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-2,5-dimethyl, trans trans*	.0012	.0012	.0042	.0073	.0096	.0111	.0120	.0125	.0129
	1-ethyl-2,5-dimethyl, trans cis*	.0175	.0178	.0315	.0368	.0368	.0350	.0328	.0307	.0288
	1-ethyl-2,6-dimethyl, cis cis	.0002	.0002	.0008	.0016	.0025	.0031	.0036	.0040	.0043
	1-ethyl-2,6-dimethyl, trans cis*	.0045	.0046	.0115	.0164	.0188	.0197	.0198	.0196	.0193
	1-ethyl-2,6-dimethyl, trans trans	.0001	.0001	.0006	.0015	.0025	.0035	.0044	.0051	.0058
	1,1,2,3-tetramethyl, cis*	.0267	.0268	.0283	.0248	.0210	.0180	.0158	.0142	.0130

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Table 17. Equilibrium mole fractions within alkylcyclohexane isomer groups --Continued

T/K		298	300	400	500	600	700	800	900	1000
	1,1,2,3-tetramethyl, trans*	.0046	.0047	.0069	.0074	.0071	.0067	.0064	.0061	.0058
	1,1,3,4-tetramethyl, cis*	.0686	.0684	.0516	.0369	.0273	.0213	.0174	.0148	.0130
	1,1,3,4-tetramethyl, trans*	.0178	.0179	.0189	.0165	.0140	.0120	.0105	.0095	.0087
	1,1,2,4-tetramethyl, cis*	.0046	.0047	.0069	.0074	.0071	.0067	.0064	.0061	.0058
	1,1,2,4-tetramethyl, trans*	.2648	.2617	.1413	.0826	.0535	.0378	.0288	.0232	.0194
	1,1,3,5-tetramethyl, cis	.0178	.0179	.0189	.0165	.0140	.0120	.0105	.0095	.0087
	1,1,3,5-tetramethyl, trans*	.0006	.0006	.0013	.0016	.0018	.0019	.0019	.0019	.0019
	1,2,2,3-tetramethyl, cis	.0006	.0006	.0013	.0016	.0018	.0019	.0019	.0019	.0019
	1,2,2,3-tetramethyl, trans*	.0023	.0023	.0034	.0037	.0036	.0034	.0032	.0030	.0029
	1,2,2,4-tetramethyl, cis*	.0089	.0089	.0094	.0083	.0070	.0060	.0053	.0047	.0043
	1,2,2,4-tetramethyl, trans*	.0003	.0003	.0009	.0015	.0019	.0021	.0023	.0025	.0026
	1,2,3,4-tetramethyl, cis cis cis	.0035	.0035	.0067	.0080	.0083	.0080	.0076	.0072	.0069
	1,2,3,4-tetramethyl, cis cis trans*	.0004	.0005	.0012	.0018	.0021	.0023	.0023	.0023	.0023
	1,2,3,4-tetramethyl, cis trans trans*	.0514	.0516	.0498	.0402	.0316	.0253	.0209	.0177	.0154
	1,2,3,4-tetramethyl, trans cis trans*	.0017	.0018	.0033	.0040	.0041	.0040	.0038	.0036	.0034
	1,2,3,4-tetramethyl, trans cis cis*	.0009	.0009	.0024	.0036	.0042	.0045	.0046	.0046	.0046
	1,2,3,4-tetramethyl, trans trans cis*	.0133	.0135	.0182	.0180	.0162	.0142	.0126	.0113	.0103
	1,2,3,5-tetramethyl, cis cis cis	.0009	.0009	.0024	.0036	.0042	.0045	.0046	.0046	.0046
	1,2,3,5-tetramethyl, trans trans trans	.0067	.0067	.0091	.0090	.0081	.0071	.0063	.0057	.0051
	1,2,3,5-tetramethyl, cis trans trans*	.0017	.0018	.0033	.0040	.0041	.0040	.0038	.0036	.0034
	1,2,3,5-tetramethyl, cis cis trans*	.0133	.0135	.0182	.0180	.0162	.0142	.0126	.0113	.0103
	1,2,3,5-tetramethyl, trans cis trans*	.0035	.0035	.0067	.0080	.0083	.0080	.0076	.0072	.0069
	1,2,3,5-tetramethyl, trans cis trans*	.0133	.0135	.0182	.0180	.0162	.0142	.0126	.0113	.0103
	1,2,3,5-tetramethyl, trans trans cis*	.1985	.1974	.1364	.0900	.0618	.0450	.0345	.0277	.0230
	1,2,3,5-tetramethyl, cis trans cis*	.0009	.0009	.0024	.0036	.0042	.0045	.0046	.0046	.0046
	1,2,4,5-tetramethyl, cis cis cis	.0133	.0135	.0182	.0180	.0162	.0142	.0126	.0113	.0103
	1,2,4,5-tetramethyl, trans trans trans*	.0002	.0002	.0006	.0009	.0011	.0011	.0012	.0012	.0011
	1,2,4,5-tetramethyl, cis trans trans	.0035	.0035	.0067	.0080	.0083	.0080	.0076	.0072	.0069
	1,2,4,5-tetramethyl, trans cis trans*	.0496	.0494	.0341	.0225	.0155	.0112	.0086	.0069	.0057
	1,2,4,5-tetramethyl, trans trans cis	.0496	.0494	.0341	.0225	.0155	.0112	.0086	.0069	.0057

Table 18. Standard heat capacity at constant pressure for alkylcyclopentane plus alkylcyclohexane isomer groups in J/K mol

T/K	C5H10	C6H12	C7H14	C8H16	C9H16	C10H20
298.15	87.81	137.24	160.46	176.95	217.66	247.85
300.00	88.47	138.90	162.02	178.42	219.21	249.64
400.00	122.36	214.37	229.47	253.63	297.22	338.60
500.00	152.62	232.43	260.28	305.14	350.40	396.03
600.00	179.24	241.57	282.86	337.29	382.62	428.02
700.00	202.23	257.43	305.79	362.51	408.55	454.35
800.00	221.58	275.10	327.33	384.50	432.22	479.63
900.00	237.30	291.05	345.67	403.07	452.77	502.18
1000.00	249.38	303.73	359.87	417.45	468.93	520.14

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8	C10-C9
298.15	49.42	23.22	16.50	40.71	30.19
300.00	50.42	23.12	16.40	40.79	30.43
400.00	92.01	15.10	24.16	43.59	41.38
500.00	79.81	27.85	44.85	45.26	45.63
600.00	62.33	41.29	54.43	45.33	45.40
700.00	55.21	48.36	56.72	46.04	45.79
800.00	53.52	52.23	57.17	47.72	47.41
900.00	53.75	54.62	57.40	49.70	49.41
1000.00	54.35	56.14	57.57	51.48	51.22

Table 19. Standard entropy for alkylcyclopentane plus alkylcyclohexane isomer groups in J/K mol

T/K	C5H10	C6H12	C7H14	C8H16	C9H16	C10H20
298.15	292.25	297.92	348.05	383.36	419.36	457.38
300.00	292.80	298.78	349.05	384.46	420.72	458.92
400.00	322.98	350.27	405.90	446.43	494.83	543.40
500.00	353.60	400.72	460.82	509.06	567.41	625.81
600.00	383.84	443.90	510.27	567.71	634.32	701.04
700.00	413.24	482.17	555.60	621.64	695.28	769.01
800.00	441.55	517.70	597.86	671.52	751.41	831.35
900.00	468.59	551.05	637.51	717.92	803.54	889.18
1000.00	494.25	582.41	674.71	761.17	852.13	943.06

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8	C10-C9
298.15	5.67	50.13	35.31	36.00	38.02
300.00	5.98	50.27	35.41	36.25	38.20
400.00	27.29	55.63	40.52	48.40	48.57
500.00	47.12	60.09	48.24	58.35	58.40
600.00	59.96	66.47	57.44	66.61	66.72
700.00	68.93	73.43	66.05	73.64	73.73
800.00	76.16	80.16	73.66	79.89	79.94
900.00	82.47	86.46	80.40	85.63	85.64
1000.00	88.16	92.30	86.46	90.96	90.94

Table 20. Standard enthalpy of formation for alkylcyclopentane plus alkylcyclohexane isomer groups in kJ/mol

T/K	C5H10	C6H12	C7H14	C8H16	C9H16	C10H20
298.15	-76.78	-122.87	-152.57	-182.04	-208.57	-234.25
300.00	-76.97	-123.05	-152.77	-182.28	-208.80	-234.50
400.00	-86.08	-128.58	-160.40	-192.06	-218.29	-244.29
500.00	-93.58	-131.47	-165.52	-197.92	-223.96	-249.81
600.00	-99.51	-134.90	-169.94	-201.80	-227.80	-253.60
700.00	-103.94	-138.22	-173.45	-204.43	-230.59	-256.55
800.00	-107.11	-140.87	-175.92	-206.09	-232.43	-258.62
900.00	-109.20	-142.61	-177.33	-206.78	-233.26	-259.62
1000.00	-110.42	-143.54	-177.84	-206.65	-233.19	-259.63

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8	C10-C9
298.15	-46.10	-29.69	-29.47	-26.53	-25.69
300.00	-46.08	-29.72	-29.51	-26.52	-25.70
400.00	-42.50	-31.82	-31.65	-26.23	-26.01
500.00	-37.89	-34.05	-32.41	-26.03	-25.85
600.00	-35.39	-35.04	-31.86	-26.00	-25.80
700.00	-34.29	-35.23	-30.98	-26.15	-25.96
800.00	-33.75	-35.06	-30.16	-26.35	-26.19
900.00	-33.41	-34.72	-29.45	-26.49	-26.36
1000.00	-33.12	-34.29	-28.81	-26.54	-26.44

Table 21. Standard Gibbs energy of formation for alkylcyclopentane plus alkylcyclohexane isomer groups in kJ/mol

T/K	C5H10	C6H12	C7H14	C8H16	C9H16	C10H20
298.15	39.41	32.29	28.31	28.98	32.38	36.03
300.00	40.12	33.24	29.42	30.27	33.86	37.68
400.00	80.99	86.35	91.45	102.76	116.34	130.08
500.00	123.16	140.41	155.02	177.20	200.70	224.36
600.00	167.06	195.07	219.52	252.57	285.97	319.52
700.00	211.89	250.37	284.76	328.56	371.88	415.33
800.00	257.19	306.02	350.34	404.76	458.01	511.39
900.00	302.89	362.02	416.25	481.21	544.42	607.76
1000.00	348.78	418.19	482.29	557.71	630.90	704.21

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8	C10-C9
298.15	-7.12	-3.97	.67	3.40	3.64
300.00	-6.88	-3.82	.85	3.59	3.82
400.00	5.76	5.10	11.31	13.58	13.74
500.00	17.25	14.61	22.18	23.51	23.66
600.00	28.01	24.45	33.05	33.40	33.54
700.00	38.48	34.39	43.80	43.32	43.45
800.00	48.83	44.32	54.42	53.25	53.37
900.00	59.13	54.23	64.95	63.21	63.33
1000.00	69.41	64.10	75.42	73.19	73.31

Table 22. Standard enthalpy for alkylcyclopentane plus alkylcyclohexane isomer groups relative to the isomer group at 298.15 K in kJ/mol

T/K	C5H10	C6H12	C7H14	C8H16	C9H18	C10H20
298.15	.00	.00	.00	.00	.00	.00
300.00	.16	.25	.30	.33	.40	.46
400.00	10.67	18.27	20.14	21.95	26.25	29.92
500.00	24.43	40.88	44.77	50.08	58.83	66.91
600.00	41.03	64.50	71.90	82.26	95.54	108.18
700.00	60.16	89.43	101.36	117.32	135.16	152.35
800.00	81.36	116.04	133.02	154.66	177.19	199.03
900.00	104.33	144.36	166.69	194.06	221.45	248.13
1000.00	128.74	174.19	202.07	235.21	267.67	299.39

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8	C10-C9
298.15	.00	.00	.00	.00	.00
300.00	.09	.04	.03	.08	.06
400.00	7.59	1.87	1.81	4.29	3.67
500.00	16.45	3.83	5.31	8.75	6.00
600.00	23.46	7.40	10.36	13.28	12.64
700.00	29.28	11.93	15.95	17.84	17.19
800.00	34.68	16.97	21.65	22.52	21.84
900.00	40.04	22.32	27.38	27.39	26.68
1000.00	45.45	27.88	33.13	32.46	31.72

Table 23. Standard enthalpy for alkylcyclopentane plus alkylcyclohexane isomer groups relative to the elements at 298.15 K in kJ/mol

T/K	C5H10	C6H12	C7H14	C8H16	C9H18	C10H20
298.15	-76.78	-122.87	-152.57	-182.04	-208.57	-234.25
300.00	-76.61	-122.62	-152.27	-181.71	-208.16	-233.79
400.00	-66.10	-104.61	-132.43	-160.09	-182.32	-204.33
500.00	-52.34	-81.99	-107.79	-131.96	-149.74	-167.34
600.00	-35.74	-58.38	-80.67	-99.78	-113.03	-126.07
700.00	-16.62	-33.44	-51.20	-64.72	-73.41	-81.91
800.00	4.58	-6.83	-19.55	-27.37	-31.38	-35.23
900.00	27.55	21.49	14.12	12.02	12.89	13.88
1000.00	51.97	51.32	49.50	53.17	59.10	65.14

Increments per carbon atom

T/K	C6-C5	C7-C6	C8-C7	C9-C8	C10-C9
298.15	-46.10	-29.69	-29.47	-26.53	-25.69
300.00	-46.01	-29.65	-29.44	-26.45	-25.63
400.00	-38.50	-27.82	-27.66	-22.24	-22.01
500.00	-29.65	-25.80	-24.17	-17.78	-17.60
600.00	-22.64	-22.29	-19.11	-13.25	-13.05
700.00	-16.82	-17.76	-13.52	-8.69	-8.50
800.00	-11.42	-12.72	-7.82	-4.01	-3.85
900.00	-6.06	-7.37	-2.10	.86	.99
1000.00	-1.65	-1.82	3.66	5.93	6.04

Table 24. Equilibrium mole fractions within the combined alkylcyclopentane and alkylcyclohexane isomer group

T/K		298	300	400	500	600	700	800	900	1000
C5H10	alkylcyclopentanes cyclopentane	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
C6H12	alkylcyclopentanes methylcyclopentane	.0420	.0441	.2692	.5463	.7169	.8059	.8537	.8812	.8977
	alkylcyclohexanes cyclohexane	.9580	.9559	.7308	.4537	.2831	.1941	.1463	.1188	.1023
C7H14	alkylcyclopentanes ethyl	.0004	.0004	.0065	.0247	.0511	.0798	.1074	.1327	.1553
	1,2-dimethyl, trans*	.0183	.0191	.0775	.1353	.1678	.1820	.1868	.1872	.1854
	1,2-dimethyl, cis	.0034	.0036	.0215	.0462	.0650	.0765	.0832	.0869	.0888
	1,3-dimethyl, trans*	.0183	.0191	.0775	.1353	.1678	.1820	.1868	.1872	.1854
	1,3-dimethyl, cis	.0183	.0191	.0775	.1353	.1678	.1820	.1868	.1872	.1854
	1,1-dimethyl	.0122	.0126	.0401	.0621	.0725	.0766	.0780	.0783	.0783
	alkylcyclohexanes methylcyclohexane	.9290	.9262	.6995	.4610	.3081	.2212	.1710	.1406	.1214
C8H16	alkylcyclopentanes 1,1,2-trimethyl*	.0048	.0050	.0229	.0443	.0571	.0616	.0617	.0601	.0579
	1-ethyl-2-methyl*	.0001	.0001	.0019	.0088	.0201	.0321	.0425	.0509	.0574
	1-ethyl-3-methyl, cis*	.0004	.0005	.0068	.0258	.0519	.0763	.0956	.1097	.1199
	1-ethyl-3-methyl, trans*	.0004	.0005	.0068	.0258	.0519	.0763	.0956	.1097	.1199
	1-ethyl-1-methyl isopropyl	.0001	.0001	.0019	.0053	.0115	.0181	.0241	.0294	.0339
	n-propyl	.0001	.0001	.0012	.0058	.0133	.0215	.0289	.0351	.0401
	1-2,3-trimethyl, cis cis	.0003	.0003	.0031	.0083	.0128	.0154	.0165	.0167	.0164
	1-2,3-trimethyl, trans trans*	.0036	.0037	.0222	.0483	.0661	.0732	.0740	.0718	.0686
	1,2,3-trimethyl, cis cis	.0096	.0100	.0399	.0707	.0852	.0870	.0831	.0773	.0715
	1,2,4-trimethyl, cis cis	.0018	.0019	.0111	.0242	.0330	.0366	.0370	.0359	.0343
	1,2,4-trimethyl, cis trans	.0018	.0019	.0111	.0242	.0330	.0366	.0370	.0359	.0343
	1,2,4-trimethyl, trans trans*	.0036	.0037	.0222	.0483	.0661	.0732	.0740	.0718	.0686
	alkylcyclohexanes ethyl	.0111	.0114	.0305	.0439	.0477	.0464	.0437	.0412	.0393
	1,1-dimethyl	.0219	.0220	.0250	.0221	.0177	.0141	.0116	.0099	.0088
	1,2-dimethyl, trans*	.1265	.1270	.1319	.1076	.0800	.0595	.0460	.0371	.0313
	1,2-dimethyl, cis	.0328	.0332	.0482	.0481	.0409	.0335	.0278	.0237	.0209
	1,3-dimethyl, cis	.4880	.4859	.3607	.2408	.1565	.1058	.0760	.0581	.0469
	1,3-dimethyl, trans*	.0328	.0332	.0482	.0481	.0409	.0335	.0278	.0237	.0209
	1,4-dimethyl, cis	.0164	.0166	.0241	.0241	.0205	.0167	.0139	.0119	.0105
	1,4-dimethyl, trans	.2440	.2430	.1804	.1204	.0783	.0529	.0380	.0290	.0234
C9H18	alkylcyclopentanes n-butyl	.0534	.0534	.0532	.0531	.0530	.0529	.0529	.0528	.0528
	1-propyl-2-methyl, cis*	.0356	.0356	.0355	.0354	.0354	.0353	.0353	.0353	.0353
	1-propyl-2-methyl, trans*	.0356	.0356	.0355	.0354	.0354	.0353	.0353	.0353	.0353
	1-propyl-3-methyl, cis*	.0356	.0356	.0355	.0354	.0354	.0353	.0353	.0353	.0353
	1-propyl-3-methyl, trans*	.0356	.0356	.0355	.0354	.0354	.0353	.0353	.0353	.0353
	1-propyl-1-methyl	.0178	.0178	.0177	.0177	.0177	.0176	.0176	.0176	.0176
	1,2-diethyl, cis	.0178	.0178	.0177	.0177	.0177	.0176	.0176	.0176	.0176
	1,2-diethyl, trans*	.0178	.0178	.0177	.0177	.0177	.0176	.0176	.0176	.0176
	1,3-diethyl, cis*	.0356	.0356	.0355	.0354	.0353	.0353	.0353	.0352	.0352
	1,3-diethyl, trans*	.0178	.0178	.0177	.0177	.0177	.0176	.0176	.0176	.0176
	1,1-diethyl	.0089	.0089	.0089	.0088	.0088	.0088	.0088	.0088	.0088
	1-ethyl-1,2-dimethyl, cis*	.0119	.0119	.0118	.0118	.0118	.0118	.0117	.0117	.0117
	1-ethyl-1,2-dimethyl, trans*	.0119	.0119	.0118	.0118	.0118	.0118	.0117	.0117	.0117
	1-ethyl-2,2-dimethyl*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0117	.0117
	1-ethyl-2,3-dimethyl, cis cis*	.0119	.0119	.0118	.0118	.0118	.0118	.0117	.0117	.0117
	1-ethyl-2,3-dimethyl, trans trans*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0117	.0117
	1-ethyl-2,3-dimethyl, trans cis*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0118	.0118
	1-ethyl-2,3-dimethyl, cis trans*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0117	.0117
	1-ethyl-2,4-dimethyl, cis cis*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0117	.0117
	1-ethyl-2,4-dimethyl, trans cis*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0118	.0118
	1-ethyl-2,4-dimethyl, cis trans*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0118	.0118
	1-ethyl-2,4-dimethyl, trans trans*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0118	.0118
	1-ethyl-1,5-dimethyl, cis cis	.0059	.0059	.0059	.0059	.0059	.0059	.0059	.0059	.0059
	1-ethyl-1,5-dimethyl, cis trans*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0117	.0117
	1-ethyl-1,5-dimethyl, trans trans*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0118	.0118
	1-ethyl-3,3-dimethyl*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0118	.0118
	1-ethyl-3,4-dimethyl, cis cis	.0059	.0059	.0059	.0059	.0059	.0059	.0059	.0059	.0059
	1-ethyl-3,4-dimethyl, trans cis*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0118	.0118
	1-ethyl-3,4-dimethyl, trans trans*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0117	.0117
	1,2,3,4-tetramethyl, cis cis cis	.0020	.0020	.0020	.0020	.0020	.0020	.0020	.0020	.0020
	1,2,3,4-tetramethyl, trans trans trans*	.0040	.0040	.0039	.0039	.0039	.0039	.0039	.0039	.0039
	1,2,3,4-tetramethyl, trans cis cis*	.0039	.0039	.0039	.0039	.0039	.0039	.0039	.0039	.0039
	1,2,3,4-tetramethyl, cis trans trans*	.0020	.0020	.0020	.0020	.0020	.0020	.0020	.0020	.0020
	1,2,3,4-tetramethyl, trans trans cis	.0020	.0020	.0020	.0020	.0020	.0020	.0020	.0020	.0020
	1,1,2,2-tetramethyl	.0010	.0010	.0010	.0010	.0010	.0010	.0010	.0010	.0010
	1,1,3,3-tetramethyl	.0010	.0010	.0010	.0010	.0010	.0010	.0010	.0010	.0010
	1,2,3,4-tetramethyl, trans cis trans*	.0019	.0019	.0019	.0020	.0020	.0020	.0020	.0020	.0020
	isobutyl	.0178	.0178	.0177	.0177	.0177	.0176	.0176	.0176	.0176
	1-methylpropyl	.0178	.0178	.0177	.0177	.0177	.0176	.0176	.0176	.0176
	1,1-dimethyl ethyl	.0020	.0020	.0020	.0020	.0020	.0020	.0020	.0020	.0020
	1-isopropyl-2-methyl, cis*	.0119	.0119	.0118	.0118	.0118	.0118	.0117	.0117	.0117
	1-isopropyl-2-methyl, trans*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0118	.0118
	1-isopropyl-3-methyl, cis*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0118	.0118
	1-isopropyl-3-methyl, trans*	.0119	.0119	.0118	.0118	.0118	.0118	.0118	.0118	.0118
	alkylcyclohexanes 1,2,3-trimethyl, trans cis	.0052	.0052	.0054	.0056	.0057	.0058	.0058	.0059	.0059
	1,2,4-trimethyl, cis cis*	.0113	.0113	.0115	.0116	.0116	.0117	.0117	.0118	.0118
	1,2,4-trimethyl, trans trans*	.0092	.0092	.0101	.0106	.0110	.0113	.0115	.0117	.0118
	1,2,4-trimethyl, trans cis*	.0113	.0113	.0115	.0116	.0116	.0117	.0117	.0118	.0118
	1,2,4-trimethyl, cis trans*	.0113	.0113	.0115	.0116	.0116	.0117	.0117	.0118	.0118
	1,3,5-trimethyl, cis cis	.0014	.0014	.0016	.0017	.0018	.0019	.0019	.0019	.0020
	1,3,5-trimethyl, cis trans	.0052	.0052	.0054	.0056	.0057	.0058	.0058	.0059	.0059
	1,1,2-trimethyl*	.0116	.0116	.0117	.0117	.0117	.0117	.0117	.0118	.0118
	isopropyl	.0176	.0176	.0176	.0176	.0176	.0176	.0177	.0177	.0177
C10H20	alkylcyclopentanes cyclopentanegroup	.0858	.0875	.2280	.4267	.5950	.7050	.7720	.8130	.8388
	alkylcyclohexanes n-butyl	.0003	.0003	.0018	.0039	.0062	.0086	.0095	.0095	.0095
	1,1-dimethyl ethyl	.0002	.0002	.0006	.0006	.0006	.0005	.0004	.0003	.0003
	1-methyl propyl*	.0014	.0015	.0056	.0086	.0089	.0081	.0071	.0064	.0058
	isobutyl	.0007	.0007	.0028	.0043	.0044	.0040	.0036	.0032	.0029

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Table 24. Equilibrium mole fractions within the combined alkylcyclopentane and alkylcyclohexane isomer group--Continued

T/K	298	300	400	500	600	700	800	900	1000
1-propyl-1-methyl	.0001	.0001	.0004	.0008	.0010	.0011	.0011	.0011	.0011
1-isopropyl-1-methyl	.0007	.0007	.0017	.0019	.0017	.0014	.0011	.0010	.0009
1,1-diethyl	.0000	.0000	.0000	.0000	.0001	.0002	.0002	.0002	.0002
1,2-diethyl, trans*	.0002	.0002	.0010	.0019	.0023	.0023	.0022	.0020	.0019
1,2-diethyl, cis	.0003	.0000	.0004	.0009	.0012	.0013	.0013	.0013	.0013
1,3-diethyl, trans*	.0000	.0000	.0000	.0000	.0012	.0013	.0013	.0013	.0013
1,3-diethyl, cis	.0007	.0007	.0028	.0043	.0044	.0040	.0036	.0032	.0029
1,4-diethyl, trans	.0004	.0004	.0014	.0022	.0022	.0020	.0018	.0016	.0015
1,1,2,2-tetramethyl	.0001	.0001	.0002	.0002	.0002	.0001	.0001	.0001	.0001
1,1,3,3-tetramethyl	.0054	.0054	.0038	.0022	.0012	.0007	.0005	.0004	.0003
1,1,4,4-tetramethyl	.0027	.0027	.0019	.0011	.0006	.0004	.0003	.0002	.0001
1-propyl-2-methyl, trans*	.0004	.0004	.0021	.0038	.0045	.0045	.0043	.0041	.0039
1-propyl-2-methyl, cis*	.0001	.0001	.0008	.0017	.0023	.0026	.0026	.0026	.0026
1-propyl-3-methyl, trans*	.0004	.0004	.0021	.0038	.0045	.0045	.0043	.0041	.0039
1-propyl-3-methyl, cis*	.0054	.0056	.0154	.0193	.0174	.0143	.0118	.0100	.0087
1-propyl-4-methyl, cis	.0002	.0002	.0010	.0019	.0023	.0023	.0022	.0020	.0019
1-propyl-4-methyl, trans	.0027	.0028	.0077	.0096	.0087	.0072	.0059	.0050	.0044
1-isopropyl-2-methyl, trans*	.0001	.0001	.0007	.0013	.0015	.0015	.0014	.0014	.0013
1-isopropyl-2-methyl, cis*	.0000	.0000	.0001	.0003	.0004	.0005	.0005	.0006	.0006
1-isopropyl-3-methyl, trans*	.0000	.0000	.0003	.0006	.0008	.0009	.0009	.0009	.0009
1-isopropyl-3-methyl, cis*	.0005	.0005	.0019	.0029	.0030	.0027	.0024	.0021	.0019
1-isopropyl-4-methyl, trans	.0002	.0002	.0009	.0014	.0015	.0013	.0012	.0011	.0010
1-isopropyl-4-methyl, cis	.0000	.0000	.0001	.0003	.0004	.0004	.0004	.0004	.0004
1-ethyl-1,2-dimethyl, trans*	.0001	.0001	.0005	.0008	.0009	.0009	.0008	.0008	.0008
1-ethyl-1,2-dimethyl, cis*	.0001	.0001	.0005	.0008	.0009	.0009	.0008	.0008	.0008
1-ethyl-1,3-dimethyl, trans*	.0014	.0015	.0034	.0039	.0034	.0028	.0023	.0020	.0018
1-ethyl-1,3-methyl, cis*	.0014	.0015	.0034	.0039	.0034	.0028	.0023	.0020	.0018
1-ethyl-1,4-dimethyl, trans	.0007	.0007	.0017	.0019	.0017	.0014	.0011	.0010	.0009
1-ethyl-1,4-dimethyl, cis	.0007	.0007	.0017	.0019	.0017	.0014	.0011	.0010	.0009
1-ethyl-2,2-dimethyl*	.0014	.0015	.0034	.0039	.0034	.0028	.0023	.0020	.0018
1-ethyl-3,3-dimethyl*	.0055	.0056	.0092	.0086	.0066	.0049	.0038	.0031	.0026
1-ethyl-4,4-dimethyl	.0028	.0028	.0046	.0043	.0033	.0024	.0019	.0015	.0013
1-ethyl-2,3-dimethyl, cis cis*	.0003	.0003	.0012	.0019	.0020	.0018	.0017	.0015	.0014
1-ethyl-2,3-dimethyl, cis trans*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-2,3-dimethyl, trans cis*	.0041	.0042	.0089	.0094	.0076	.0058	.0045	.0037	.0031
1-ethyl-2,3-dimethyl, trans trans*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-3,4-dimethyl, cis cis*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-3,4-dimethyl, trans cis*	.0160	.0162	.0244	.0211	.0149	.0103	.0075	.0057	.0046
1-ethyl-3,4-dimethyl, cis trans*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-3,4-dimethyl, trans trans*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-3,5-dimethyl, cis cis	.0308	.0310	.0333	.0236	.0146	.0092	.0062	.0045	.0035
1-ethyl-3,5-dimethyl, trans cis*	.0041	.0042	.0089	.0094	.0076	.0058	.0045	.0037	.0031
1-ethyl-3,5-dimethyl, trans trans	.0021	.0021	.0045	.0047	.0038	.0029	.0023	.0018	.0016
1-ethyl-2,4-dimethyl, cis cis*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-2,4-dimethyl, trans trans*	.0160	.0162	.0244	.0211	.0149	.0103	.0075	.0057	.0046
1-ethyl-2,4-dimethyl, cis trans*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-2,4-dimethyl, trans cis*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-2,5-dimethyl, cis cis*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-2,5-dimethyl, trans trans*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-2,5-dimethyl, cis trans*	.0011	.0011	.0033	.0042	.0039	.0033	.0027	.0023	.0021
1-ethyl-2,6-dimethyl, cis cis	.0001	.0001	.0006	.0009	.0010	.0009	.0008	.0008	.0007
1-ethyl-2,6-dimethyl, trans cis*	.0041	.0042	.0089	.0094	.0076	.0058	.0045	.0037	.0031
1-ethyl-2,6-dimethyl, trans trans	.0001	.0001	.0004	.0008	.0010	.0010	.0010	.0010	.0009
1,1,2,3-tetramethyl, cis*	.0244	.0245	.0219	.0142	.0085	.0053	.0036	.0027	.0021
1,1,2,3-tetramethyl, trans*	.0042	.0043	.0053	.0042	.0029	.0020	.0015	.0011	.0009
1,1,3,4-tetramethyl, cis*	.0627	.0624	.0399	.0212	.0111	.0063	.0040	.0028	.0021
1,1,3,4-tetramethyl, trans*	.0163	.0163	.0146	.0095	.0057	.0035	.0024	.0018	.0014
1,1,2,4-tetramethyl, cis*	.0042	.0043	.0053	.0042	.0029	.0020	.0015	.0011	.0009
1,1,2,4-tetramethyl, trans*	.2421	.2388	.1091	.0474	.0216	.0112	.0066	.0043	.0031
1,1,3,5-tetramethyl, cis	.0163	.0163	.0146	.0095	.0057	.0035	.0024	.0018	.0014
1,1,3,5-tetramethyl, trans*	.0005	.0006	.0010	.0009	.0007	.0006	.0004	.0004	.0003
1,2,2,3-tetramethyl, cis	.0005	.0006	.0010	.0009	.0007	.0006	.0004	.0004	.0003
1,2,2,3-tetramethyl, trans*	.0021	.0021	.0037	.0021	.0014	.0010	.0007	.0006	.0005
1,2,2,4-tetramethyl, cis*	.0081	.0082	.0073	.0047	.0028	.0018	.0012	.0009	.0007
1,2,2,4-tetramethyl, trans*	.0003	.0003	.0007	.0008	.0008	.0006	.0005	.0005	.0004
1,2,3,4-tetramethyl, cis cis cis	.0032	.0032	.0051	.0046	.0033	.0024	.0017	.0014	.0011
1,2,3,4-tetramethyl, cis cis trans*	.0004	.0004	.0009	.0010	.0009	.0007	.0005	.0004	.0004
1,2,3,4-tetramethyl, cis trans trans*	.0470	.0471	.0385	.0231	.0128	.0075	.0048	.0033	.0025
1,2,3,4-tetramethyl, trans cis trans*	.0016	.0016	.0026	.0023	.0017	.0012	.0009	.0007	.0006
1,2,3,4-tetramethyl, trans cis cis*	.0008	.0008	.0019	.0021	.0017	.0013	.0011	.0009	.0007
1,2,3,4-tetramethyl, trans trans cis*	.0122	.0123	.0141	.0103	.0065	.0042	.0029	.0021	.0017
1,2,3,5-tetramethyl, cis cis cis	.0008	.0008	.0019	.0021	.0017	.0013	.0011	.0009	.0007
1,2,3,5-tetramethyl, trans trans trans	.0061	.0062	.0070	.0052	.0033	.0021	.0014	.0011	.0008
1,2,3,5-tetramethyl, cis trans trans*	.0016	.0016	.0026	.0023	.0017	.0012	.0009	.0007	.0006
1,2,3,5-tetramethyl, cis cis trans*	.0122	.0123	.0141	.0103	.0065	.0042	.0029	.0021	.0017
1,2,3,5-tetramethyl, trans cis trans*	.0032	.0032	.0051	.0046	.0033	.0024	.0017	.0014	.0011
1,2,3,5-tetramethyl, trans trans cis*	.0122	.0123	.0141	.0103	.0065	.0042	.0029	.0021	.0017
1,2,3,5-tetramethyl, cis trans cis*	.1815	.1802	.1053	.0516	.0250	.0133	.0079	.0052	.0037
1,2,3,5-tetramethyl, cis trans cis*	.0008	.0008	.0019	.0021	.0017	.0013	.0011	.0009	.0007
1,2,4,5-tetramethyl, cis cis cis	.0122	.0123	.0141	.0103	.0065	.0042	.0029	.0021	.0017
1,2,4,5-tetramethyl, trans trans trans*	.0002	.0002	.0005	.0005	.0004	.0003	.0003	.0002	.0002
1,2,4,5-tetramethyl, cis trans trans	.0042	.0042	.0051	.0046	.0033	.0024	.0017	.0014	.0011
1,2,4,5-tetramethyl, trans cis trans*	.0454	.0450	.0263	.0129	.0063	.0033	.0020	.0013	.0009
1,2,4,5-tetramethyl, trans trans cis	.0454	.0450	.0263	.0129	.0063	.0033	.0020	.0013	.0009

Table 25. Standard heat capacity at constant pressure for alkylcyclopentanes in J/K mol

T/K		298.15	300	400	500	600	700	800	900	1000
C5H10	cyclopentane	87.81	88.47	122.36	152.62	179.24	202.23	221.58	237.30	249.38
C6H12	methylcyclopentane	104.09	104.90	146.63	183.75	216.27	244.19	267.50	286.22	300.33
C7H14	ethyl	132.73	133.64	180.14	221.58	257.96	289.30	315.58	336.81	352.99
	1,2-dimethyl, trans*	131.67	132.60	179.80	221.79	258.57	290.13	316.48	337.61	353.53
	1,2-dimethyl, cis	126.02	126.97	175.35	218.34	255.93	288.14	314.95	336.37	352.40
	1,3-dimethyl, trans*	131.67	132.60	179.80	221.79	258.57	290.13	316.48	337.61	353.53
	1,3-dimethyl, cis	131.67	132.60	179.80	221.79	258.57	290.13	316.48	337.61	353.53
	1,1-dimethyl	136.08	136.03	184.27	226.98	264.16	295.80	321.92	342.52	357.58
C8H16	1,1,2-trimethyl*	151.36	152.46	208.53	258.11	301.18	337.76	367.85	391.44	408.53
	1-ethyl-2-methyl*	149.01	150.07	204.40	252.71	294.99	331.26	361.51	385.73	403.94
	1-ethyl-3-methyl, cis*	154.66	155.70	208.86	256.16	297.63	333.25	363.03	386.97	405.06
	1-ethyl-3-methyl, trans*	154.66	155.70	208.86	256.16	297.63	333.25	363.03	386.97	405.06
	1-ethyl-1-methyl	158.08	159.14	213.32	261.35	303.21	338.92	368.48	391.87	409.11
	isopropyl	154.66	155.70	208.86	256.16	297.63	333.25	363.03	386.97	405.06
	n-propyl	155.73	156.75	209.19	255.95	297.02	332.42	362.14	386.17	404.52
	1-2-3-trimethyl, cis cis	142.30	143.40	199.61	249.47	292.96	330.10	360.88	385.29	403.35
	1-2-3-trimethyl, trans trans*	147.95	149.03	204.07	252.92	295.60	332.09	362.40	386.53	404.48
	1,2,3-trimethyl, cis cis	153.60	154.66	208.52	256.38	298.24	334.08	363.93	387.77	405.60
	1,2,4-trimethyl, cis cis	147.95	149.03	204.07	252.92	295.60	332.09	362.40	386.53	404.48
	1,2,4-trimethyl, cis trans*	147.95	149.03	204.07	252.92	295.60	332.09	362.40	386.53	404.48
	1,2,4-trimethyl, trans trans*	147.95	149.03	204.07	252.92	295.60	332.09	362.40	386.53	404.48
C9H18	n-butyl	178.72	179.86	238.24	290.32	336.08	375.54	408.69	435.53	456.06
	1-propyl-2-methyl, cis*	172.00	173.18	233.45	287.08	334.05	374.38	408.06	435.09	455.47
	1-propyl-2-methyl, trans*	177.66	178.81	237.91	290.53	336.69	376.37	409.58	436.33	456.60
	1-propyl-3-methyl, cis*	177.66	178.81	237.91	290.53	336.69	376.37	409.58	436.33	456.60
	1-propyl-3-methyl, trans*	177.66	178.81	237.91	290.53	336.69	376.37	409.58	436.33	456.60
	1-propyl-1-methyl	181.07	182.24	242.37	295.72	342.27	382.05	415.03	441.23	460.64
	1,2-diethyl, cis	172.00	173.18	233.45	287.08	334.05	374.38	408.06	435.09	455.47
	1,2-diethyl, trans*	177.66	178.81	237.91	290.53	336.69	376.37	409.58	436.33	456.60
	1,3-diethyl, cis*	177.66	178.81	237.91	290.53	336.69	376.37	409.58	436.33	456.60
	1,3-diethyl, trans*	177.66	178.81	237.91	290.53	336.69	376.37	409.58	436.33	456.60
	1,1-diethyl	181.07	182.24	242.37	295.72	342.27	382.05	415.03	441.23	460.64
	1-ethyl-1,2-dimethyl, cis*	174.35	175.57	237.58	292.48	340.24	380.88	414.40	440.79	460.06
	1-ethyl-1,2-dimethyl, trans*	174.35	175.57	237.58	292.48	340.24	380.88	414.40	440.79	460.06
	1-ethyl-2,2-dimethyl*	174.35	175.57	237.58	292.48	340.24	380.88	414.40	440.79	460.06
	1-ethyl-2,3-dimethyl, cis cis*	165.29	166.50	228.66	283.84	332.02	373.22	407.43	434.65	454.89
	1-ethyl-2,3-dimethyl, trans trans*	170.94	172.13	233.12	287.29	334.66	375.21	408.96	435.89	456.01
	1-ethyl-2,3-dimethyl, trans cis*	176.60	177.76	237.57	290.75	337.29	377.20	410.48	437.12	457.13
	1-ethyl-2,3-dimethyl, cis trans*	170.94	172.13	233.12	287.29	334.66	375.21	408.96	435.89	456.01
	1-ethyl-2,4-dimethyl, cis cis*	170.94	172.13	233.12	287.29	334.66	375.21	408.96	435.89	456.01
	1-ethyl-2,4-dimethyl, trans cis*	176.60	177.76	237.57	290.75	337.29	377.20	410.48	437.12	457.13
	1-ethyl-2,4-dimethyl, cis trans*	170.94	172.13	233.12	287.29	334.66	375.21	408.96	435.89	456.01
	1-ethyl-2,4-dimethyl, trans trans*	176.60	177.76	237.57	290.75	337.29	377.20	410.48	437.12	457.13
	1-ethyl-1,5-dimethyl, cis cis	165.29	166.50	228.66	283.84	332.02	373.22	407.43	434.65	454.89
	1-ethyl-1,5-dimethyl, cis trans*	170.94	172.13	233.12	287.29	334.66	375.21	408.96	435.89	456.01
	1-ethyl-1,5-dimethyl, trans trans*	176.60	177.76	237.57	290.75	337.29	377.20	410.48	437.12	457.13
	1-ethyl-3,3-dimethyl*	180.01	181.20	242.04	295.93	342.88	382.88	415.93	442.03	461.18
	1-ethyl-3,4-dimethyl, cis cis	170.94	172.13	233.12	287.29	334.66	375.21	408.96	435.89	456.01
	1-ethyl-3,4-dimethyl, trans cis*	176.60	177.76	237.57	290.75	337.29	377.20	410.48	437.12	457.13
	1-ethyl-3,4-dimethyl, trans trans*	170.94	172.13	233.12	287.29	334.66	375.21	408.96	435.89	456.01
	1,2,3,4-tetramethyl, cis cis cis	158.57	159.83	223.88	280.60	329.99	372.06	406.80	434.21	454.30
	1,2,3,4-tetramethyl, trans trans trans*	164.23	165.46	228.33	284.05	332.63	374.05	408.33	435.45	455.43
	1,2,3,4-tetramethyl, trans cis cis*	169.88	171.09	232.79	287.51	335.26	376.04	409.85	436.69	456.55
	1,2,3,4-tetramethyl, cis trans trans*	164.23	165.46	228.33	284.05	332.63	374.05	408.33	435.45	455.43
	1,2,3,4-tetramethyl, trans trans cis	169.88	171.09	232.79	287.51	335.26	376.04	409.85	436.69	456.55
	1,1,2,2-tetramethyl	165.40	166.69	232.80	290.96	341.16	383.40	417.69	444.02	462.40
	1,1,3,3-tetramethyl	182.36	183.58	246.17	301.33	349.07	389.38	422.27	447.73	465.77
	1,2,3,4-tetramethyl, trans cis trans*	175.54	176.72	237.24	290.97	337.90	378.04	411.38	437.92	457.67
	isobutyl	177.66	178.81	237.91	290.53	336.69	376.37	409.58	436.33	456.60
	1-methylpropyl	177.66	178.81	237.91	290.53	336.69	376.37	409.58	436.33	456.60
	1,1-dimethylethyl	180.01	181.20	242.04	295.93	342.88	382.88	415.93	442.03	461.18
	1-isopropyl-2-methyl, cis*	170.94	172.13	233.12	287.29	334.66	375.21	408.96	435.89	456.01
	1-isopropyl-2-methyl, trans*	176.60	177.76	237.57	290.75	337.29	377.20	410.48	437.12	457.13
	1-isopropyl-3-methyl, cis*	176.60	177.76	237.57	290.75	337.29	377.20	410.48	437.12	457.13
	1-isopropyl-3-methyl, trans*	176.60	177.76	237.57	290.75	337.29	377.20	410.48	437.12	457.13

THERMODYNAMIC PROPERTIES OF ALKYL CYCLOPENTANES AND ALKYL CYCLOHEXANES 1123

Table 26. Standard entropy for alkylcyclopentanes in J/K mol

T/K		298.15	300	400	500	600	700	800	900	1000
C5H10	cyclopentane	292.25	292.80	322.98	353.60	383.84	413.24	441.55	468.59	494.25
C6H12	methylcyclopentane	339.59	340.23	376.24	413.03	449.47	484.97	519.15	551.78	582.71
C7H14	ethyl	379.00	379.82	424.76	469.50	513.19	555.37	595.78	634.22	670.59
	1,2-dimethyl, trans*	367.77	368.59	413.33	458.06	501.82	544.12	584.64	623.19	659.63
	1,2-dimethyl, cis	367.77	368.56	411.84	455.68	498.89	540.83	581.12	619.51	655.82
	1,3-dimethyl, trans*	367.77	368.59	413.33	458.06	501.82	544.12	584.64	623.19	659.63
	1,3-dimethyl, cis	367.77	368.59	413.33	458.06	501.82	544.12	584.64	623.19	659.63
	1,1-dimethyl	355.57	356.41	402.28	448.09	492.84	536.01	577.27	616.43	653.35
C8H16	1,1,2-trimethyl*	395.28	396.22	447.91	499.89	550.86	600.12	647.25	692.01	734.19
	1-ethyl-2-methyl*	412.95	413.87	464.63	515.54	565.45	613.72	660.00	704.03	745.67
	1-ethyl-3-methyl, cis*	412.95	413.91	466.12	517.92	568.38	617.01	663.51	707.71	749.47
	1-ethyl-3-methyl, trans*	412.95	413.91	466.12	517.92	568.38	617.01	663.51	707.71	749.47
	1-ethyl-1-methyl	400.74	401.72	455.07	507.95	559.39	608.89	656.15	700.96	743.19
	isopropyl	407.19	408.15	460.36	512.15	562.61	611.24	657.75	701.95	743.71
	n-propyl	418.41	419.38	471.79	523.60	573.98	622.50	668.89	712.99	754.67
	1-2-3-trimethyl, cis cis	395.96	396.84	445.95	495.96	545.39	593.42	639.58	683.55	725.14
	1-2-3-trimethyl, trans trans*	401.72	402.64	453.20	504.10	554.08	602.47	648.86	693.00	734.70
	1,2,3-trimethyl, cis cis	395.96	396.91	448.93	500.71	551.24	599.99	646.61	690.91	732.74
	1,2,4-trimethyl, cis cis	395.96	396.88	447.44	498.34	548.32	596.70	643.09	687.23	728.94
	1,2,4-trimethyl, cis trans	395.96	396.88	447.44	498.34	548.32	596.70	643.09	687.23	728.94
	1,2,4-trimethyl, trans trans*	401.72	402.64	453.20	504.10	554.08	602.47	648.86	693.00	734.70
C9H18	n-butyl	457.83	458.94	518.82	577.70	634.77	689.62	742.00	791.75	838.75
	1-propyl-2-methyl, cis*	452.36	453.43	511.67	569.64	626.24	680.84	733.11	782.80	829.75
	1-propyl-2-methyl, trans*	452.36	453.47	513.15	572.02	629.16	684.13	736.63	786.48	833.55
	1-propyl-3-methyl, cis*	452.36	453.47	513.15	572.02	629.16	684.13	736.63	786.48	833.55
	1-propyl-3-methyl, trans*	452.36	453.47	513.15	572.02	629.16	684.13	736.63	786.48	833.55
	1-propyl-1-methyl	440.16	441.28	502.11	562.05	620.18	676.02	729.26	779.72	827.27
	1,2-diethyl, cis	446.60	447.67	505.90	563.88	620.47	676.08	727.35	777.03	823.99
	1,2-diethyl, trans*	446.60	447.70	507.39	566.25	623.40	678.37	730.86	780.71	827.79
	1,3-diethyl, cis*	452.36	453.47	513.15	572.02	629.16	684.13	736.63	786.48	833.55
	1,3-diethyl, trans*	446.60	447.70	507.39	566.25	623.40	678.37	730.86	780.71	827.79
	1,1-diethyl	434.39	435.52	496.34	556.28	614.42	670.25	723.50	773.96	821.51
	1-ethyl-1,2-dimethyl, cis*	434.69	435.78	494.95	553.99	611.65	667.24	720.37	770.77	818.27
	1-ethyl-1,2-dimethyl, trans*	434.69	435.78	494.95	553.99	611.65	667.24	720.37	770.77	818.27
	1-ethyl-2,2-dimethyl*	434.69	435.78	494.95	553.99	611.65	667.24	720.37	770.77	818.27
	1-ethyl-2,3-dimethyl, cis cis*	441.14	442.16	498.74	555.82	611.94	666.30	718.45	768.08	814.98
	1-ethyl-2,3-dimethyl, trans trans*	441.14	442.20	500.23	558.20	614.87	669.59	721.97	771.76	818.79
	1-ethyl-2,3-dimethyl, trans cis*	441.14	442.23	501.72	560.57	617.80	672.87	725.49	775.44	822.59
	1-ethyl-2,3-dimethyl, cis trans*	441.14	442.20	500.23	558.20	614.87	669.59	721.97	771.76	818.79
	1-ethyl-2,4-dimethyl, cis cis*	441.14	442.20	500.23	558.20	614.87	669.59	721.97	771.76	818.79
	1-ethyl-2,4-dimethyl, trans cis*	441.14	442.23	501.72	560.57	617.80	672.87	725.49	775.44	822.59
	1-ethyl-2,4-dimethyl, cis trans*	441.14	442.20	500.23	558.20	614.87	669.59	721.97	771.76	818.79
	1-ethyl-2,4-dimethyl, trans trans*	441.14	442.23	501.72	560.57	617.80	672.87	725.49	775.44	822.59
	1-ethyl-1,5-dimethyl, cis cis	435.37	436.40	492.98	550.06	606.18	660.54	712.69	762.32	809.22
	1-ethyl-1,5-dimethyl, cis trans*	441.14	442.20	500.23	558.20	614.87	669.59	721.97	771.76	818.79
	1-ethyl-1,5-dimethyl, trans trans*	441.14	442.23	501.72	560.57	617.80	672.87	725.49	775.44	822.59
	1-ethyl-1,3-dimethyl*	434.69	435.81	496.44	556.36	614.57	670.52	723.88	774.45	822.07
	1-ethyl-3,4-dimethyl, cis cis	435.37	436.43	494.47	552.43	609.10	663.83	716.21	766.00	813.02
	1-ethyl-3,4-dimethyl, trans cis*	441.14	442.23	501.72	560.57	617.80	672.87	725.49	775.44	822.59
	1-ethyl-3,4-dimethyl, trans trans*	441.14	442.20	500.23	558.20	614.87	669.59	721.97	771.76	818.79
	1,2,3,4-tetramethyl, cis cis cis	424.15	425.13	480.06	536.24	591.88	646.00	698.03	747.60	794.45
	1,2,3,4-tetramethyl, trans trans trans*	429.91	430.93	487.31	544.38	600.57	655.05	707.31	757.04	804.02
	1,2,3,4-tetramethyl, trans cis cis*	429.91	430.97	488.80	546.75	603.50	658.33	710.83	760.72	807.82
	1,2,3,4-tetramethyl, cis trans trans*	424.15	425.17	481.55	538.62	594.81	649.29	701.55	751.28	798.26
	1,2,3,4-tetramethyl, trans trans cis	424.15	425.20	483.04	540.99	597.74	652.57	705.07	754.96	802.06
	1,1,2,2-tetramethyl	405.50	406.52	463.72	522.07	579.67	635.54	689.06	739.86	787.66
	1,1,3,3-tetramethyl	405.50	406.63	468.19	529.19	588.46	645.39	699.61	750.89	799.07
	1,2,3,4-tetramethyl, trans cis trans*	424.15	425.24	484.53	543.36	600.67	655.85	708.59	758.64	805.86
	isobutyl	446.60	447.70	507.39	566.25	623.40	678.37	730.86	780.71	827.79
	1-methylpropyl	446.60	447.70	507.39	566.25	623.40	678.37	730.86	780.71	827.79
	1,1-dimethylethyl	419.80	420.91	481.54	541.47	599.68	655.63	708.99	759.55	807.17
	1-isopropyl-2-methyl, cis*	441.14	442.20	500.23	558.20	614.87	669.59	721.97	771.76	818.79
	1-isopropyl-2-methyl, trans*	441.14	442.23	501.72	560.57	617.80	672.87	725.49	775.44	822.59
	1-isopropyl-3-methyl, cis*	441.14	442.23	501.72	560.57	617.80	672.87	725.49	775.44	822.59
	1-isopropyl-3-methyl, trans*	441.14	442.23	501.72	560.57	617.80	672.87	725.49	775.44	822.59

Table 27. Standard enthalpy of formation for alkylcyclopentanes in kJ/mol

T/K		298.15	300	400	500	600	700	800	900	1000
C5H10	cyclopentane	-76.78	-76.97	-86.08	-93.58	-99.51	-103.94	-107.11	-109.20	-110.42
C6H12	methylcyclopentane	-102.59	-102.83	-113.83	-122.81	-129.83	-135.01	-138.66	-141.01	-142.35
C7H14	ethyl	-124.06	-124.31	-136.14	-145.79	-153.35	-158.89	-162.75	-165.18	-166.47
	1,2-dimethyl, trans*	-136.77	-137.03	-148.93	-158.59	-166.10	-171.57	-175.34	-177.68	-178.90
	1,2-dimethyl, cis	-132.59	-132.85	-145.25	-155.31	-163.13	-168.83	-172.78	-175.25	-176.59
	1,3-dimethyl, trans*	-136.77	-137.03	-148.93	-158.59	-166.10	-171.57	-175.34	-177.68	-178.90
	1,3-dimethyl, cis	-136.77	-137.03	-148.93	-158.59	-166.10	-171.57	-175.34	-177.68	-178.90
	1,1-dimethyl	-139.41	-139.66	-151.16	-160.33	-167.30	-172.21	-175.43	-177.68	-178.01
C8H16	1,1,2-trimethyl*	-165.23	-165.51	-178.91	-189.56	-197.63	-203.28	-206.97	-209.06	-209.94
	1-ethyl-2-methyl*	-149.87	-150.16	-163.89	-175.02	-183.67	-189.96	-194.30	-196.99	-198.39
	1-ethyl-3-methyl, cis*	-154.05	-154.34	-167.56	-178.30	-186.64	-192.71	-196.87	-199.42	-200.71
	1-ethyl-3-methyl, trans*	-154.05	-154.34	-167.56	-178.30	-186.64	-192.71	-196.87	-199.42	-200.71
	1-ethyl-1-methyl	-153.34	-153.62	-166.44	-176.70	-184.50	-190.00	-193.61	-195.64	-196.47
	isopropyl	-150.71	-150.99	-164.21	-174.95	-183.30	-189.36	-193.52	-196.08	-197.36
	n-propyl	-144.68	-144.96	-158.12	-168.85	-177.24	-183.38	-187.63	-190.27	-191.62
	1-2-3-trimethyl, cis cis	-158.41	-158.71	-173.00	-184.54	-193.45	-199.90	-204.32	-207.06	-208.51
	1-2-3-trimethyl, trans trans*	-162.59	-162.88	-176.68	-187.82	-196.42	-202.64	-206.89	-209.49	-210.83
	1,2,3-trimethyl, cis cis	-166.77	-167.06	-180.35	-191.09	-199.39	-205.38	-209.46	-211.93	-213.14
	1,2,4-trimethyl, cis cis	-162.59	-162.88	-176.68	-187.82	-196.42	-202.64	-206.89	-209.49	-210.83
	1,2,4-trimethyl, cis trans	-162.59	-162.88	-176.68	-187.82	-196.42	-202.64	-206.89	-209.49	-210.83
	1,2,4-trimethyl, trans trans*	-162.59	-162.88	-176.68	-187.82	-196.42	-202.64	-206.89	-209.49	-210.83
C9H18	n-butyl	-165.31	-165.62	-180.10	-191.91	-201.13	-207.86	-212.50	-215.95	-216.77
	1-propyl-2-methyl, cis*	-170.50	-170.82	-185.87	-198.08	-207.56	-214.45	-219.18	-222.08	-223.55
	1-propyl-2-methyl, trans*	-174.68	-174.99	-189.54	-201.36	-210.54	-217.19	-221.75	-224.51	-225.86
	1-propyl-3-methyl, cis*	-174.68	-174.99	-189.54	-201.36	-210.54	-217.19	-221.75	-224.51	-225.86
	1-propyl-3-methyl, trans*	-174.68	-174.99	-189.54	-201.36	-210.54	-217.19	-221.75	-224.51	-225.86
	1-propyl-1-methyl	-173.97	-174.27	-188.42	-199.76	-208.39	-214.48	-218.48	-220.72	-221.63
	1,2-diethyl, cis	-167.15	-167.47	-182.52	-194.73	-204.21	-211.10	-215.83	-218.73	-220.20
	1,2-diethyl, trans*	-171.33	-171.65	-186.19	-198.01	-207.19	-213.84	-218.40	-221.16	-222.51
	1,3-diethyl, cis*	-171.33	-171.65	-186.19	-198.01	-207.19	-213.84	-218.40	-221.16	-222.51
	1,3-diethyl, trans*	-171.33	-171.65	-186.19	-198.01	-207.19	-213.84	-218.40	-221.16	-222.51
	1,1-diethyl	-167.28	-167.58	-181.73	-193.06	-201.70	-207.79	-211.79	-214.03	-214.93
	1-ethyl-1,2-dimethyl, cis*	-179.16	-179.48	-194.19	-205.93	-214.82	-221.07	-225.15	-227.45	-228.40
	1-ethyl-1,2-dimethyl, trans*	-179.16	-179.48	-194.19	-205.93	-214.82	-221.07	-225.15	-227.45	-228.40
	1-ethyl-2,2-dimethyl*	-182.51	-182.82	-197.54	-209.27	-218.17	-224.42	-228.50	-230.79	-231.75
	1-ethyl-2,3-dimethyl, cis cis*	-175.69	-176.02	-191.64	-204.25	-213.99	-221.03	-225.85	-228.80	-230.32
	1-ethyl-2,3-dimethyl, trans trans*	-179.87	-180.19	-195.31	-207.53	-216.97	-223.78	-228.42	-231.23	-232.63
	1-ethyl-2,3-dimethyl, trans cis*	-184.05	-184.37	-198.98	-210.80	-219.94	-226.52	-230.99	-233.67	-234.95
	1-ethyl-2,3-dimethyl, cis trans*	-179.87	-180.19	-195.31	-207.53	-216.97	-223.78	-228.42	-231.23	-232.63
	1-ethyl-2,4-dimethyl, cis cis*	-179.87	-180.19	-195.31	-207.53	-216.97	-223.78	-228.42	-231.23	-232.63
	1-ethyl-2,4-dimethyl, trans cis*	-184.05	-184.37	-198.98	-210.80	-219.94	-226.52	-230.99	-233.67	-234.95
	1-ethyl-2,4-dimethyl, cis trans*	-179.87	-180.19	-195.31	-207.53	-216.97	-223.78	-228.42	-231.23	-232.63
	1-ethyl-2,4-dimethyl, trans trans*	-184.05	-184.37	-198.98	-210.80	-219.94	-226.52	-230.99	-233.67	-234.95
	1-ethyl-1,5-dimethyl, cis cis	-175.69	-176.02	-191.64	-204.25	-213.99	-221.03	-225.85	-228.80	-230.32
	1-ethyl-1,5-dimethyl, cis trans*	-179.87	-180.19	-195.31	-207.53	-216.97	-223.78	-228.42	-231.23	-232.63
	1-ethyl-1,5-dimethyl, trans trans*	-184.05	-184.37	-198.98	-210.80	-219.94	-226.52	-230.99	-233.67	-234.95
	1-ethyl-3,3-dimethyl*	-186.69	-187.00	-201.21	-212.55	-221.14	-227.16	-231.07	-233.23	-234.06
	1-ethyl-3,4-dimethyl, cis cis	-179.87	-180.19	-195.31	-207.53	-216.97	-223.78	-228.42	-231.23	-232.63
	1-ethyl-3,4-dimethyl, trans cis*	-184.05	-184.37	-198.98	-210.80	-219.94	-226.52	-230.99	-233.67	-234.95
	1-ethyl-3,4-dimethyl, trans trans*	-179.87	-180.19	-195.31	-207.53	-216.97	-223.78	-228.42	-231.23	-232.63
	1,2,3,4-tetramethyl, cis cis cis	-184.22	-184.57	-200.76	-213.77	-223.77	-230.97	-235.87	-238.87	-240.44
	1,2,3,4-tetramethyl, trans trans trans*	-188.41	-188.74	-204.43	-217.04	-226.74	-233.71	-238.44	-241.30	-242.75
	1,2,3,4-tetramethyl, trans cis cis*	-192.59	-192.91	-208.10	-220.32	-229.72	-236.46	-241.01	-243.74	-245.07
	1,2,3,4-tetramethyl, cis trans trans*	-188.41	-188.74	-204.43	-217.04	-226.74	-233.71	-238.44	-241.30	-242.75
	1,2,3,4-tetramethyl, trans trans cis	-192.59	-192.91	-208.10	-220.32	-229.72	-236.46	-241.01	-243.74	-245.07
	1,1,2,2-tetramethyl	-189.49	-189.83	-205.22	-217.26	-226.18	-232.25	-236.04	-238.00	-238.66
	1,1,3,3-tetramethyl	-202.05	-202.35	-216.23	-227.09	-235.10	-240.48	-243.74	-245.29	-245.61
	1,2,3,4-tetramethyl, trans cis trans*	-196.77	-197.09	-211.77	-223.60	-232.69	-239.20	-243.58	-246.17	-247.39
	isobutyl	-171.33	-171.65	-186.19	-198.01	-207.19	-213.84	-218.40	-221.16	-222.51
	1-methylpropyl	-167.99	-168.30	-182.84	-194.66	-203.84	-210.50	-215.05	-217.81	-219.17
	1,1-dimethylethyl	-176.52	-176.85	-191.17	-202.51	-211.10	-217.12	-221.03	-223.19	-224.02
	1-isopropyl-2-methyl, cis*	-180.71	-181.02	-195.63	-207.46	-216.59	-223.17	-227.64	-230.32	-231.60
	1-isopropyl-2-methyl, trans*	-180.71	-181.02	-195.63	-207.46	-216.59	-223.17	-227.64	-230.32	-231.60
	1-isopropyl-3-methyl, cis*	-180.71	-181.02	-195.63	-207.46	-216.59	-223.17	-227.64	-230.32	-231.60
	1-isopropyl-3-methyl, trans*	-180.71	-181.02	-195.63	-207.46	-216.59	-223.17	-227.64	-230.32	-231.60

THERMODYNAMIC PROPERTIES OF ALKYL CYCLOPENTANES AND ALKYL CYCLOHEXANES 1125

Table 28. Standard Gibbs energy of formation for alkylcyclopentanes in kJ/mol

T/K		298.15	300	400	500	600	700	800	900	1000
C5H10	cyclopentane	39.41	40.12	80.59	123.16	167.06	211.89	257.19	302.89	348.78
C6H12	methylcyclopentane	40.15	41.02	90.71	142.92	196.73	251.62	307.07	362.97	419.09
C7H14	ethyl	47.60	48.65	108.18	170.41	234.36	299.47	365.18	431.37	497.77
	1,2-dimethyl, trans*	38.23	39.30	99.96	163.34	228.43	294.68	361.50	428.79	496.30
	1,2-dimethyl, cis	42.41	43.48	104.23	167.80	233.16	299.72	366.88	434.54	502.42
	1,3-dimethyl, trans*	38.23	39.30	99.96	163.34	228.43	294.68	361.50	428.79	496.30
	1,3-dimethyl, cis	38.23	39.30	99.96	163.34	228.43	294.68	361.50	428.79	496.30
	1,1-dimethyl	39.23	40.32	102.15	166.57	232.61	299.71	367.31	435.31	503.47
C8H16	1,1,2-trimethyl*	42.24	43.51	115.32	190.15	266.85	344.78	423.29	502.25	581.39
	1-ethyl-2-methyl*	52.33	53.56	123.65	196.87	272.06	348.58	425.77	503.49	581.46
	1-ethyl-3-methyl, cis*	48.14	49.38	119.38	192.40	267.33	343.54	420.38	497.75	575.34
	1-ethyl-3-methyl, trans*	48.14	49.38	119.38	192.40	267.33	343.54	420.38	497.75	575.34
	1-ethyl-1-methyl	52.49	53.75	124.92	198.99	274.86	351.92	429.54	507.61	585.86
	isopropyl	53.21	54.46	125.04	198.63	274.13	350.92	428.34	506.28	584.45
	n-propyl	55.89	57.11	126.56	199.01	273.37	349.02	425.32	502.16	579.23
	1-2-3-trimethyl, cis cis	48.86	50.12	122.01	197.14	274.32	352.86	432.08	511.85	591.87
	1-2-3-trimethyl, trans trans*	42.95	44.21	115.43	189.79	266.13	343.78	422.09	500.92	579.99
	1,2,3-trimethyl, cis cis	40.49	41.76	113.47	188.21	264.85	342.77	421.31	500.36	579.64
	1,2,4-trimethyl, cis cis	44.67	45.94	117.74	192.68	269.58	347.81	426.70	506.11	585.75
	1,2,4-trimethyl, cis trans	44.67	45.94	117.74	192.68	269.58	347.81	426.70	506.11	585.75
	1,2,4-trimethyl, trans trans*	42.95	44.21	115.43	189.79	266.13	343.78	422.09	500.92	579.99
C9H18	n-butyl	64.17	65.58	144.94	227.61	312.38	398.57	485.47	572.95	660.68
	1-propyl-2-methyl, cis*	60.61	62.03	142.03	225.47	311.07	398.13	485.91	574.28	662.92
	1-propyl-2-methyl, trans*	56.43	57.84	137.76	221.00	306.34	393.08	480.53	568.54	656.80
	1-propyl-3-methyl, cis*	56.43	57.84	137.76	221.00	306.34	393.08	480.53	568.54	656.80
	1-propyl-3-methyl, trans*	56.43	57.84	137.76	221.00	306.34	393.08	480.53	568.54	656.80
	1-propyl-1-methyl	60.78	62.22	143.30	227.59	313.87	401.47	489.68	578.40	667.31
	1,2-diethyl, cis	65.68	67.10	147.68	231.69	317.87	405.51	493.87	582.81	672.03
	1,2-diethyl, trans*	61.49	62.92	143.42	227.23	313.14	400.46	488.48	577.07	665.91
	1,3-diethyl, cis*	59.78	61.19	141.11	224.35	309.68	396.43	483.87	571.88	660.15
	1,3-diethyl, trans*	61.49	62.92	143.42	227.23	313.14	400.46	488.48	577.07	665.91
	1,1-diethyl	69.19	70.64	152.30	237.16	324.02	412.20	500.99	590.28	679.77
	1-ethyl-1,2-dimethyl, cis*	57.22	58.67	140.39	225.45	312.56	401.03	490.13	579.73	669.54
	1-ethyl-1,2-dimethyl, trans*	57.22	58.67	140.39	225.45	312.56	401.03	490.13	579.73	669.54
	1-ethyl-2,2-dimethyl*	53.87	55.32	137.04	222.10	309.21	397.68	486.78	576.39	666.20
	1-ethyl-2,3-dimethyl, cis cis*	58.77	60.21	141.43	226.20	313.21	401.72	490.96	580.80	670.91
	1-ethyl-2,3-dimethyl, trans trans*	54.59	56.02	137.16	221.74	308.48	396.67	485.58	575.06	664.79
	1-ethyl-2,3-dimethyl, trans cis*	50.40	51.84	132.89	217.28	303.75	391.63	480.19	569.31	658.67
	1-ethyl-2,3-dimethyl, cis trans*	54.59	56.02	137.16	221.74	308.48	396.67	485.58	575.06	664.79
	1-ethyl-2,4-dimethyl, cis cis*	54.59	56.02	137.16	221.74	308.48	396.67	485.58	575.06	664.79
	1-ethyl-2,4-dimethyl, trans cis*	50.40	51.84	132.89	217.28	303.75	391.63	480.19	569.31	658.67
	1-ethyl-2,4-dimethyl, cis trans*	54.59	56.02	137.16	221.74	308.48	396.67	485.58	575.06	664.79
	1-ethyl-2,4-dimethyl, trans cis*	50.40	51.84	132.89	217.28	303.75	391.63	480.19	569.31	658.67
	1-ethyl-1,5-dimethyl, cis cis	60.49	61.94	143.73	229.09	316.67	405.75	495.57	585.99	676.67
	1-ethyl-1,5-dimethyl, cis trans*	54.59	56.02	137.16	221.74	308.48	396.67	485.58	575.06	664.79
	1-ethyl-1,5-dimethyl, trans trans*	50.40	51.84	132.89	217.28	303.75	391.63	480.19	569.31	658.67
	1-ethyl-3,3-dimethyl*	49.69	51.14	132.78	217.63	304.48	392.64	481.40	570.64	660.08
	1-ethyl-3,4-dimethyl, cis cis	56.31	57.75	139.47	224.62	311.94	400.71	490.19	580.24	670.56
	1-ethyl-3,4-dimethyl, trans cis*	50.40	51.84	132.89	217.28	303.75	391.63	480.19	569.31	658.67
	1-ethyl-3,4-dimethyl, trans trans*	54.59	56.02	137.16	221.74	308.48	396.67	485.58	575.06	664.79
	1,2,3,4-tetramethyl, cis cis cis	55.30	56.77	139.78	226.48	315.47	405.99	497.28	589.16	681.32
	1,2,3,4-tetramethyl, trans trans trans*	49.40	50.86	133.21	219.13	307.28	396.92	487.28	578.23	669.44
	1,2,3,4-tetramethyl, trans cis cis*	45.22	46.67	128.95	214.67	302.55	391.88	481.90	572.49	663.32
	1,2,3,4-tetramethyl, cis trans trans*	51.12	52.58	135.52	222.02	310.74	400.95	491.89	583.42	675.20
	1,2,3,4-tetramethyl, trans trans cis	46.93	48.40	131.25	217.55	306.01	395.91	486.51	577.67	669.08
	1,1,2,2-tetramethyl	55.59	57.09	141.85	230.07	320.38	412.04	504.29	597.01	689.89
	1,1,3,3-tetramethyl	43.04	44.54	129.05	216.68	306.19	396.91	488.14	579.78	671.54
	1,2,3,4-tetramethyl, trans cis trans*	42.75	44.22	126.98	213.09	301.28	390.87	481.13	571.93	662.97
	isobutyl	61.49	62.92	143.42	227.23	313.14	400.46	488.48	577.07	665.91
	1-methylpropyl	64.84	66.27	146.76	230.58	316.49	403.81	491.83	580.42	669.26
	1,1-dimethylethyl	64.17	65.65	148.78	235.13	323.46	413.11	503.35	594.09	685.02
	1-isopropyl-2-methyl, cis*	57.94	59.37	140.51	225.09	311.83	400.02	488.92	578.40	668.14
	1-isopropyl-2-methyl, trans*	53.75	55.19	136.24	220.63	307.10	394.98	483.54	572.66	662.02
	1-isopropyl-3-methyl, cis*	53.75	55.19	136.24	220.63	307.10	394.98	483.54	572.66	662.02
	1-isopropyl-3-methyl, trans*	53.75	55.19	136.24	220.63	307.10	394.98	483.54	572.66	662.02

Table 29. Standard heat capacity at constant pressure for alkylcyclohexanes in J/K mol

T/K		298.15	300	400	500	600	700	800	900	1000
C6H12	cyclohexane	113.24	114.08	156.89	195.19	228.96	258.21	282.93	303.14	318.82
C7H14	methylcyclohexane	135.17	136.14	185.61	229.78	268.62	302.16	330.38	353.29	370.89
C8H16	ethyl	158.17	159.25	214.67	264.15	307.68	345.28	376.94	402.65	422.43
	1,1-dimethyl	160.52	161.63	218.80	269.54	313.87	351.78	383.28	408.35	427.01
	1,2-dimethyl, trans*	157.11	158.20	214.33	264.36	308.29	346.11	377.83	403.45	422.96
	1,2-dimethyl, cis	157.11	158.20	214.33	264.36	308.29	346.11	377.83	403.45	422.96
	1,3-dimethyl, cis	157.11	158.20	214.33	264.36	308.29	346.11	377.83	403.45	422.96
	1,3-dimethyl, trans*	157.11	158.20	214.33	264.36	308.29	346.11	377.83	403.45	422.96
	1,4-dimethyl, cis	157.11	158.20	214.33	264.36	308.29	346.11	377.83	403.45	422.96
	1,4-dimethyl, trans	157.11	158.20	214.33	264.36	308.29	346.11	377.83	403.45	422.96
C9H18	n-propyl	181.16	182.35	243.72	298.52	346.74	388.40	423.49	452.01	473.96
	1-ethyl-1-methyl	183.51	184.74	247.85	303.92	352.93	394.91	429.83	457.71	478.55
	1-ethyl-2-methyl, cis*	180.10	181.31	243.39	298.73	347.35	389.23	424.39	452.81	474.50
	1-ethyl-2-methyl, trans*	180.10	181.31	243.39	298.73	347.35	389.23	424.39	452.81	474.50
	1-ethyl-3-methyl, cis*	180.10	181.31	243.39	298.73	347.35	389.23	424.39	452.81	474.50
	1-ethyl-3-methyl, trans*	180.10	181.31	243.39	298.73	347.35	389.23	424.39	452.81	474.50
	1-ethyl-4-methyl, cis*	180.10	181.31	243.39	298.73	347.35	389.23	424.39	452.81	474.50
	1-ethyl-4-methyl, trans*	180.10	181.31	243.39	298.73	347.35	389.23	424.39	452.81	474.50
	1,2,3-trimethyl, cis cis	179.04	180.26	243.05	298.95	347.95	390.06	425.28	453.61	475.04
	1,2,3-trimethyl, trans trans*	179.04	180.26	243.05	298.95	347.95	390.06	425.28	453.61	475.04
	1,2,3-trimethyl, trans cis	179.04	180.26	243.05	298.95	347.95	390.06	425.28	453.61	475.04
	1,2,4-trimethyl, cis cis*	179.04	180.26	243.05	298.95	347.95	390.06	425.28	453.61	475.04
	1,2,4-trimethyl, trans trans*	179.04	180.26	243.05	298.95	347.95	390.06	425.28	453.61	475.04
	1,2,4-trimethyl, trans cis*	179.04	180.26	243.05	298.95	347.95	390.06	425.28	453.61	475.04
	1,2,4-trimethyl, cis trans*	179.04	180.26	243.05	298.95	347.95	390.06	425.28	453.61	475.04
	1,3,5-trimethyl, cis cis	179.04	180.26	243.05	298.95	347.95	390.06	425.28	453.61	475.04
	1,3,5-trimethyl, cis trans	179.04	180.26	243.05	298.95	347.95	390.06	425.28	453.61	475.04
	1,1,2-trimethyl*	182.45	183.70	247.52	304.13	353.54	395.74	430.73	458.51	479.08
	isopropyl	180.10	181.31	243.39	298.73	347.35	389.23	424.39	452.81	474.50
C10H20	n-butyl	204.15	205.46	272.77	332.89	385.80	431.52	470.04	501.37	525.49
	1,1-dimethylethyl	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1-methylpropyl*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	isobutyl	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-propyl-1-methyl	206.50	207.85	276.90	338.29	391.99	438.03	476.38	507.07	530.08
	1-isopropyl-1-methyl	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1,1-diethyl	206.50	207.85	276.90	338.29	391.99	438.03	476.38	507.07	530.08
	1,2-diethyl, trans*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1,2-diethyl, cis	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1,3-diethyl, trans*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1,3-diethyl, cis	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1,4-diethyl, trans	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1,1,2,2-tetramethyl	207.79	209.19	280.70	343.90	398.79	445.36	483.62	513.57	535.21
	1,1,3,3-tetramethyl	207.79	209.19	280.70	343.90	398.79	445.36	483.62	513.57	535.21
	1,1,4,4-tetramethyl	207.79	209.19	280.70	343.90	398.79	445.36	483.62	513.57	535.21
	1-propyl-2-methyl, trans*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-propyl-2-methyl, cis*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-propyl-3-methyl, trans*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-propyl-3-methyl, cis*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-propyl-4-methyl, cis	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-propyl-4-methyl, trans	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-isopropyl-2-methyl, trans*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-isopropyl-2-methyl, cis*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-isopropyl-3-methyl, trans*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-isopropyl-3-methyl, cis*	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-isopropyl-4-methyl, trans	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-isopropyl-4-methyl, cis	203.09	204.42	272.44	333.10	386.41	432.35	470.94	502.16	526.03
	1-ethyl-1,2-dimethyl, trans*	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1-ethyl-1,2-dimethyl, cis*	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1-ethyl-1,3-dimethyl, trans*	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1-ethyl-1,3-dimethyl, cis*	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1-ethyl-1,4-dimethyl, trans	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1-ethyl-1,4-dimethyl, cis	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1-ethyl-2,2-dimethyl*	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1-ethyl-3,3-dimethyl*	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1-ethyl-4,4-dimethyl	205.44	206.80	276.57	338.50	392.60	438.86	477.28	507.87	530.62
	1-ethyl-2,3-dimethyl, cis cis*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,3-dimethyl, cis trans*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,3-dimethyl, trans trans*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-3,4-dimethyl, cis cis*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-3,4-dimethyl, trans cis*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-3,4-dimethyl, cis trans*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-3,4-dimethyl, trans trans*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-3,5-dimethyl, cis cis	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-3,5-dimethyl, trans cis*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-3,5-dimethyl, trans trans	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,4-dimethyl, cis cis*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,4-dimethyl, trans trans*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,4-dimethyl, cis trans*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,4-dimethyl, trans cis*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,5-dimethyl, cis cis*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,5-dimethyl, cis trans*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,5-dimethyl, trans trans*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,5-dimethyl, trans cis*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,6-dimethyl, cis cis	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,6-dimethyl, trans cis*	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57
	1-ethyl-2,6-dimethyl, trans trans	202.03	203.37	272.11	333.32	387.01	433.19	471.83	502.96	526.57

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Table 29. Standard heat capacity at constant pressure for alkylcyclohexanes in J/K mol--Continued

T/K	298.15	300	400	500	600	700	800	900	1000
1,1,2,3-tetramethyl, cis*	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,1,2,3-tetramethyl, trans*	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,1,3,4-tetramethyl, cis*	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,1,3,4-tetramethyl, trans*	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,1,2,4-tetramethyl, cis*	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,1,2,4-tetramethyl, trans*	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,1,3,5-tetramethyl, cis	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,1,3,5-tetramethyl, trans*	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,2,2,3-tetramethyl, cis	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,2,2,3-tetramethyl, trans*	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,2,2,4-tetramethyl, cis*	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,2,2,4-tetramethyl, trans*	204.38	205.76	276.24	338.72	393.20	439.69	478.18	508.67	531.16
1,2,3,4-tetramethyl, cis cis cis	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,4-tetramethyl, cis cis trans*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,4-tetramethyl, cis trans trans*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,4-tetramethyl, trans cis trans*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,4-tetramethyl, trans cis cis*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,4-tetramethyl, trans trans cis*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,5-tetramethyl, cis cis cis	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,5-tetramethyl, trans trans trans	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,5-tetramethyl, cis trans trans*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,5-tetramethyl, cis cis trans*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,5-tetramethyl, trans cis trans*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,5-tetramethyl, trans trans cis*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,3,5-tetramethyl, cis trans cis*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,4,5-tetramethyl, cis cis cis	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,4,5-tetramethyl, trans trans trans*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,4,5-tetramethyl, cis trans trans	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,4,5-tetramethyl, trans cis trans*	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11
1,2,4,5-tetramethyl, trans trans cis	200.97	202.32	271.77	333.54	387.62	434.02	472.73	503.76	527.11

Table 30. Standard entropy for alkylcyclohexanes in J/K mol

T/K	298.15	300	400	500	600	700	800	900	1000
C6H12 cyclohexane	294.59	295.29	334.08	373.29	411.93	449.48	485.62	520.16	552.95
C7H14 methylcyclohexane	343.44	344.27	390.34	436.60	482.01	526.01	568.26	608.54	646.72
C8H16 ethyl	382.85	383.83	437.38	490.70	542.80	593.13	641.37	687.31	730.81
1,1-dimethyl	359.42	360.41	414.89	469.29	522.45	573.76	622.86	669.52	713.56
1,2-dimethyl, trans*	371.62	372.60	425.94	479.26	531.43	581.87	630.23	676.27	719.84
1,2-dimethyl, cis	371.62	372.60	425.94	479.26	531.43	581.87	630.23	676.27	719.84
1,3-dimethyl, cis	371.62	372.60	425.94	479.26	531.43	581.87	630.23	676.27	719.84
1,3-dimethyl, trans*	371.62	372.60	425.94	479.26	531.43	581.87	630.23	676.27	719.84
1,4-dimethyl, cis	365.86	366.83	420.18	473.49	525.67	576.11	624.47	670.51	714.08
1,4-dimethyl, trans	365.86	366.83	420.18	473.49	525.67	576.11	624.47	670.51	714.08
C9H18 n-propyl	422.26	423.39	484.41	544.80	603.59	660.25	714.48	766.07	814.89
1-ethyl-1-methyl	404.59	405.73	467.69	529.15	589.00	646.65	701.74	754.04	803.41
1-ethyl-2-methyl, cis*	416.80	417.92	478.74	539.12	597.98	654.76	709.10	760.80	809.69
1-ethyl-2-methyl, trans*	416.80	417.92	478.74	539.12	597.98	654.76	709.10	760.80	809.69
1-ethyl-3-methyl, cis*	416.80	417.92	478.74	539.12	597.98	654.76	709.10	760.80	809.69
1-ethyl-3-methyl, trans*	416.80	417.92	478.74	539.12	597.98	654.76	709.10	760.80	809.69
1-ethyl-4-methyl, cis*	416.80	417.92	478.74	539.12	597.98	654.76	709.10	760.80	809.69
1-ethyl-4-methyl, trans*	416.80	417.92	478.74	539.12	597.98	654.76	709.10	760.80	809.69
1,2,3-trimethyl, cis cis	399.81	400.92	461.54	521.91	580.85	637.74	692.20	744.00	792.96
1,2,3-trimethyl, trans trans*	405.57	406.68	467.31	527.68	586.62	643.50	697.97	749.76	798.72
1,2,3-trimethyl, trans cis	399.81	400.92	461.54	521.91	580.85	637.74	692.20	744.00	792.96
1,2,4-trimethyl, cis cis*	405.57	406.68	467.31	527.68	586.62	643.50	697.97	749.76	798.72
1,2,4-trimethyl, trans trans*	405.57	406.68	467.31	527.68	586.62	643.50	697.97	749.76	798.72
1,2,4-trimethyl, trans cis*	405.57	406.68	467.31	527.68	586.62	643.50	697.97	749.76	798.72
1,2,4-trimethyl, cis trans*	405.57	406.68	467.31	527.68	586.62	643.50	697.97	749.76	798.72
1,3,5-trimethyl, cis cis	390.68	391.79	452.41	512.78	571.72	628.61	683.07	734.86	783.82
1,3,5-trimethyl, cis trans	399.81	400.92	461.54	521.91	580.85	637.74	692.20	744.00	792.96
1,1,2-trimethyl*	399.13	400.26	462.02	523.47	583.39	641.15	696.36	748.77	798.21
isopropyl	411.04	412.15	472.98	533.36	592.22	649.00	703.34	755.03	803.92

Table 30. Standard entropy for alkylcyclohexanes in J/K mol--Continued

T/K		298.15	300	400	500	600	700	800	900	1000
C10H20	n-butyl	461.68	462.94	531.44	598.90	664.38	727.38	787.59	844.83	898.97
	1,1-dimethylethyl	423.65	424.92	494.16	562.67	629.29	693.38	754.58	812.64	867.39
	1-methylpropyl*	456.21	457.47	525.77	593.22	658.77	721.88	782.22	839.56	893.77
	isobutyl	450.45	451.71	520.01	587.45	653.01	716.12	776.45	833.80	888.01
	1-propyl-1-methyl	444.01	445.29	514.72	583.25	649.79	713.77	774.85	832.81	887.49
	1-isopropyl-1-methyl	432.78	434.05	503.29	571.80	638.42	702.51	763.71	821.77	876.53
	1,1-diethyl	438.24	439.52	508.96	577.49	644.03	708.01	769.09	827.04	881.73
	1,2-diethyl, trans*	450.45	451.71	520.01	587.45	653.01	716.12	776.45	833.80	888.01
	1,2-diethyl, cis	450.45	451.71	520.01	587.45	653.01	716.12	776.45	833.80	888.01
	1,3-diethyl, trans*	450.45	451.71	520.01	587.45	653.01	716.12	776.45	833.80	888.01
	1,3-diethyl, cis	450.45	451.71	520.01	587.45	653.01	716.12	776.45	833.80	888.01
	1,4-diethyl, trans	444.69	445.95	514.25	581.69	647.25	710.36	770.69	828.03	882.24
	1,1,2,2-tetramethyl	409.35	410.64	480.81	550.39	618.07	683.15	745.21	803.98	859.28
	1,1,3,3-tetramethyl	409.35	410.64	480.81	550.39	618.07	683.15	745.21	803.98	859.28
	1,1,4,4-tetramethyl	403.58	404.87	475.05	544.63	612.30	677.38	739.44	798.22	853.52
	1-propyl-2-methyl, trans*	456.21	457.47	525.77	593.22	658.77	721.88	782.22	839.56	893.77
	1-propyl-2-methyl, cis*	456.21	457.47	525.77	593.22	658.77	721.88	782.22	839.56	893.77
	1-propyl-3-methyl, trans*	456.21	457.47	525.77	593.22	658.77	721.88	782.22	839.56	893.77
	1-propyl-3-methyl, cis*	456.21	457.47	525.77	593.22	658.77	721.88	782.22	839.56	893.77
	1-propyl-4-methyl, cis	450.45	451.71	520.01	587.45	653.01	716.12	776.45	833.80	888.01
	1-propyl-4-methyl, trans	450.45	451.71	520.01	587.45	653.01	716.12	776.45	833.80	888.01
	1-isopropyl-2-methyl, trans*	447.08	448.34	516.64	584.08	649.64	712.75	773.08	830.43	884.63
	1-isopropyl-2-methyl, cis*	447.08	448.34	516.64	584.08	649.64	712.75	773.08	830.43	884.63
	1-isopropyl-3-methyl, trans*	447.08	448.34	516.64	584.08	649.64	712.75	773.08	830.43	884.63
	1-isopropyl-3-methyl, cis*	447.08	448.34	516.64	584.08	649.64	712.75	773.08	830.43	884.63
	1-isopropyl-4-methyl, trans	441.31	442.58	510.87	578.32	643.88	706.99	767.32	824.66	878.87
	1-isopropyl-4-methyl, cis	441.31	442.58	510.87	578.32	643.88	706.99	767.32	824.66	878.87
	1-ethyl-1,2-dimethyl, trans*	438.54	439.82	509.05	577.57	644.18	708.28	769.47	827.53	882.29
	1-ethyl-1,2-dimethyl, cis*	438.54	439.82	509.05	577.57	644.18	708.28	769.47	827.53	882.29
	1-ethyl-1,3-dimethyl, trans*	438.54	439.82	509.05	577.57	644.18	708.28	769.47	827.53	882.29
	1-ethyl-1,3-dimethyl, cis*	438.54	439.82	509.05	577.57	644.18	708.28	769.47	827.53	882.29
	1-ethyl-1,4-dimethyl, trans	432.78	434.05	503.29	571.80	638.42	702.51	763.71	821.77	876.53
	1-ethyl-1,4-dimethyl, cis	432.78	434.05	503.29	571.80	638.42	702.51	763.71	821.77	876.53
	1-ethyl-2,2-dimethyl*	438.54	439.82	509.05	577.57	644.18	708.28	769.47	827.53	882.29
	1-ethyl-2,3-dimethyl*	438.54	439.82	509.05	577.57	644.18	708.28	769.47	827.53	882.29
	1-ethyl-4,4-dimethyl	432.78	434.05	503.29	571.80	638.42	702.51	763.71	821.77	876.53
	1-ethyl-2,3-dimethyl, cis cis*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,3-dimethyl, cis trans*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,3-dimethyl, trans cis*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,3-dimethyl, trans trans*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-3,4-dimethyl, cis cis*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-3,4-dimethyl, cis trans*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-3,4-dimethyl, trans cis*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-3,4-dimethyl, trans trans*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-3,5-dimethyl, cis cis	439.22	440.48	508.58	576.01	641.64	704.86	765.32	822.76	877.04
	1-ethyl-3,5-dimethyl, trans cis*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-3,5-dimethyl, trans trans	439.22	440.48	508.58	576.01	641.64	704.86	765.32	822.76	877.04
	1-ethyl-2,4-dimethyl, cis cis*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,4-dimethyl, trans trans*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,4-dimethyl, cis trans*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,4-dimethyl, trans cis*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,5-dimethyl, cis cis*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,5-dimethyl, cis trans*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,5-dimethyl, trans trans*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,5-dimethyl, trans cis*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,6-dimethyl, cis cis	439.22	440.48	508.58	576.01	641.64	704.86	765.32	822.76	877.04
	1-ethyl-2,6-dimethyl, trans cis*	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1-ethyl-2,6-dimethyl, trans trans	444.99	446.24	514.34	581.77	647.41	710.63	771.08	828.52	882.80
	1,1,2,3-tetramethyl, cis*	430.69	431.96	500.99	569.49	636.19	700.39	761.71	819.87	874.69
	1,1,2,3-tetramethyl, trans*	427.32	428.58	497.62	566.12	632.82	697.02	758.34	816.50	871.32
	1,1,3,4-tetramethyl, cis*	427.32	428.58	497.62	566.12	632.82	697.02	758.34	816.50	871.32
	1,1,3,4-tetramethyl, trans*	427.32	428.58	497.62	566.12	632.82	697.02	758.34	816.50	871.32
	1,1,2,4-tetramethyl, cis*	427.32	428.58	497.62	566.12	632.82	697.02	758.34	816.50	871.32
	1,1,2,4-tetramethyl, trans*	427.32	428.58	497.62	566.12	632.82	697.02	758.34	816.50	871.32
	1,1,3,5-tetramethyl, cis	427.32	428.58	497.62	566.12	632.82	697.02	758.34	816.50	871.32
	1,1,3,5-tetramethyl, trans*	421.55	422.82	491.86	560.36	627.05	691.26	752.57	810.73	865.56
	1,2,2,3-tetramethyl, cis	421.55	422.82	491.86	560.36	627.05	691.26	752.57	810.73	865.56
	1,2,2,3-tetramethyl, trans*	421.55	422.82	491.86	560.36	627.05	691.26	752.57	810.73	865.56
	1,2,2,4-tetramethyl, cis*	421.55	422.82	491.86	560.36	627.05	691.26	752.57	810.73	865.56
	1,2,2,4-tetramethyl, trans*	427.32	428.58	497.62	566.12	632.82	697.02	758.34	816.50	871.32
	1,2,3,4-tetramethyl, cis cis cis	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,3,4-tetramethyl, cis cis trans*	428.00	429.24	497.14	564.57	630.27	693.61	754.18	811.72	866.08
	1,2,3,4-tetramethyl, cis trans trans*	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,3,4-tetramethyl, trans cis trans*	428.00	429.24	497.14	564.57	630.27	693.61	754.18	811.72	866.08
	1,2,3,4-tetramethyl, trans cis cis*	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,3,4-tetramethyl, trans trans cis*	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,3,5-tetramethyl, cis cis cis	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,3,5-tetramethyl, trans trans trans	428.00	429.24	497.14	564.57	630.27	693.61	754.18	811.72	866.08
	1,2,3,5-tetramethyl, cis trans trans*	428.00	429.24	497.14	564.57	630.27	693.61	754.18	811.72	866.08
	1,2,3,5-tetramethyl, cis cis trans*	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,3,5-tetramethyl, trans cis trans*	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,3,5-tetramethyl, trans cis cis*	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,3,5-tetramethyl, trans trans cis*	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,4,5-tetramethyl, cis cis cis	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,4,5-tetramethyl, trans trans trans*	422.23	423.48	491.38	558.80	624.51	687.85	748.41	805.96	860.31
	1,2,4,5-tetramethyl, cis trans trans	433.76	435.01	502.91	570.33	636.04	699.37	759.94	817.49	871.84
	1,2,4,5-tetramethyl, trans cis trans*	422.23	423.48	491.38	558.80	624.51	687.85	748.41	805.96	860.31
	1,2,4,5-tetramethyl, trans trans cis	422.23	423.48	491.38	558.80	624.51	687.85	748.41		

THERMODYNAMIC PROPERTIES OF ALKYLCYCLOPENTANES AND ALKYLCYCLOHEXANES 1129

Table 31. Standard enthalpy of formation for alkylcyclohexanes in kJ/mol

T/K		298.15	300	400	500	600	700	800	900	1000
C6H12	cyclohexane	-123.76	-123.98	-134.02	-141.90	-147.72	-151.57	-153.74	-154.48	-154.04
C7H14	methylcyclohexane	-153.76	-154.01	-165.44	-174.41	-181.02	-185.38	-187.86	-188.72	-188.29
C8H16	ethyl	-171.04	-171.32	-184.07	-194.12	-201.56	-206.52	-209.39	-210.46	-210.09
	1,1-dimethyl	-179.70	-179.97	-192.40	-201.97	-208.82	-213.14	-215.37	-215.83	-214.94
	1,2-dimethyl, trans*	-180.41	-180.69	-193.51	-203.57	-210.97	-215.85	-218.63	-219.62	-219.18
	1,2-dimethyl, cis	-177.07	-177.34	-190.16	-200.22	-207.62	-212.50	-215.28	-216.27	-215.83
	1,3-dimethyl, cis	-183.76	-184.04	-196.86	-206.91	-214.31	-219.20	-221.98	-222.96	-222.53
	1,3-dimethyl, trans*	-177.07	-177.34	-190.16	-200.22	-207.62	-212.50	-215.28	-216.27	-215.83
	1,4-dimethyl, cis	-177.07	-177.34	-190.16	-200.22	-207.62	-212.50	-215.28	-216.27	-215.83
	1,4-dimethyl, trans	-183.76	-184.04	-196.86	-206.91	-214.31	-219.20	-221.98	-222.96	-222.53
C9H18	n-propyl	-191.67	-191.97	-206.05	-217.18	-225.45	-231.00	-234.26	-235.54	-235.24
	1-ethyl-1-methyl	-193.64	-193.94	-207.68	-218.33	-226.02	-230.93	-233.55	-234.22	-233.40
	1-ethyl-2-methyl, cis*	-191.00	-191.31	-205.45	-216.58	-224.82	-230.29	-233.46	-234.66	-234.29
	1-ethyl-2-methyl, trans*	-197.69	-198.00	-212.14	-223.28	-231.51	-236.99	-240.16	-241.35	-240.99
	1-ethyl-3-methyl, cis*	-201.04	-201.35	-215.49	-226.62	-234.86	-240.34	-243.51	-244.70	-244.33
	1-ethyl-3-methyl, trans*	-194.35	-194.65	-208.80	-219.93	-228.16	-233.64	-236.81	-238.01	-237.64
	1-ethyl-4-methyl, cis*	-194.35	-194.65	-208.80	-219.93	-228.16	-233.64	-236.81	-238.01	-237.64
	1-ethyl-4-methyl, trans*	-201.04	-201.35	-215.49	-226.62	-234.86	-240.34	-243.51	-244.70	-244.33
	1,2,3-trimethyl, cis cis	-200.37	-200.68	-214.89	-226.03	-234.22	-239.62	-242.71	-243.82	-243.38
	1,2,3-trimethyl, trans trans*	-200.37	-200.68	-214.89	-226.03	-234.22	-239.62	-242.71	-243.82	-243.38
	1,2,3-trimethyl, trans cis	-207.07	-207.37	-221.59	-232.72	-240.91	-246.32	-249.40	-250.51	-250.07
	1,2,4-trimethyl, cis cis*	-203.72	-204.03	-218.24	-229.38	-237.57	-242.97	-246.05	-247.16	-246.73
	1,2,4-trimethyl, trans trans*	-210.41	-210.72	-224.93	-236.07	-244.26	-249.67	-252.75	-253.86	-253.42
	1,2,4-trimethyl, trans cis*	-203.72	-204.03	-218.24	-229.38	-237.57	-242.97	-246.05	-247.16	-246.73
	1,2,4-trimethyl, cis trans*	-203.72	-204.03	-218.24	-229.38	-237.57	-242.97	-246.05	-247.16	-246.73
	1,3,5-trimethyl, cis cis	-213.76	-214.07	-228.28	-239.42	-247.61	-253.01	-256.10	-257.21	-256.77
	1,3,5-trimethyl, cis trans	-207.07	-207.37	-221.59	-232.72	-240.91	-246.32	-249.40	-250.51	-250.07
	1,1,2-trimethyl*	-203.01	-203.31	-217.12	-227.78	-235.43	-240.26	-242.79	-243.38	-242.49
	isopropyl	-197.69	-198.00	-212.14	-223.28	-231.51	-236.99	-240.16	-241.35	-240.99
C10H20	n-butyl	-212.30	-212.63	-228.03	-240.24	-249.35	-255.49	-259.14	-260.63	-260.40
	1,1-dimethylethyl	-223.63	-223.96	-239.10	-250.83	-259.32	-264.75	-267.66	-268.46	-267.65
	1-methylpropyl*	-218.32	-218.66	-234.12	-246.34	-255.40	-261.47	-265.03	-266.44	-266.14
	isobutyl	-218.32	-218.66	-234.12	-246.34	-255.40	-261.47	-265.03	-266.44	-266.14
	1-propyl-1-methyl	-214.26	-214.59	-229.66	-241.39	-249.91	-255.42	-258.42	-259.31	-258.56
	1-isopropyl-1-methyl	-223.63	-223.96	-239.10	-250.83	-259.32	-264.75	-267.66	-268.46	-267.65
	1,1-diethyl	-207.57	-207.90	-222.97	-234.69	-243.22	-248.72	-251.73	-252.61	-251.86
	1,2-diethyl, trans*	-214.97	-215.31	-230.78	-242.99	-252.06	-258.13	-261.69	-263.09	-262.79
	1,2-diethyl, cis	-211.63	-211.96	-227.43	-239.64	-248.71	-254.78	-258.34	-259.75	-259.44
	1,3-diethyl, trans*	-211.63	-211.96	-227.43	-239.64	-248.71	-254.78	-258.34	-259.75	-259.44
	1,3-diethyl, cis	-218.32	-218.66	-234.12	-246.34	-255.40	-261.47	-265.03	-266.44	-266.14
	1,4-diethyl, trans	-218.32	-218.66	-234.12	-246.34	-255.40	-261.47	-265.03	-266.44	-266.14
	1,1,2,2-tetramethyl	-225.60	-225.93	-240.73	-251.99	-259.89	-264.68	-266.95	-267.14	-265.80
	1,1,3,3-tetramethyl	-235.64	-235.97	-250.78	-262.03	-269.93	-274.72	-276.99	-277.18	-275.85
	1,1,4,4-tetramethyl	-235.64	-235.97	-250.78	-262.03	-269.93	-274.72	-276.99	-277.18	-275.85
	1-propyl-2-methyl, trans*	-214.97	-215.31	-230.78	-242.99	-252.06	-258.13	-261.69	-263.09	-262.79
	1-propyl-2-methyl, cis*	-211.63	-211.96	-227.43	-239.64	-248.71	-254.78	-258.34	-259.75	-259.44
	1-propyl-3-methyl, trans*	-214.97	-215.31	-230.78	-242.99	-252.06	-258.13	-261.69	-263.09	-262.79
	1-propyl-3-methyl, cis*	-221.67	-222.00	-237.47	-249.68	-258.75	-264.82	-268.38	-269.79	-269.49
	1-propyl-4-methyl, cis	-214.97	-215.31	-230.78	-242.99	-252.06	-258.13	-261.69	-263.09	-262.79
	1-propyl-4-methyl, trans	-221.67	-222.00	-237.47	-249.68	-258.75	-264.82	-268.38	-269.79	-269.49
	1-isopropyl-2-methyl, trans*	-214.97	-215.31	-230.78	-242.99	-252.06	-258.13	-261.69	-263.09	-262.79
	1-isopropyl-2-methyl, cis*	-208.28	-208.61	-224.08	-236.29	-245.36	-251.43	-254.99	-256.40	-256.10
	1-isopropyl-3-methyl, trans*	-211.63	-211.96	-227.43	-239.64	-248.71	-254.78	-258.34	-259.75	-259.44
	1-isopropyl-3-methyl, cis*	-218.32	-218.66	-234.12	-246.34	-255.40	-261.47	-265.03	-266.44	-266.14
	1-isopropyl-4-methyl, trans	-218.32	-218.66	-234.12	-246.34	-255.40	-261.47	-265.03	-266.44	-266.14
	1-isopropyl-4-methyl, cis	-211.63	-211.96	-227.43	-239.64	-248.71	-254.78	-258.34	-259.75	-259.44
	1-ethyl-1,2-dimethyl, trans*	-216.94	-217.27	-232.41	-244.14	-252.62	-258.06	-260.97	-261.77	-260.95
	1-ethyl-1,2-dimethyl, cis*	-216.94	-217.27	-232.41	-244.14	-252.62	-258.06	-260.97	-261.77	-260.95
	1-ethyl-1,3-dimethyl, trans*	-223.63	-223.96	-239.10	-250.83	-259.32	-264.75	-267.66	-268.46	-267.65
	1-ethyl-1,3-dimethyl, cis*	-223.63	-223.96	-239.10	-250.83	-259.32	-264.75	-267.66	-268.46	-267.65
	1-ethyl-1,4-dimethyl, trans	-223.63	-223.96	-239.10	-250.83	-259.32	-264.75	-267.66	-268.46	-267.65
	1-ethyl-1,4-dimethyl, cis	-223.63	-223.96	-239.10	-250.83	-259.32	-264.75	-267.66	-268.46	-267.65
	1-ethyl-2,2-dimethyl*	-223.63	-223.96	-239.10	-250.83	-259.32	-264.75	-267.66	-268.46	-267.65
	1-ethyl-3,3-dimethyl*	-226.98	-227.31	-242.45	-254.18	-262.66	-268.10	-271.01	-271.81	-270.99
	1-ethyl-4,4-dimethyl	-226.98	-227.31	-242.45	-254.18	-262.66	-268.10	-271.01	-271.81	-270.99
	1-ethyl-2,3-dimethyl, cis cis*	-217.65	-217.99	-233.52	-245.74	-254.76	-260.76	-264.23	-265.56	-265.19
	1-ethyl-2,3-dimethyl, cis trans*	-221.00	-221.34	-236.87	-249.09	-258.11	-264.11	-267.58	-268.90	-268.53
	1-ethyl-2,3-dimethyl, trans cis*	-224.35	-224.68	-240.22	-252.43	-261.46	-267.46	-270.93	-272.25	-271.88
	1-ethyl-2,3-dimethyl, trans trans*	-221.00	-221.34	-236.87	-249.09	-258.11	-264.11	-267.58	-268.90	-268.53
	1-ethyl-3,4-dimethyl, cis cis*	-221.00	-221.34	-236.87	-249.09	-258.11	-264.11	-267.58	-268.90	-268.53
	1-ethyl-3,4-dimethyl, cis trans*	-227.69	-228.03	-243.56	-255.78	-264.81	-270.80	-274.28	-275.60	-275.23
	1-ethyl-3,4-dimethyl, trans trans*	-221.00	-221.34	-236.87	-249.09	-258.11	-264.11	-267.58	-268.90	-268.53
	1-ethyl-3,4-dimethyl, trans cis*	-221.00	-221.34	-236.87	-249.09	-258.11	-264.11	-267.58	-268.90	-268.53
	1-ethyl-3,5-dimethyl, cis cis	-231.04	-231.38	-246.91	-259.13	-268.15	-274.15	-277.62	-278.94	-278.57
	1-ethyl-3,5-dimethyl, trans cis*	-224.35	-224.68	-240.22	-252.43	-261.46	-267.46	-270.93	-272.25	-271.88
	1-ethyl-3,5-dimethyl, trans trans	-224.35	-224.68	-240.22	-252.43	-261.46	-267.46	-270.93	-272.25	-271.88
	1-ethyl-2,4-dimethyl, cis cis*	-221.00	-221.34	-236.87	-249.09	-258.11	-264.11	-267.58	-268.90	-268.53
	1-ethyl-2,4-dimethyl, trans trans*	-227.69	-228.03	-243.56	-255.78	-264.81	-270.80	-274.28	-275.60	-275.23
	1-ethyl-2,4-dimethyl, cis trans*	-221.00	-221.34	-236.87	-249.09	-258.11	-264.11	-267.58	-268.90	-268.53
	1-ethyl-2,4-dimethyl, trans cis*	-221.00	-221.34	-236.87	-249.09	-258.11	-264.11	-267.58	-268.90	-268.53
	1-ethyl-2,5-dimethyl, cis cis*	-221.00	-221.34	-236.87	-249.09	-258.11	-264.11	-267.58	-268.90	-268.53
	1-ethyl-2,5-dimethyl, trans trans*	-221.00	-221.34	-236.87	-249.09	-258.11	-264.11	-267.58	-268.90	-268.53
	1-ethyl-2,5-dimethyl, trans cis*	-227.69	-228.03	-243.56	-255.78	-264.81	-270.80	-274.28	-275.60	-275.23
	1-ethyl-2,6-dimethyl, cis cis	-217.65	-217.99	-233.52	-245.74	-254.76	-260.76	-264.23	-265.56	-265.19
	1-ethyl-2,6-dimethyl, trans cis*	-224.35	-224.68	-240.22	-252.43	-261.46	-267.46	-270.93	-272.25	-271.88
	1-ethyl-2,6-dimethyl, trans trans	-214.30	-214.64	-230.18	-242.39	-251.42	-257.41	-260.89	-262.21	-261.84

Table 31. Standard enthalpy of formation for alkylcyclohexanes in kJ/mol--Continued

T/K		298.15	300	400	500	600	700	800	900	1000
	1,1,2,3-tetramethyl, cis*	-233.01	-233.34	-248.54	-260.28	-268.72	-274.08	-276.91	-277.62	-276.73
	1,1,2,3-tetramethyl, trans*	-229.66	-229.99	-245.20	-256.93	-265.37	-270.73	-273.56	-274.27	-273.39
	1,1,3,4-tetramethyl, cis*	-236.35	-236.69	-251.89	-263.63	-272.07	-277.43	-280.25	-280.97	-280.08
	1,1,3,4-tetramethyl, trans*	-233.01	-233.34	-248.54	-260.28	-268.72	-274.08	-276.91	-277.62	-276.73
	1,1,2,4-tetramethyl, cis*	-229.66	-229.99	-245.20	-256.93	-265.37	-270.73	-273.56	-274.27	-273.39
	1,1,2,4-tetramethyl, trans*	-239.70	-240.03	-255.24	-266.98	-275.42	-280.77	-283.60	-284.32	-283.43
	1,1,3,5-tetramethyl, cis	-233.01	-233.34	-248.54	-260.28	-268.72	-274.08	-276.91	-277.62	-276.73
	1,1,3,5-tetramethyl, trans*	-226.31	-226.64	-241.85	-253.59	-262.03	-267.39	-270.21	-270.93	-270.04
	1,2,2,3-tetramethyl, cis	-226.31	-226.64	-241.85	-253.59	-262.03	-267.39	-270.21	-270.93	-270.04
	1,2,2,3-tetramethyl, trans*	-229.66	-229.99	-245.20	-256.93	-265.37	-270.73	-273.56	-274.27	-273.39
	1,2,2,4-tetramethyl, cis*	-233.01	-233.34	-248.54	-260.28	-268.72	-274.08	-276.91	-277.62	-276.73
	1,2,2,4-tetramethyl, trans*	-222.97	-223.30	-238.50	-250.24	-258.68	-264.04	-266.86	-267.58	-266.69
	1,2,3,4-tetramethyl, cis cis cis	-227.02	-227.36	-242.96	-255.19	-264.17	-270.09	-273.48	-274.71	-274.27
	1,2,3,4-tetramethyl, cis cis trans*	-223.68	-224.01	-239.62	-251.84	-260.82	-266.74	-270.13	-271.36	-270.93
	1,2,3,4-tetramethyl, cis trans trans*	-233.72	-234.06	-249.66	-261.88	-270.86	-276.79	-280.17	-281.41	-280.97
	1,2,3,4-tetramethyl, trans cis trans*	-227.02	-227.36	-242.96	-255.19	-264.17	-270.09	-273.48	-274.71	-274.27
	1,2,3,4-tetramethyl, trans cis cis*	-223.68	-224.01	-239.62	-251.84	-260.82	-266.74	-270.13	-271.36	-270.93
	1,2,3,4-tetramethyl, trans trans cis*	-230.37	-230.71	-246.31	-258.53	-267.52	-273.44	-276.82	-278.06	-277.62
	1,2,3,5-tetramethyl, cis cis cis	-223.68	-224.01	-239.62	-251.84	-260.82	-266.74	-270.13	-271.36	-270.93
	1,2,3,5-tetramethyl, trans trans trans	-230.37	-230.71	-246.31	-258.53	-267.52	-273.44	-276.82	-278.06	-277.62
	1,2,3,5-tetramethyl, cis trans trans*	-227.02	-227.36	-242.96	-255.19	-264.17	-270.09	-273.48	-274.71	-274.27
	1,2,3,5-tetramethyl, cis cis trans*	-230.37	-230.71	-246.31	-258.53	-267.52	-273.44	-276.82	-278.06	-277.62
	1,2,3,5-tetramethyl, trans cis trans*	-227.02	-227.36	-242.96	-255.19	-264.17	-270.09	-273.48	-274.71	-274.27
	1,2,3,5-tetramethyl, trans cis trans*	-230.37	-230.71	-246.31	-258.53	-267.52	-273.44	-276.82	-278.06	-277.62
	1,2,3,5-tetramethyl, trans trans cis*	-237.07	-237.40	-253.01	-265.23	-274.21	-280.13	-283.52	-284.75	-284.32
	1,2,3,5-tetramethyl, cis trans cis*	-223.68	-224.01	-239.62	-251.84	-260.82	-266.74	-270.13	-271.36	-270.93
	1,2,4,5-tetramethyl, cis cis cis	-230.37	-230.71	-246.31	-258.53	-267.52	-273.44	-276.82	-278.06	-277.62
	1,2,4,5-tetramethyl, trans trans trans*	-223.68	-224.01	-239.62	-251.84	-260.82	-266.74	-270.13	-271.36	-270.93
	1,2,4,5-tetramethyl, cis trans trans	-227.02	-227.36	-242.96	-255.19	-264.17	-270.09	-273.48	-274.71	-274.27
	1,2,4,5-tetramethyl, trans cis trans*	-237.07	-237.40	-253.01	-265.23	-274.21	-280.13	-283.52	-284.75	-284.32
	1,2,4,5-tetramethyl, trans trans cis	-237.07	-237.40	-253.01	-265.23	-274.21	-280.13	-283.52	-284.75	-284.32

Table 32. Standard Gibbs energy of formation for alkylcyclohexanes in kJ/mol

T/K		298.15	300	400	500	600	700	800	900	1000
C6H12	cyclohexane	32.39	33.35	87.39	143.70	201.37	259.91	318.81	377.96	437.15
C7H14	methylcyclohexane	28.50	29.61	92.64	158.24	225.40	293.54	362.09	430.94	499.82
C8H16	ethyl	40.13	41.42	114.37	190.19	267.75	346.43	425.58	505.07	584.62
	1,1-dimethyl	38.46	39.79	115.04	193.05	272.70	353.37	434.41	515.71	597.01
	1,2-dimethyl, trans*	34.10	35.42	109.50	186.46	265.17	344.98	425.25	505.85	586.50
	1,2-dimethyl, cis	37.45	38.77	112.85	189.81	268.52	348.33	428.60	509.20	589.85
	1,3-dimethyl, cis	30.76	32.07	106.15	183.12	261.82	341.64	421.90	502.50	583.15
	1,3-dimethyl, trans*	37.45	38.77	112.85	189.81	268.52	348.33	428.60	509.20	589.85
	1,4-dimethyl, cis	39.17	40.49	115.15	192.69	271.98	352.36	433.21	514.38	595.61
	1,4-dimethyl, trans	32.48	33.80	108.46	186.00	265.28	345.67	426.51	507.69	588.92
C9H18	n-propyl	48.42	49.89	132.75	218.79	306.76	395.98	485.73	575.86	666.08
	1-ethyl-1-methyl	51.72	53.22	137.81	225.46	314.95	405.58	496.64	588.01	679.40
	1-ethyl-2-methyl, cis*	50.71	52.19	135.62	222.22	310.76	400.54	490.83	581.50	672.23
	1-ethyl-2-methyl, trans*	44.02	45.50	128.92	215.53	304.07	393.84	484.13	574.80	665.54
	1-ethyl-3-methyl, cis*	40.67	42.15	125.58	212.18	300.72	390.50	480.78	571.45	662.19
	1-ethyl-3-methyl, trans*	47.37	48.85	132.27	218.88	307.42	397.19	487.48	578.15	668.89
	1-ethyl-4-methyl, cis*	47.37	48.85	132.27	218.88	307.42	397.19	487.48	578.15	668.89
	1-ethyl-4-methyl, trans*	40.67	42.15	125.58	212.18	300.72	390.50	480.78	571.45	662.19
	1,2,3-trimethyl, cis cis	46.41	47.92	133.05	221.38	311.64	403.12	495.10	587.46	679.87
	1,2,3-trimethyl, trans trans*	44.69	46.19	130.75	218.50	308.18	399.09	490.49	582.27	674.11
	1,2,3-trimethyl, trans cis	39.71	41.23	126.36	214.69	304.94	396.43	488.41	580.76	673.18
	1,2,4-trimethyl, cis cis*	41.34	42.84	127.40	215.15	304.83	395.74	487.15	578.93	670.76
	1,2,4-trimethyl, trans trans*	34.65	36.15	120.71	208.46	298.14	389.05	480.45	572.23	664.07
	1,2,4-trimethyl, trans cis*	41.34	42.84	127.40	215.15	304.83	395.74	487.15	578.93	670.76
	1,2,4-trimethyl, cis trans*	41.34	42.84	127.40	215.15	304.83	395.74	487.15	578.93	670.76
	1,3,5-trimethyl, cis cis	35.74	37.27	123.32	212.56	303.73	396.13	489.02	582.29	675.62
	1,3,5-trimethyl, cis trans	39.71	41.23	126.36	214.69	304.94	396.43	488.41	580.76	673.18
	1,1,2-trimethyl*	43.97	45.49	130.63	218.86	308.91	400.09	491.69	583.60	675.51
	isopropyl	45.74	47.23	131.23	218.41	307.53	397.88	488.74	579.99	671.30

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Table 32. Standard Gibbs energy of formation for alkylcyclohexanes in kJ/mol--Continued

T/K		298.15	300	400	500	600	700	800	900	1000
C10H20	n-butyl	56.70	58.35	151.13	247.39	345.77	445.53	545.87	646.65	747.53
	1,1-dimethylethyl	56.70	58.42	154.97	254.91	356.85	460.07	563.76	667.80	771.87
	1-methylpropyl*	52.31	53.96	147.30	244.13	343.08	443.39	544.28	645.59	747.00
	isobutyl	54.03	55.69	149.61	247.01	346.54	447.43	548.89	650.78	752.76
	1-propyl-1-methyl	60.00	61.68	156.19	254.06	353.96	455.12	556.78	658.80	760.86
	1-isopropyl-1-methyl	53.98	55.68	151.32	250.34	351.37	453.67	556.45	659.58	762.73
	1,1-diethyl	68.42	70.11	165.19	263.64	364.11	465.85	568.09	670.68	773.31
	1,2-diethyl, trans*	57.37	59.04	152.96	250.36	349.88	450.77	552.23	654.13	756.11
	1,2-diethyl, cis	60.72	62.39	156.30	253.71	353.23	454.12	555.58	657.47	759.45
	1,3-diethyl, trans*	60.72	62.39	156.30	253.71	353.23	454.12	555.58	657.47	759.45
	1,3-diethyl, cis	54.03	55.69	149.61	247.01	346.54	447.43	548.89	650.78	752.76
	1,4-diethyl, trans	55.74	57.42	151.92	249.89	349.99	451.46	553.50	655.97	758.52
	1,1,2,2-tetramethyl	59.00	60.74	158.68	259.89	363.02	467.30	571.97	676.91	781.82
	1,1,3,3-tetramethyl	48.96	50.70	148.64	249.85	352.98	457.26	561.93	666.87	771.78
	1,1,4,4-tetramethyl	50.68	52.43	150.94	252.73	356.43	461.29	566.54	672.06	777.54
	1-propyl-2-methyl, trans*	55.65	57.31	150.65	247.48	346.42	446.74	547.62	648.94	750.34
	1-propyl-2-methyl, cis*	59.00	60.66	154.00	250.82	349.77	450.09	550.97	652.29	753.69
	1-propyl-3-methyl, trans*	55.65	57.31	150.65	247.48	346.42	446.74	547.62	648.94	750.34
	1-propyl-3-methyl, cis*	48.96	50.62	143.96	240.78	339.73	440.04	540.93	642.24	743.65
	1-propyl-4-methyl, cis	57.37	59.04	152.96	250.36	349.88	450.77	552.23	654.13	756.11
	1-propyl-4-methyl, trans	50.68	52.35	146.26	243.66	343.19	444.08	545.54	647.43	749.41
	1-isopropyl-2-methyl, trans*	58.38	60.05	154.31	252.04	351.91	453.13	554.93	657.16	759.48
	1-isopropyl-2-methyl, cis*	65.07	66.75	161.00	258.74	358.60	459.83	561.62	663.85	766.17
	1-isopropyl-3-methyl, trans*	61.72	63.40	157.65	255.39	355.25	456.48	558.28	660.51	762.82
	1-isopropyl-3-methyl, cis*	55.03	56.70	150.96	248.70	348.56	449.79	551.58	653.81	756.13
	1-isopropyl-4-methyl, trans	56.75	58.43	153.26	251.58	352.02	453.82	556.19	659.00	761.89
	1-isopropyl-4-methyl, cis	63.44	65.13	159.96	258.27	358.71	460.51	562.89	665.69	768.59
	1-ethyl-1,2-dimethyl, trans*	58.96	60.65	155.71	254.15	354.61	456.33	558.53	661.09	763.66
	1-ethyl-1,2-dimethyl, cis*	58.96	60.65	155.71	254.15	354.61	456.33	558.53	661.09	763.66
	1-ethyl-1,3-dimethyl, trans*	52.26	53.95	149.01	247.46	347.92	449.64	551.84	654.39	756.97
	1-ethyl-1,3-dimethyl, cis*	52.26	53.95	149.01	247.46	347.92	449.64	551.84	654.39	756.97
	1-ethyl-1,4-dimethyl, trans	63.98	65.68	161.92	250.34	351.07	453.07	555.45	658.50	762.70
	1-ethyl-1,4-dimethyl, cis	53.98	55.68	151.32	250.34	351.37	453.67	556.45	659.58	762.73
	1-ethyl-2,2-dimethyl*	52.26	53.95	149.01	247.46	347.92	449.64	551.84	654.39	756.97
	1-ethyl-3,3-dimethyl*	48.91	50.60	145.67	244.11	344.57	446.29	548.49	651.05	753.62
	1-ethyl-4,4-dimethyl	50.63	52.33	147.97	246.99	348.03	450.33	553.10	656.23	759.39
	1-ethyl-2,3-dimethyl, cis cis*	56.32	58.00	152.48	250.45	350.54	451.98	553.99	656.41	758.91
	1-ethyl-2,3-dimethyl, cis trans*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-2,3-dimethyl, trans cis*	49.63	51.31	145.78	243.75	343.84	445.29	547.29	649.72	752.22
	1-ethyl-2,3-dimethyl, trans trans*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-3,4-dimethyl, cis cis*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-3,4-dimethyl, trans cis*	46.28	47.96	142.44	240.41	340.49	441.94	543.94	646.37	748.87
	1-ethyl-3,4-dimethyl, cis trans*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-3,4-dimethyl, trans trans*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-3,5-dimethyl, cis cis	44.65	46.34	141.39	239.94	340.61	442.63	545.21	648.21	751.29
	1-ethyl-3,5-dimethyl, trans cis*	49.63	51.31	145.78	243.75	343.84	445.29	547.29	649.72	752.22
	1-ethyl-3,5-dimethyl, trans trans	51.35	53.04	148.09	246.63	347.30	449.32	551.90	654.90	757.98
	1-ethyl-2,4-dimethyl, cis cis*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-2,4-dimethyl, trans trans*	46.28	47.96	142.44	240.41	340.49	441.94	543.94	646.37	748.87
	1-ethyl-2,4-dimethyl, cis trans*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-2,4-dimethyl, trans cis*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-2,5-dimethyl, cis cis*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-2,5-dimethyl, cis trans*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-2,5-dimethyl, trans trans*	52.98	54.65	149.13	247.10	347.19	448.63	550.64	653.06	755.57
	1-ethyl-2,5-dimethyl, trans cis*	46.28	47.96	142.44	240.41	340.49	441.94	543.94	646.37	748.87
	1-ethyl-2,6-dimethyl, cis cis	58.04	59.73	154.78	253.33	353.99	456.02	558.60	661.60	764.68
	1-ethyl-2,6-dimethyl, trans cis*	49.63	51.31	145.78	243.75	343.84	445.29	547.29	649.72	752.22
	1-ethyl-2,6-dimethyl, trans trans	59.67	61.35	155.82	253.79	353.88	455.33	557.33	659.76	762.26
	1,1,2,3-tetramethyl, cis*	45.23	46.94	142.80	242.05	343.31	445.83	548.81	652.14	755.47
	1,1,2,3-tetramethyl, trans*	49.58	51.29	147.49	247.08	348.68	451.53	554.85	658.52	762.19
	1,1,3,4-tetramethyl, cis*	42.89	44.60	140.80	240.39	341.99	444.84	548.16	651.82	755.50
	1,1,3,4-tetramethyl, trans*	46.24	47.95	144.14	243.73	345.33	448.19	551.51	655.17	758.85
	1,1,2,4-tetramethyl, cis*	49.58	51.29	147.49	247.08	348.68	451.53	554.85	658.52	762.19
	1,1,2,4-tetramethyl, trans*	39.54	41.25	137.45	237.04	338.64	441.49	544.81	648.47	752.15
	1,1,3,6-tetramethyl, cis	46.24	47.95	144.14	243.73	345.33	448.19	551.51	655.17	758.85
	1,1,3,5-tetramethyl, trans*	54.65	56.37	153.14	253.31	355.49	458.92	562.81	667.05	771.30
	1,2,2,3-tetramethyl, cis	54.65	56.37	153.14	253.31	355.49	458.92	562.81	667.05	771.30
	1,2,2,3-tetramethyl, trans*	51.30	53.02	149.80	249.96	352.14	455.57	559.46	663.70	767.96
	1,2,2,4-tetramethyl, cis*	47.95	49.68	146.45	246.61	348.79	452.22	556.12	660.36	764.61
	1,2,2,4-tetramethyl, trans*	56.28	57.99	154.19	253.77	355.37	458.23	561.55	665.21	768.89
	1,2,3,4-tetramethyl, cis cis cis	50.30	52.00	147.61	246.72	347.95	450.53	553.65	657.19	760.79
	1,2,3,4-tetramethyl, cis cis trans*	55.36	57.07	153.26	252.95	354.76	457.91	561.61	665.72	769.90
	1,2,3,4-tetramethyl, cis trans trans*	43.60	45.30	140.91	240.03	341.26	443.84	546.96	650.49	754.10
	1,2,3,4-tetramethyl, trans cis trans*	52.02	53.73	149.91	249.61	351.41	454.56	558.26	662.37	766.55
	1,2,3,4-tetramethyl, trans cis cis*	53.65	55.34	150.96	250.07	351.30	453.88	557.00	660.53	764.14
	1,2,3,4-tetramethyl, trans trans cis*	46.95	48.65	144.26	243.38	344.61	447.18	550.31	653.84	757.44
	1,2,3,5-tetramethyl, cis cis cis	53.65	55.34	150.96	250.07	351.30	453.88	557.00	660.53	764.14
	1,2,3,5-tetramethyl, trans trans trans	48.67	50.38	146.57	246.26	348.06	451.22	554.92	659.03	763.21
	1,2,3,5-tetramethyl, cis trans trans*	52.02	53.73	149.91	249.61	351.41	454.56	558.26	662.37	766.55
	1,2,3,5-tetramethyl, cis cis trans*	46.95	48.65	144.26	243.38	344.61	447.18	550.31	653.84	757.44
	1,2,3,5-tetramethyl, trans cis trans*	50.30	52.00	147.61	246.72	347.95	450.53	553.65	657.19	760.79
	1,2,3,5-tetramethyl, trans cis trans*	46.95	48.65	144.26	243.38	344.61	447.18	550.31	653.84	757.44
	1,2,3,5-tetramethyl, trans trans cis*	40.26	41.96	137.57	236.68	337.91	440.49	543.61	647.15	750.75
	1,2,3,5-tetramethyl, cis trans cis*	53.65	55.34	150.96	250.07	351.30	453.88	557.00	660.53	764.14
	1,2,4,5-tetramethyl, cis cis cis	46.95	48.65	144.26	243.38	344.61	447.18	550.31	653.84	757.44
	1,2,4,5-tetramethyl, trans trans trans*	57.08	58.80	155.57	255.83	358.22	461.95	566.22	670.91	775.66
	1,2,4,5-tetramethyl, cis trans trans	50.30	52.00	147.61	246.72	347.95	450.53	553.65	657.19	760.79
	1,2,4,5-tetramethyl, trans cis trans*	43.69	45.41	142.18	242.45	344.83	448.56	552.83	657.52	762.27
	1,2,4,5-tetramethyl, trans trans cis	43.69	45.41	142.18	242.45	344.83	448.56	552.83	657.52	762.27

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