

Standard Chemical Thermodynamic Properties of Alkene Isomer Groups

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The chemical thermodynamic properties of alkene isomer groups from C_4H_8 to C_8H_{12} in the ideal gas phase have been calculated from 298.15 to 1000 K from tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher isomer groups, the properties of isomers of C_7H_{14} to C_8H_{16} have been estimated using Benson group values. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 298.15 to 1000 K. For isomer group properties increments per carbon atom have been calculated to show the extent to which thermodynamic properties of higher isomer groups may be obtained by linear extrapolation. Values of C_p° , S° , $\Delta_f H^\circ$, and $\Delta_f G^\circ$ are given for all species from C_2H_4 to C_8H_{16} in joules for a standard state pressure of 1 bar.

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

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1. Introduction

Earlier papers in this series have presented isomer group thermodynamic properties¹ for the alkanes² and alkylbenzenes.³ Significantly less thermodynamic data are available on the alkenes than on the alkanes, partly because

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of the larger number of isomers and the more rapid increase in numbers of isomers with carbon number.^{4,5} The alkene isomer group thermodynamic properties are especially important because of their large number of isomers and their high reactivity, which makes it more likely that they will be in equilibrium with each other.⁶ The thermodynamic properties have been calculated for the C_4H_8 , C_5H_{10} , and C_6H_{12} isomer groups,⁷ which is as far as data on individual species goes. However, since the increments in isomer group properties per carbon atom vary somewhat for lower members of homologous series, it is of special interest to see what the Benson group method⁸ can tell us about the properties of higher homologs. The standard thermodynamic properties of all alkenes through C_8H_{16} have been calculated using the Benson method.

2. Standard Thermodynamic Properties of Alkene Isomer Groups

When isomers are in chemical equilibrium it has been known for some time^{9,10} that they can be aggregated in calculations of equilibrium mole fractions by use of the standard Gibbs energy of formation $\Delta_f G^\circ(I)$ of the isomer group defined by

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

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

$$r_i = y_i/y_I = \exp\{\Delta_f G^\circ(I) - \Delta_f G_i^\circ\}/RT\}, \quad (2)$$

where y_I is the sum of the mole fractions of the individual isomers. The corresponding equations for the other standard thermodynamic properties $C_P^\circ(I)$, $S^\circ(I)$, and $\Delta_f H^\circ(I)$ can be derived by differentiating Eq. (1) with respect to temperature.³ When standard Gibbs energies of formation of isomer groups are used to calculate equilibrium constants for reactions of ideal gases the equilibrium expression is written in terms of equilibrium mole fractions of isomer groups.

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

$$\Delta_f G^\circ(I) = \Delta_f H^\circ(I) - T [S^\circ(I) - nS_{graphite}^\circ - nS_{H_2(g)}^\circ], \quad (3)$$

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. The numbers of chiral molecules and isomers of the alkenes are shown in Table 1. 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. Therefore the numbers of lines in tables in this article do not correspond to the total numbers of isomers; the numbers of lines, chiral molecules, and isomers are given in Table 1.

Table 1. Numbers of isomers of alkenes

	Number of lines	Number of chiral centers	Total Isomers
C_2H_4	1		1
C_3H_6	1		1
C_4H_8	4		4
C_5H_{10}	6		6
C_6H_{12}	17	1	18
C_7H_{14}	36	6	42
C_8H_{16}	93	25	118

The basic information on the chemical thermodynamic properties of the alkenes comes from statistical mechanical calculations and correlations by Kilpatrick, Prosen, Pitzer, and Rossini,^{11,12} published in 1946. Their tables for the ideal gases at 298.15 to 1000 K for all of the isomers through C_6H_{12} and for the *n*-alk-1-enes through $C_{20}H_{40}$ have been modified in subsequent tabulations.¹²⁻¹⁴ The values used in this article are from an Errata (1 December 1972) from Stull, Westrum, and Sinke; this Errata brings their values for $\Delta_f H^\circ(298.15 \text{ K})$ into considerably better agreement with the values selected by Cox and Pilcher.¹⁵

3. Calculations of Standard Thermodynamic Properties of Alkenes Using the Benson Method

Since data are available for the calculation of isomer group properties only for C_4H_8 , C_5H_{10} , and C_6H_{12} , they do not provide a very good basis for extrapolation to higher carbon numbers. Therefore the Benson group method has been used to calculate the properties for all isomers through C_8H_{16} in the ideal gas state.

In order to make these calculations, the structure of each alkene species was divided into the following Benson groups: $C(H)_3(C)$, $C(H)_2(C)_2$, $C(H)(C)_3$, $C_d(H)_2$, $C_d(H)(C)$, $C_d(C)_2$, $C(C)_4$, $C(C_d)(C)_3$, $C(C_d)(C)(H)_2$, and $C(C_d)(C)_2(H)$. In addition, the total symmetry number (TSN), number of optical isomers (OPT), cis, gauche, 2-cis, 3-ene, but-2-ene, and *t*-butyl corrections were tabulated. In view of some of the uncertainties in some of these group values indicated by Benson, the 1,5-H repulsions, which affect only several of the most highly branched species were omitted. In calculating symmetry numbers, a report by Davies, Syverud, and Steiner¹⁶ was very helpful.

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

The matrix of numbers of contributions was then matrix multiplied by a matrix of the Benson values to obtain for

Table 2. Root mean square deviations between alkene 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									
C ₂ H ₄	.96	.93	.75	.80	.55	.16	.12	.13	.27
C ₃ H ₆	.50	.52	.63	.24	.21	.39	.58	.50	.00
C ₄ H ₈	1.25	1.25	.97	.71	.63	.74	.94	.80	.37
C ₅ H ₁₀	5.23	5.85	4.52	3.37	2.33	1.61	1.43	1.17	1.07
C ₆ H ₁₂	5.68	5.65	5.29	4.67	3.74	3.25	3.24	3.25	2.46
Standard entropy in J/K mol									
C ₂ H ₄	.06	.03	.22	.36	.49	.57	.57	.54	.54
C ₃ H ₆	.03	.01	.20	.29	.33	.37	.44	.48	.55
C ₄ H ₈	3.17	3.15	3.06	2.99	2.91	2.92	2.92	2.96	2.98
C ₅ H ₁₀	3.46	3.46	3.90	4.40	4.74	4.95	5.07	5.15	5.22
C ₆ H ₁₂	3.89	3.88	3.96	4.47	5.02	5.44	5.76	6.06	6.30
Standard enthalpy of formation in kJ/mol									
C ₂ H ₄	.08	.06	.04	.03	.09	.16	.16	.11	.14
C ₃ H ₆	.96	.97	.87	.82	.77	.74	.69	.65	.64
C ₄ H ₈	1.71	1.72	1.67	1.68	1.70	1.74	1.74	1.73	1.77
C ₅ H ₁₀	2.90	2.89	2.74	2.70	2.71	2.71	2.69	2.66	2.65
C ₆ H ₁₂	2.67	2.68	2.74	2.87	2.88	3.16	3.39	3.62	3.79
Standard Gibbs energy of formation in kJ/mol									
C ₂ H ₄	.10	.07	.11	.10	.16	.19	.27	.31	.31
C ₃ H ₆	.94	.93	.93	.97	1.00	1.07	1.10	1.16	1.25
C ₄ H ₈	2.53	2.52	2.81	3.10	3.38	3.70	3.95	4.26	4.58
C ₅ H ₁₀	2.39	2.38	2.35	2.42	2.60	2.90	3.22	3.65	4.10
C ₆ H ₁₂	3.11	3.12	3.35	3.60	3.92	4.27	4.68	5.10	5.56

each isomer the sum of the contributions to $\Delta_f H^\circ_{298}$, S°_{int298} , $C_P^\circ_{300}$, $C_P^\circ_{400}$, $C_P^\circ_{500}$, $C_P^\circ_{600}$, $C_P^\circ_{800}$, and $C_P^\circ_{1000}$. In further steps in the calculation, the heat capacity values were fit to the equation

$$C_P^\circ = \alpha + \beta T + \gamma T^2, \quad (4)$$

using the least-squares criteria, and the values of α , β , and γ were used to calculate C_P° , S° , and $\Delta_f H^\circ$ from 298.15 to 1000 K,

$$S^\circ = S_0^\circ + \alpha \ln T + \beta T + (\gamma/2)T^2 - R \ln (TSN/OPT), \quad (5)$$

$$\Delta_f H^\circ = \Delta_f H_0^\circ + \alpha T + (\beta/2)T^2 + (\gamma/3)T^3$$

$$- n(H^\circ - H_{298}^\circ)_{graph} - n(H^\circ - H_{298}^\circ)_{H_2}. \quad (6)$$

The values of $\Delta_f G^\circ$ at various temperatures were then calculated using Eq. (3).

Table 2 shows how well the chemical thermodynamic properties calculated using the Benson method agree with the corrected values from Stull, Westrum, and Sinke⁷ for C₂H₄ through C₆H₁₂. 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. For C₂H₄ and C₃H₆ this yields the magnitudes of the deviations, and for the higher homologous series it yields the root-mean-square deviations at various temperatures. The average root-mean-square deviation in $\Delta_f G^\circ$ for C₆H₁₂ over the temperature range is 4 kJ mol⁻¹.

4. Tables of Standard Thermodynamic Properties of Alkene Isomer Groups

Since the International Union of Pure and Applied Chemistry has recently recommended that thermodynamic

data be given in SI units for a standard state pressure of 1 bar (10⁵ 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 $R \ln (1.013 25) = 0.109 \text{ J K}^{-1} \text{ mol}^{-1}$ at any temperature and the standard Gibbs energy of formation is reduced by $[RT \ln (1.013 25)]\delta$, where δ is the net increase (1 - n) in moles of gas in the formation reaction.¹⁷

The remaining tables in this paper have all been calculated using corrected values from Stull, Westrum, and Sinke for C₂H₄ to C₆H₁₂ and values calculated using the Benson method for C₇H₁₄ and C₈H₁₆ species. Tables 3-8 give isomer group properties and the increments per carbon atom. Table 7 gives $H^\circ(I, T) - H^\circ(I, 298.15 \text{ K})$, the standard enthalpy for an isomer group relative to the isomer group at 298.15 K. Table 8 gives values for $H^\circ(I, T) - H^\circ(I, 298.15 \text{ K}) + \Delta_f H^\circ(I, 298.15 \text{ K})$, the standard enthalpy for the isomer group relative to the elements at 298.15 K. This quantity allows the direct calculation of heat effects when the reactants and products are at different temperatures.

The increments per carbon atom are of interest because they indicate the extent to which we can estimate thermodynamic properties of isomer groups of higher carbon numbers. Since the data for C₆H₁₂ and below come from earlier calculations and the data for C₇H₁₄ and C₈H₁₆ come from the Benson method, the C₇-C₆ increment is in a sense less certain. When Benson values for C₆H₁₂ are used, the C₇-C₆ and C₈-C₇ increments are nearly the same. The increments do change with carbon number for the first several isomer groups and tend to approach constant values. The increment in the enthalpy of formation at 298.15 K is of special interest because the -20.6 kJ mol⁻¹ found by Prosen and Rossini¹⁸ for the *n*-alkanes satisfactorily fits the ex-

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

T/K	C2H4	C3H6	C4H8	C5H10	C6H12	C7H14	C8H16
298.15	43.56	63.89	98.54	113.77	141.03	171.6	192.1
300.00	43.72	64.18	99.00	115.02	141.65	172.5	193.1
400.00	53.97	79.91	119.82	146.39	177.17	211.5	238.9
500.00	63.43	94.64	137.73	173.73	208.75	244.8	278.2
600.00	71.55	107.53	153.46	196.05	234.83	274.4	313.0
700.00	78.49	118.70	167.29	214.31	256.07	300.5	343.3
800.00	84.52	128.37	179.44	229.69	274.79	322.8	369.2
900.00	89.79	136.82	190.02	242.78	290.80	341.2	390.4
1000.00	94.43	144.18	199.31	254.13	304.79	355.6	407.0

Table 3a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	20.33	34.65	15.22	27.26	30.6	20.5
300.00	20.46	34.82	16.02	26.63	30.8	20.6
400.00	25.94	39.90	26.57	30.79	34.3	27.4
500.00	31.21	43.09	35.99	35.03	36.0	33.5
600.00	35.98	45.93	42.59	38.78	39.5	38.6
700.00	40.21	48.59	47.02	41.76	44.4	42.9
800.00	43.85	51.07	50.25	45.10	48.0	46.4
900.00	47.03	53.20	52.76	48.02	50.4	49.2
1000.00	49.75	55.13	54.82	50.66	50.8	51.3

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

T/K	C2H4	C3H6	C4H8	C5H10	C6H12	C7H14	C8H16
298.15	219.56	267.05	298.83	342.26	388.00	426.9	472.5
300.00	219.85	267.47	299.48	342.98	388.90	428.0	473.7
400.00	233.87	288.09	330.94	380.41	434.58	483.1	535.7
500.00	246.92	307.55	359.62	416.07	477.57	534.0	593.3
600.00	259.23	325.96	386.18	449.80	517.93	581.3	647.2
700.00	270.81	343.41	410.87	481.41	555.74	625.6	697.7
800.00	281.69	359.89	434.04	511.04	591.19	667.2	745.3
900.00	291.94	375.54	455.80	538.89	624.50	706.3	790.1
1000.00	301.65	390.31	476.32	565.06	655.87	743.1	832.1

Table 4a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	47.49	31.78	43.43	45.74	38.9	45.5
300.00	47.61	32.02	43.49	45.93	39.1	45.7
400.00	54.22	42.84	49.47	54.18	48.6	52.5
500.00	60.63	52.07	56.45	61.50	56.4	59.3
600.00	66.73	60.22	63.62	68.14	63.3	65.9
700.00	72.59	67.46	70.54	74.33	69.8	72.2
800.00	78.20	74.15	77.00	80.15	76.0	78.1
900.00	83.60	80.26	83.09	85.61	81.8	83.8
1000.00	88.66	86.01	88.73	90.82	87.2	89.1

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

T/K	C2H4	C3H6	C4H8	C5H10	C6H12	C7H14	C8H16
298.15	52.30	20.42	-15.80	-41.76	-66.24	-88.1	-110.1
300.00	52.26	20.33	-15.91	-41.91	-66.42	-88.3	-110.3
400.00	49.25	15.73	-20.66	-48.50	-74.09	-96.5	-120.0
500.00	46.61	11.72	-24.78	-53.74	-80.40	-103.4	-128.2
600.00	44.35	8.28	-28.25	-57.76	-85.13	-108.9	-134.6
700.00	42.47	5.48	-31.02	-60.77	-88.85	-113.1	-139.4
800.00	40.88	3.22	-33.18	-62.95	-91.55	-116.1	-142.8
900.00	39.54	1.46	-34.76	-64.35	-93.33	-117.9	-144.9
1000.00	38.53	.17	-35.74	-65.09	-94.25	-118.9	-146.0

Table 5a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-31.88	-36.22	-25.96	-24.48	-21.8	-22.0
300.00	-31.92	-36.24	-26.00	-24.51	-21.8	-22.1
400.00	-33.51	-36.39	-27.84	-25.59	-22.4	-23.6
500.00	-34.89	-36.50	-28.96	-26.66	-23.0	-24.8
600.00	-36.07	-36.53	-29.51	-27.37	-23.8	-25.7
700.00	-36.99	-36.50	-29.75	-28.07	-24.3	-26.3
800.00	-37.66	-36.41	-29.76	-28.60	-24.5	-26.7
900.00	-38.07	-36.23	-29.59	-28.98	-24.6	-26.9
1000.00	-38.37	-35.91	-29.35	-29.16	-24.7	-27.0

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

T/K	C2H4	C3H6	C4H8	C5H10	C6H12	C7H14	C8H16
298.15	68.15	62.78	57.75	59.52	62.10	69.4	74.4
300.00	68.27	63.03	58.20	60.14	62.88	70.3	75.6
400.00	74.06	77.99	83.67	95.23	107.17	124.5	139.1
500.00	80.60	94.04	110.23	131.77	153.23	180.5	204.8
600.00	87.59	110.84	137.55	169.26	200.37	237.9	272.0
700.00	94.97	128.18	165.43	207.36	248.28	296.0	340.2
800.00	102.55	145.86	193.63	245.77	296.59	354.7	409.0
900.00	110.35	163.79	222.10	284.49	345.26	413.6	478.0
1000.00	118.31	181.93	250.72	323.32	394.08	472.7	547.3

Table 6a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-5.36	-5.04	1.77	2.58	7.3	5.1
300.00	-5.24	-4.84	1.94	2.74	7.4	5.2
400.00	3.93	5.68	11.56	11.95	17.3	14.6
500.00	13.44	16.19	21.54	21.46	27.3	24.3
600.00	23.24	26.71	31.70	31.11	37.5	34.2
700.00	33.21	37.25	41.93	40.91	47.7	44.2
800.00	43.31	47.77	52.14	50.82	58.1	54.3
900.00	53.44	58.31	62.39	60.77	68.4	64.4
1000.00	63.62	68.79	72.60	70.76	78.6	74.6

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

T/K	C2H4	C3H6	C4H8	C5H10	C6H12	C7H14	C8H16
298.15	.00	.00	.00	.00	.00	.0	.0
300.00	.10	.13	.18	.20	.25	.3	.4
400.00	4.94	7.30	11.12	13.24	16.13	19.6	22.0
500.00	10.80	16.04	24.01	29.25	35.32	42.4	47.9
600.00	17.56	26.13	38.57	47.77	57.63	68.4	77.5
700.00	25.10	37.46	54.64	68.31	82.18	97.2	110.4
800.00	33.26	49.82	71.97	90.51	108.72	128.4	146.0
900.00	41.94	63.10	90.44	114.16	137.01	161.6	184.0
1000.00	51.19	77.18	109.97	139.05	166.86	196.5	224.0

Table 7a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	.00	.00	.00	.00	.0	.0
300.00	.03	.05	.02	.05	.1	.0
400.00	2.36	3.82	2.11	2.89	3.5	2.4
500.00	5.23	7.97	5.24	6.07	7.1	5.5
600.00	8.57	12.44	9.20	9.86	10.8	9.1
700.00	12.36	17.18	13.67	13.87	15.0	13.2
800.00	16.57	22.15	18.53	18.22	19.7	17.6
900.00	21.16	27.35	23.71	22.85	24.6	22.4
1000.00	25.99	32.79	29.08	27.80	29.6	27.5

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

T/K	C2H4	C3H6	C4H8	C5H10	C6H12	C7H14	C8H16
298.15	52.30	20.42	-15.80	-41.76	-66.24	-88.1	-110.1
300.00	52.40	20.55	-15.62	-41.56	-65.99	-87.8	-109.7
400.00	57.24	27.72	-4.68	-28.52	-50.11	-68.5	-88.1
500.00	63.10	36.46	8.21	-12.51	-30.92	-45.6	-62.2
600.00	69.86	46.54	22.77	6.01	-8.61	-19.7	-32.6
700.00	77.40	57.87	38.83	26.55	15.94	9.1	.3
800.00	85.56	70.24	56.17	48.75	42.48	40.3	35.9
900.00	94.24	83.51	74.64	72.40	70.77	73.5	73.9
1000.00	103.49	97.60	94.17	97.29	100.62	108.4	113.9

Table 8a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-31.88	-36.22	-25.96	-24.48	-21.8	-22.0
300.00	-31.85	-36.17	-25.93	-24.43	-21.8	-22.0
400.00	-29.52	-32.40	-23.84	-21.59	-18.4	-19.6
500.00	-26.65	-28.25	-20.72	-18.41	-14.7	-16.5
600.00	-23.31	-23.78	-16.76	-14.62	-11.0	-12.9
700.00	-19.52	-19.04	-12.29	-10.61	-6.8	-8.8
800.00	-15.32	-14.07	-7.42	-6.27	-2.2	-4.4
900.00	-10.72	-8.88	-2.24	-1.63	2.8	.4
1000.00	-5.89	-3.43	3.13	3.32	7.8	5.4

perimental data for higher members of the series of *n*-alkyl halides, *n*-alkyl thiols, and *n*-alk-1-enes. For the alkane isomer groups, $\Delta_f H^\circ(1,298.15 \text{ K})$ approaches $-25.3 \text{ kJ mol}^{-1}$. At higher temperatures the increments per carbon atom approach more nearly constant values, perhaps because the equilibrium distribution becomes more uniform, reflecting the greater influence of the entropies. The entropies of the various species in an isomer group are more nearly the same than their enthalpies of formation.

The increments per carbon atom for $\Delta_f G^\circ(I)$ at C_7H_{14} and C_8H_{16} are a little larger than those calculated earlier by Alberty⁷ from data up to C_6H_{12} .

5. Equilibrium Mole Fractions Within Alkene Isomer Groups

The equilibrium mole fractions within isomer groups calculated from standard Gibbs energies of formation are given in Table 9 for the ideal gas state. Since the uncertainties in $\Delta_f G^\circ(I)$ and $\Delta_f G^\circ_i$ are about the same, the uncertainty in the difference is nearly independent of the relative values of the two parameters, but the absolute uncertainty does increase with temperature. The usual equation for the propa-

gation of variance indicates that the equilibrium mole fractions are uncertain by about 15% at the lower temperature and 10% at the higher temperatures. This makes it difficult to indicate the uncertainties in the table. It could be done by using exponential notation, but this makes it difficult to compare the mole fractions of various isomers.

Compounds are named in tables according to the IUPAC Revised and Collected Recommendations for the *Nomenclature of Organic Chemistry*, 1978.¹⁹ For example, the two forms of 3-methyl-1-pentene are represented by 3(R) and 3(S), and the racemic mixture is represented by 3(RS)-methyl-1-pentene.

6. Standard Thermodynamic Properties of Individual Alkene Species

The values of C_p° , S° , $\Delta_f H^\circ$, and $\Delta_f G^\circ$ for all the alkene species through C_8H_{16} are given in Tables 10–13 in joules for a standard state pressure of 1 bar. The values of C_2H_4 through C_6H_{12} have been converted from the tables of Stull, Westrum, and Sinke,¹⁴ and the values for C_7H_{14} and C_8H_{16} have been calculated using the Benson method.⁸ The values for chiral forms are for the racemates.

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Table 9. Equilibrium mole fractions within alkene isomer groups

T/K	298.15	300	400	500	600	700	800	900	1000
C4H8									
1-butene	.0041	.0043	.0194	.0449	.0755	.1080	.1401	.1693	.1964
cis-2-butene	.0365	.0377	.0835	.1191	.1440	.1581	.1660	.1703	.1723
trans-2-butene	.1169	.1180	.1798	.2156	.2342	.2416	.2452	.2462	.2439
2-methyl-1-propene	.8425	.8400	.7174	.6204	.5463	.4923	.4486	.4142	.3874
C5H10									
1-pentene	.0003	.0004	.0029	.0095	.0203	.0338	.0485	.0636	.0781
cis-2-pentene	.0066	.0068	.0253	.0509	.0768	.0986	.1162	.1300	.1392
trans-2-pentene	.0143	.0147	.0388	.0655	.0894	.1067	.1199	.1286	.1344
2-methyl-1-butene	.0815	.0825	.1401	.1810	.2102	.2271	.2365	.2405	.2422
2-methyl-2-butene	.8952	.8936	.7852	.6763	.5752	.4936	.4271	.3741	.3326
3-methyl-1-butene	.0020	.0021	.0077	.0168	.0281	.0402	.0519	.0632	.0735
C6H12									
1-hexene	.0000	.0000	.0004	.0016	.0039	.0073	.0113	.0158	.0203
trans-2-hexene	.0029	.0030	.0098	.0187	.0276	.0353	.0415	.0465	.0503
cis-2-hexene	.0031	.0032	.0121	.0243	.0364	.0470	.0555	.0622	.0673
trans-3-hexene	.0018	.0019	.0058	.0109	.0160	.0204	.0242	.0273	.0296
cis-3-hexene	.0002	.0002	.0013	.0033	.0061	.0089	.0117	.0142	.0164
2-methyl-1-pentene	.0316	.0321	.0623	.0890	.1093	.1251	.1363	.1438	.1498
3(RS)-methyl-1-pentene	.0003	.0003	.0017	.0047	.0093	.0149	.0213	.0279	.0346
4-methyl-1-pentene	.0002	.0002	.0009	.0020	.0031	.0041	.0050	.0057	.0063
2-methyl-2-pentene	.4104	.4104	.3623	.3070	.2615	.2255	.1964	.1739	.1560
trans-3-methyl-2-pentene	.1370	.1380	.1747	.1875	.1854	.1766	.1678	.1581	.1491
cis-3-methyl-2-pentene	.0620	.0627	.0885	.0994	.1022	.1008	.0971	.0930	.0888
trans-4-methyl-2-pentene	.0138	.0139	.0225	.0297	.0349	.0387	.0415	.0435	.0448
cis-4-methyl-2-pentene	.0050	.0052	.0118	.0187	.0244	.0286	.0319	.0344	.0362
3,3-dimethyl-1-butene	.0007	.0007	.0011	.0013	.0014	.0014	.0014	.0013	.0013
2,3-dimethyl-1-butene	.0709	.0717	.0715	.0721	.0719	.0714	.0704	.0695	.0687
2,3-dimethyl-2-butene	.2559	.2523	.1620	.1100	.0788	.0588	.0456	.0370	.0305
2-ethyl-1-butene	.0041	.0042	.0114	.0199	.0279	.0350	.0410	.0460	.0500
C7H14									
1-heptene	.0000	.0000	.0004	.0015	.0037	.0068	.0106	.0147	.0189
trans-2-heptene	.0027	.0028	.0099	.0190	.0278	.0351	.0409	.0453	.0488
trans-3-heptene	.0018	.0019	.0071	.0142	.0212	.0273	.0323	.0364	.0396
2-methyl-1-hexene	.0018	.0019	.0066	.0129	.0193	.0250	.0299	.0340	.0374
3(RS)-methyl-1-hexene	.0004	.0004	.0024	.0058	.0102	.0147	.0191	.0231	.0268
4(RS)-methyl-1-hexene	.0007	.0007	.0032	.0075	.0125	.0175	.0222	.0265	.0302
5-methyl-1-hexene	.0003	.0003	.0016	.0038	.0063	.0088	.0111	.0132	.0151
2-methyl-2-hexene	.0321	.0325	.0486	.0549	.0556	.0540	.0514	.0487	.0461
cis-3-methyl-2-hexene	.0321	.0325	.0486	.0549	.0556	.0540	.0514	.0487	.0461
trans-3-methyl-2-hexene	.0321	.0325	.0486	.0549	.0556	.0540	.0514	.0487	.0461
cis-4(RS)-methyl-2-hexene	.0075	.0077	.0173	.0248	.0293	.0317	.0328	.0332	.0331
trans-4(RS)-methyl-2-hexene	.0404	.0410	.0625	.0726	.0757	.0754	.0737	.0714	.0690
cis-5-methyl-2-hexene	.0057	.0058	.0119	.0159	.0180	.0189	.0191	.0190	.0186
trans-5-methyl-2-hexene	.0308	.0311	.0428	.0466	.0466	.0450	.0430	.0409	.0399
cis-2-methyl-3-hexene	.0025	.0026	.0062	.0092	.0112	.0123	.0130	.0133	.0134
trans-2-methyl-3-hexene	.0025	.0026	.0062	.0092	.0112	.0123	.0130	.0133	.0134
cis-3-methyl-3-hexene	.0093	.0095	.0186	.0247	.0279	.0293	.0297	.0295	.0291
trans-3-methyl-3-hexene	.0502	.0507	.0672	.0723	.0721	.0698	.0667	.0636	.0607
2,3(RS)-dimethyl-1-pentene	.0119	.0121	.0223	.0298	.0346	.0375	.0394	.0405	.0411
2,4-dimethyl-1-pentene	.0210	.0212	.0287	.0317	.0324	.0321	.0314	.0306	.0298
3(RS),4-dimethyl-1-pentene	.0049	.0050	.0102	.0143	.0171	.0188	.0200	.0208	.0214
2,3-dimethyl-2-pentene	.3806	.3773	.2382	.1581	.1116	.0831	.0648	.0523	.0436
2,4-dimethyl-2-pentene	.1030	.1027	.0818	.0632	.0499	.0405	.0339	.0290	.0254
cis-3,4-dimethyl-2-pentene	.1030	.1027	.0818	.0632	.0499	.0405	.0339	.0290	.0254
trans-3,4-dimethyl-2-pentene	.1030	.1027	.0818	.0632	.0499	.0405	.0339	.0290	.0254
2-ethyl-3-methyl-1-butene	.0023	.0024	.0058	.0091	.0117	.0138	.0154	.0166	.0176
3,3-dimethyl-1-pentene	.0009	.0009	.0020	.0031	.0039	.0046	.0052	.0057	.0061
4,4-dimethyl-1-pentene	.0017	.0017	.0024	.0028	.0030	.0032	.0033	.0034	.0034
cis-4,4-dimethyl-2-pentene	.0000	.0000	.0001	.0002	.0003	.0004	.0004	.0005	.0006
trans-4,4-dimethyl-2-pentene	.0002	.0002	.0004	.0006	.0008	.0009	.0010	.0011	.0012
2,3,3-trimethyl-1-butene	.0001	.0001	.0001	.0003	.0004	.0005	.0005	.0006	.0007
2-ethyl-1-pentene	.0007	.0008	.0034	.0079	.0131	.0184	.0233	.0279	.0319
3-ethyl-1-pentene	.0002	.0002	.0012	.0029	.0051	.0073	.0095	.0116	.0134
3-ethyl-2-pentene	.0126	.0128	.0252	.0334	.0378	.0397	.0402	.0400	.0394
cis-2-heptene	.0005	.0005	.0027	.0065	.0108	.0147	.0182	.0210	.0234
cis-3-heptene	.0003	.0004	.0020	.0048	.0082	.0115	.0144	.0169	.0190
C8H16									
1-octene	.0000	.0000	.0001	.0005	.0014	.0027	.0044	.0063	.0083
trans-2-octene	.0007	.0008	.0031	.0067	.0105	.0139	.0169	.0194	.0213
cis-2-octene	.0001	.0001	.0009	.0023	.0041	.0059	.0075	.0090	.0102
trans-3-octene	.0005	.0005	.0023	.0050	.0080	.0109	.0134	.0155	.0173
cis-3-octene	.0001	.0001	.0006	.0017	.0031	.0046	.0060	.0072	.0083
trans-4-octene	.0003	.0003	.0015	.0034	.0054	.0073	.0090	.0105	.0117
cis-4-octene	.0001	.0001	.0004	.0012	.0021	.0031	.0040	.0049	.0056
2-methyl-1-heptene	.0005	.0005	.0021	.0045	.0073	.0099	.0124	.0145	.0164

Table 9. Equilibrium mole fractions within alkene isomer groups--Continued

T/K	298.15	300	400	500	600	700	800	900	1000
C8H16									
3(RS)-methyl-1-heptene	.0001	.0001	.0008	.0021	.0038	.0058	.0079	.0099	.0117
4(RS)-methyl-1-heptene	.0002	.0002	.0010	.0026	.0047	.0070	.0092	.0113	.0132
5(RS)-methyl-1-heptene	.0002	.0002	.0010	.0026	.0047	.0070	.0092	.0113	.0132
6-methyl-1-heptene	.0001	.0001	.0005	.0013	.0024	.0035	.0046	.0056	.0066
2-methyl-1-2-heptene	.0473	.0475	.0556	.0564	.0542	.0510	.0478	.0448	.0421
trans-3-methyl-1-2-heptene	.0087	.0089	.0154	.0193	.0210	.0215	.0213	.0208	.0202
cis-3-methyl-1-2-heptene	.0087	.0089	.0154	.0193	.0210	.0215	.0213	.0208	.0202
trans-4(RS)-methyl-1-2-heptene	.0110	.0112	.0198	.0255	.0285	.0300	.0305	.0305	.0302
cis-4(RS)-methyl-1-2-heptene	.0020	.0021	.0055	.0087	.0111	.0126	.0136	.0142	.0145
trans-5(RS)-methyl-1-2-heptene	.0168	.0170	.0272	.0328	.0351	.0358	.0355	.0349	.0341
cis-5(RS)-methyl-1-2-heptene	.0031	.0032	.0075	.0112	.0136	.0150	.0158	.0162	.0163
trans-6-methyl-1-2-heptene	.0084	.0085	.0136	.0164	.0176	.0179	.0178	.0174	.0170
cis-6-methyl-1-2-heptene	.0016	.0016	.0038	.0056	.0068	.0075	.0079	.0081	.0082
trans-2-methyl-1-3-heptene	.0037	.0038	.0071	.0095	.0109	.0117	.0121	.0122	.0123
cis-2-methyl-1-3-heptene	.0007	.0007	.0020	.0032	.0042	.0049	.0054	.0057	.0059
trans-3-methyl-1-3-heptene	.0025	.0026	.0059	.0087	.0105	.0117	.0123	.0126	.0127
cis-3-methyl-1-3-heptene	.0025	.0026	.0059	.0087	.0105	.0117	.0123	.0126	.0127
trans-4-methyl-1-3-heptene	.0025	.0026	.0059	.0087	.0105	.0117	.0123	.0126	.0127
cis-4-methyl-1-3-heptene	.0025	.0026	.0059	.0087	.0105	.0117	.0123	.0126	.0127
trans-5(RS)-methyl-1-3-heptene	.0074	.0075	.0143	.0190	.0218	.0233	.0241	.0245	.0245
cis-5(RS)-methyl-1-3-heptene	.0014	.0014	.0040	.0065	.0084	.0098	.0107	.0113	.0118
trans-6-methyl-1-3-heptene	.0056	.0057	.0098	.0122	.0134	.0139	.0141	.0140	.0138
cis-6-methyl-1-3-heptene	.0010	.0011	.0027	.0042	.0052	.0059	.0063	.0065	.0066
3(RS)-ethyl-1-hexene	.0001	.0001	.0008	.0021	.0038	.0058	.0079	.0099	.0117
4-ethyl-1-hexene	.0001	.0001	.0005	.0013	.0024	.0035	.0046	.0056	.0066
trans-3-ethyl-1-hexene	.0034	.0035	.0080	.0117	.0143	.0158	.0166	.0171	.0172
cis-3-ethyl-1-hexene	.0034	.0035	.0080	.0117	.0143	.0158	.0166	.0171	.0172
trans-4-ethyl-1-hexene	.0055	.0056	.0099	.0127	.0143	.0150	.0152	.0152	.0151
cis-4-ethyl-1-hexene	.0010	.0010	.0028	.0044	.0055	.0063	.0068	.0071	.0072
3-ethyl-3-hexene	.0013	.0014	.0041	.0072	.0097	.0116	.0130	.0140	.0147
2,3(RS)-dimethyl-1-hexene	.0006	.0006	.0020	.0036	.0051	.0063	.0072	.0080	.0086
2,4(RS)-dimethyl-1-hexene	.0021	.0022	.0051	.0076	.0095	.0107	.0116	.0121	.0125
2,5-dimethyl-1-hexene	.0057	.0058	.0091	.0111	.0122	.0128	.0130	.0131	.0131
3,3-dimethyl-1-hexene	.0002	.0003	.0006	.0011	.0015	.0018	.0021	.0024	.0027
3(RS),4(RS)-dimethyl-1-hexene	.0013	.0014	.0033	.0050	.0064	.0075	.0083	.0089	.0094
3(RS),3(RS)-dimethyl-1-hexene	.0013	.0014	.0033	.0050	.0064	.0075	.0083	.0089	.0094
4,4-dimethyl-1-hexene	.0014	.0014	.0023	.0030	.0034	.0038	.0040	.0043	.0045
4(RS),5-dimethyl-1-hexene	.0020	.0021	.0045	.0065	.0079	.0089	.0097	.0102	.0106
2,3-dimethyl-1-hexene	.0191	.0192	.0220	.0217	.0203	.0187	.0171	.0157	.0145
2,4(RS)-dimethyl-2-hexene	.0560	.0560	.0519	.0444	.0376	.0322	.0280	.0248	.0222
2,5-dimethyl-2-hexene	.0993	.0986	.0667	.0472	.0352	.0275	.0224	.0187	.0161
trans-3,4(RS)-dimethyl-1-hexene	.0560	.0560	.0519	.0444	.0376	.0322	.0280	.0248	.0222
cis-3,4(RS)-dimethyl-1-hexene	.0560	.0560	.0519	.0444	.0376	.0322	.0280	.0248	.0222
trans-3,5-dimethyl-1-hexene	.0993	.0986	.0667	.0472	.0352	.0275	.0224	.0187	.0161
cis-3,5-dimethyl-1-hexene	.0993	.0986	.0667	.0472	.0352	.0275	.0224	.0187	.0161
trans-4,4-dimethyl-1-hexene	.0231	.0230	.0171	.0133	.0109	.0093	.0083	.0075	.0069
cis-4,4-dimethyl-1-hexene	.0043	.0043	.0047	.0046	.0042	.0039	.0037	.0035	.0033
trans-4(RS),5-dimethyl-1-hexene	.1250	.1241	.0858	.0624	.0479	.0385	.0320	.0275	.0241
cis-4(RS),5-dimethyl-1-hexene	.0231	.0232	.0238	.0213	.0186	.0162	.0143	.0128	.0116
trans-5,5-dimethyl-1-hexene	.0003	.0003	.0005	.0006	.0007	.0007	.0008	.0008	.0008
cis-5,5-dimethyl-1-hexene	.0000	.0001	.0001	.0002	.0003	.0003	.0004	.0004	.0004
trans-2,2-dimethyl-3-hexene	.0002	.0002	.0003	.0004	.0005	.0006	.0006	.0006	.0006
cis-2,2-dimethyl-3-hexene	.0000	.0000	.0001	.0002	.0002	.0002	.0003	.0003	.0003
trans-2,3-dimethyl-3-hexene	.0081	.0081	.0099	.0100	.0094	.0088	.0081	.0075	.0070
cis-2,3-dimethyl-3-hexene	.0081	.0081	.0099	.0100	.0094	.0088	.0081	.0075	.0070
trans-2,4-dimethyl-3-hexene	.0081	.0081	.0099	.0100	.0094	.0088	.0081	.0075	.0070
cis-2,4-dimethyl-3-hexene	.0081	.0081	.0099	.0100	.0094	.0088	.0081	.0075	.0070
trans-2,5-dimethyl-3-hexene	.0275	.0275	.0225	.0181	.0149	.0125	.0109	.0096	.0087
cis-2,5-dimethyl-3-hexene	.0225	.0226	.0301	.0301	.0229	.0226	.0224	.0202	.0201
trans-3,4-dimethyl-3-hexene	.0024	.0024	.0045	.0059	.0067	.0071	.0072	.0072	.0071
cis-3,4-dimethyl-3-hexene	.0012	.0012	.0023	.0030	.0034	.0035	.0036	.0036	.0036
3-ethyl-2-methyl-1-pentene	.0016	.0016	.0035	.0052	.0065	.0075	.0081	.0086	.0090
3-ethyl-3-methyl-1-pentene	.0002	.0003	.0006	.0011	.0015	.0018	.0021	.0024	.0027
3(RS)-ethyl-4-methyl-1-pentene	.0013	.0014	.0033	.0050	.0064	.0075	.0083	.0089	.0094
2-propyl-1-pentene	.0001	.0001	.0005	.0014	.0025	.0037	.0048	.0059	.0070
3-ethyl-2-methyl-1-pentene	.0016	.0016	.0030	.0040	.0045	.0048	.0049	.0049	.0048
trans-3-ethyl-4-methyl-1-pentene	.0109	.0110	.0135	.0135	.0128	.0118	.0109	.0102	.0095
cis-3-ethyl-4-methyl-1-pentene	.0109	.0110	.0135	.0135	.0128	.0118	.0109	.0102	.0095
2,3,3-trimethyl-1-pentene	.0029	.0029	.0033	.0033	.0033	.0032	.0032	.0032	.0032
2,3(RS),4-trimethyl-1-pentene	.0366	.0365	.0307	.0256	.0219	.0191	.0171	.0156	.0144
2,4,4-trimethyl-1-pentene	.0001	.0001	.0002	.0002	.0003	.0004	.0004	.0005	.0005
2,3,4-trimethyl-1-pentene	.0264	.0262	.0198	.0151	.0120	.0098	.0082	.0071	.0062
2,4,4-trimethyl-2-pentene	.0002	.0003	.0004	.0004	.0004	.0004	.0004	.0004	.0004
trans-3,4,4-trimethyl-1-pentene	.0002	.0003	.0004	.0004	.0004	.0004	.0004	.0004	.0004
cis-3,4,4-trimethyl-2-pentene	.0002	.0002	.0003	.0003	.0003	.0003	.0003	.0003	.0003
2-ethyl-3,3-dimethyl-1-butene	.0000	.0000	.0000	.0001	.0001	.0001	.0002	.0002	.0003
2-ethyl-1-hexene	.0002	.0002	.0011	.0028	.0049	.0073	.0097	.0119	.0140
3-methyl-2-isopropyl-4-butene	.0010	.0010	.0015	.0018	.0020	.0021	.0021	.0021	.0021
2-isopropyl-1-pentene	.0006	.0006	.0018	.0032	.0044	.0055	.0064	.0071	.0077
2-ethyl-3(RS)-methyl-1-pentene	.0013	.0013	.0037	.0064	.0089	.0110	.0127	.0142	.0154
2-ethyl-4-methyl-1-pentene	.0022	.0023	.0047	.0068	.0083	.0094	.0102	.0107	.0111
3,3,4-trimethyl-1-pentene	.0028	.0028	.0028	.0026	.0025	.0023	.0022	.0022	.0021
3(RS),4,4-trimethyl-1-pentene	.0000	.0000	.0001	.0002	.0003	.0003	.0004	.0004	.0005
5,5-dimethyl-1-hexene	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0003

CHEMICAL THERMODYNAMIC PROPERTIES OF ALKENE ISOMER GROUPS

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Table 10. Standard heat capacity at constant pressure for alkenes in J/K mol

T/K	298.15	300	400	500	600	700	800	900	1000
C2H4 ethylene	43.56	43.72	53.97	63.43	71.55	78.49	84.52	89.79	94.43
C3H6 propene	63.89	64.18	79.91	94.64	107.53	118.70	128.37	136.82	144.18
C4H8 1-butene	85.65	86.06	108.95	129.41	147.03	161.96	174.89	186.15	195.89
cis-2-butene	78.91	79.33	101.80	122.97	141.42	157.32	171.00	182.84	193.09
trans-2-butene	87.82	88.20	108.87	128.37	145.60	160.58	173.64	184.93	194.89
2-methyl-1-propene	89.12	89.50	111.17	130.71	147.70	162.38	175.14	186.31	196.02
C5H10 1-pentene	109.58	110.08	138.49	164.14	186.44	205.27	221.54	235.64	247.73
cis-2-pentene	101.75	102.30	132.09	159.20	182.51	201.88	218.78	233.30	245.94
trans-2-pentene	108.45	108.95	136.69	162.13	184.18	203.09	219.45	233.68	246.06
2-methyl-1-butene	109.96	118.87	138.91	164.85	187.11	206.10	222.38	236.48	248.66
2-methyl-2-butene	105.02	105.52	133.60	159.28	181.67	201.00	217.78	232.30	244.97
3-methyl-1-butene	118.62	119.12	147.53	171.42	192.05	209.83	225.31	238.61	250.33
C6H12 1-hexene	132.34	132.97	167.49	198.61	225.52	248.28	267.86	284.76	299.32
trans-2-hexene	132.38	132.97	166.10	197.07	223.43	246.44	266.10	282.84	297.90
cis-2-hexene	125.69	126.31	161.50	194.14	221.75	245.18	265.27	282.84	297.90
trans-3-hexene	132.84	133.47	168.20	199.16	225.52	247.69	267.36	283.68	298.74
cis-3-hexene	123.64	124.31	161.08	194.14	222.59	245.60	265.68	282.84	297.90
2-methyl-1-pentene	135.56	136.23	170.71	201.25	227.61	250.20	269.45	286.19	300.41
3(RS)-methyl-1-pentene	142.42	143.05	177.82	207.53	232.63	253.97	272.80	288.70	302.50
4-methyl-1-pentene	126.48	127.36	162.76	194.14	221.33	244.35	264.01	280.75	295.81
2-methyl-2-pentene	126.61	127.28	163.18	194.97	222.59	245.18	265.27	282.42	297.48
trans-3-methyl-2-pentene	126.61	127.28	163.18	194.97	222.59	245.18	265.27	282.42	297.48
cis-3-methyl-2-pentene	126.61	127.28	163.18	194.97	222.59	245.18	265.27	282.42	297.48
trans-4-methyl-2-pentene	141.42	142.00	175.31	204.18	229.28	251.04	269.87	286.19	300.41
cis-4-methyl-2-pentene	133.55	134.18	167.57	200.00	226.35	248.53	267.78	284.51	299.16
3,3-dimethyl-1-butene	126.48	127.15	162.76	195.39	223.43	246.44	266.10	281.58	297.06
2,3-dimethyl-1-butene	143.47	144.10	178.24	207.11	231.79	253.13	271.96	287.86	302.08
2,3-dimethyl-2-butene	123.60	124.18	156.82	188.45	216.65	241.29	262.67	281.37	297.65
2-ethyl-1-butene	133.55	134.22	170.29	201.67	228.03	250.20	269.45	286.19	300.83
C7H14 1-heptene	154.9	155.7	196.2	232.5	264.6	292.4	316.1	335.5	350.8
trans-2-heptene	153.8	154.5	194.5	230.4	262.2	290.1	313.8	333.6	349.3
trans-3-heptene	152.3	153.1	193.9	230.5	262.8	290.9	314.7	334.4	349.7
2-methyl-1-hexene	157.6	158.4	198.2	233.9	265.5	293.0	316.4	335.8	351.0
3(RS)-methyl-1-hexene	153.9	154.7	196.0	232.8	265.3	293.4	317.1	336.4	351.3
4(RS)-methyl-1-hexene	153.9	154.7	195.9	232.7	265.2	293.2	317.0	336.3	351.3
5-methyl-1-hexene	153.9	154.7	195.9	232.7	265.2	293.2	317.0	336.3	351.3
2-methyl-2-hexene	150.8	151.5	192.0	228.3	260.5	288.6	312.7	332.6	348.4
cis-3-methyl-2-hexene	150.8	151.5	192.0	228.3	260.5	288.6	312.7	332.6	348.4
trans-3-methyl-2-hexene	150.8	151.5	192.0	228.3	260.5	288.6	312.7	332.6	348.4
cis-4(RS)-methyl-2-hexene	147.1	147.9	189.8	227.3	260.3	289.0	313.3	333.2	348.6
trans-4(RS)-methyl-2-hexene	152.7	153.5	194.2	230.7	263.0	291.0	314.8	334.4	349.8
cis-5-methyl-2-hexene	147.0	147.9	189.7	227.1	260.2	288.9	313.2	333.1	348.7
trans-5-methyl-2-hexene	152.7	153.5	194.1	230.6	262.8	290.9	314.7	334.4	349.8
cis-2-methyl-3-hexene	145.7	146.5	189.2	227.4	260.9	289.9	314.2	333.9	349.1
trans-2-methyl-3-hexene	145.7	146.5	189.2	227.4	260.9	289.9	314.2	333.9	349.1
cis-3-methyl-3-hexene	149.3	150.1	191.4	228.4	261.1	289.5	313.6	333.4	348.9
trans-3-methyl-3-hexene	155.0	155.8	195.9	231.9	263.7	291.5	315.1	334.6	350.0
2,3(RS)-dimethyl-1-pentene	156.6	157.4	197.9	234.2	266.2	293.9	317.4	336.6	351.5
2,4-dimethyl-1-pentene	156.5	157.3	197.8	234.1	266.1	293.8	317.3	336.6	351.6
3(RS),4-dimethyl-1-pentene	152.9	153.7	195.6	233.0	265.9	294.2	318.0	337.2	351.8
2,3-dimethyl-2-pentene	147.7	148.5	189.4	226.2	258.6	287.2	311.5	331.6	347.6
2,4-dimethyl-2-pentene	149.7	150.5	191.7	228.6	261.2	289.6	313.6	333.4	348.9
cis-3,4-dimethyl-2-pentene	149.7	150.5	191.7	228.6	261.2	289.6	313.6	333.4	348.9
trans-3,4-dimethyl-2-pentene	149.7	150.5	191.7	228.6	261.2	289.6	313.6	333.4	348.9
2-ethyl-3-methyl-1-butene	155.2	156.0	197.4	234.3	266.8	294.8	318.3	337.4	352.0
3,3-dimethyl-1-pentene	156.3	157.1	200.0	238.1	271.3	299.8	323.4	342.2	366.1
4,4-dimethyl-1-pentene	156.2	157.1	200.0	238.1	271.3	299.8	323.3	342.0	355.9
cis-4,4-dimethyl-2-pentene	149.4	150.3	193.8	232.5	266.4	295.4	319.6	339.0	353.5
trans-4,4-dimethyl-2-pentene	155.1	155.9	198.3	236.0	269.0	297.4	321.1	340.2	354.6
2,3,3-trimethyl-1-butene	158.9	159.7	201.9	239.4	272.2	300.3	323.7	342.4	366.4
2-ethyl-1-pentene	156.2	157.0	197.6	234.0	266.0	293.8	317.3	336.6	351.5
3-ethyl-1-pentene	153.9	154.7	196.0	232.8	265.3	293.4	317.1	336.4	351.3
3-ethyl-2-pentene	149.3	150.1	191.4	228.4	261.1	289.5	313.6	333.4	348.9
cis-2-heptene	148.1	148.9	190.0	226.9	259.6	288.1	312.3	332.3	348.1
cis-3-heptene	146.7	147.5	189.5	227.0	260.2	288.9	313.2	333.1	348.6
C8H16 1-octene	177.9	178.8	225.3	266.9	303.6	335.5	362.6	384.9	402.3
trans-2-octene	176.7	177.6	223.5	264.7	301.3	333.2	360.4	382.9	400.8
cis-2-octene	171.1	172.0	219.1	261.3	298.7	331.2	358.9	381.7	399.7
trans-3-octene	175.3	176.2	223.0	264.9	301.9	334.0	361.3	383.7	401.3
cis-3-octene	169.7	170.6	218.5	261.4	299.2	332.0	359.8	382.5	400.1
trans-4-octene	175.3	176.2	223.0	264.9	301.9	334.0	361.3	383.7	401.3
cis-4-octene	169.7	170.6	218.5	261.4	299.2	332.0	359.8	382.5	400.1
2-methyl-1-heptene	180.6	181.5	227.2	268.2	304.5	336.1	363.0	385.1	402.6

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

T/K	298.15	300	400	500	600	700	800	900	1000
C8H16									
3(RS)-methyl-1-heptene	176.9	177.8	225.0	267.2	304.3	336.5	363.6	385.7	402.8
4(RS)-methyl-1-heptene	176.9	177.8	224.9	267.1	304.2	336.4	363.5	385.7	402.8
5(RS)-methyl-1-heptene	176.9	177.8	224.9	267.1	304.2	336.4	363.5	385.7	402.8
6-methyl-1-heptene	176.9	177.8	224.9	267.1	304.2	336.4	363.5	385.7	402.8
2-methyl-2-heptene	179.4	180.3	225.5	266.1	302.2	333.7	360.7	383.2	401.1
trans-3-methyl-2-heptene	173.7	174.6	221.0	262.7	299.6	331.8	359.2	381.9	399.9
cis-3-methyl-2-heptene	173.7	174.6	221.0	262.7	299.6	331.8	359.2	381.9	399.9
trans-4(RS)-methyl-2-heptene	175.7	176.6	223.3	265.1	302.0	334.1	361.4	383.8	401.3
cis-4(RS)-methyl-2-heptene	170.1	171.0	218.8	261.6	299.4	332.1	359.8	382.5	400.2
trans-5(RS)-methyl-2-heptene	175.7	176.6	223.2	265.0	301.9	334.0	361.3	383.7	401.3
cis-5(RS)-methyl-2-heptene	170.0	171.0	218.7	261.5	299.3	332.0	359.8	382.5	400.2
trans-6-methyl-2-heptene	175.7	176.6	223.2	265.0	301.9	334.0	361.3	383.7	401.3
cis-6-methyl-2-heptene	170.0	171.0	218.7	261.5	299.3	332.0	359.8	382.5	400.2
trans-2-methyl-3-heptene	174.3	175.2	222.7	265.2	302.6	335.0	362.3	384.5	401.7
cis-2-methyl-3-heptene	168.6	169.6	218.3	261.7	300.6	333.0	360.8	383.3	400.6
trans-3-methyl-3-heptene	172.3	173.2	220.5	262.8	300.1	332.6	360.1	382.7	400.4
cis-3-methyl-3-heptene	172.3	173.2	220.5	262.8	300.1	332.6	360.1	382.7	400.4
trans-4-methyl-3-heptene	172.3	173.2	220.5	262.8	300.1	332.6	360.1	382.7	400.4
cis-4-methyl-3-heptene	172.3	173.2	220.5	262.8	300.1	332.6	360.1	382.7	400.4
trans-5(RS)-methyl-3-heptene	174.3	175.2	222.7	265.2	302.6	335.0	362.3	384.5	401.7
cis-5(RS)-methyl-3-heptene	168.6	169.6	218.3	261.7	300.6	333.0	360.8	383.3	400.6
trans-6-methyl-3-heptene	174.3	175.2	222.6	265.1	302.5	334.8	362.2	384.5	401.8
cis-6-methyl-3-heptene	168.6	169.6	218.2	261.6	299.8	332.9	360.7	383.3	400.7
3(RS)-ethyl-1-hexene	176.9	177.8	225.0	267.2	304.3	336.5	363.6	385.7	402.8
4-ethyl-1-hexene	176.9	177.8	224.9	267.1	304.2	336.4	363.5	385.7	402.8
trans-3-ethyl-2-hexene	172.3	173.2	220.5	262.8	300.1	332.6	360.1	382.7	400.4
cis-3-ethyl-2-hexene	172.3	173.2	220.5	262.8	300.1	332.6	360.1	382.7	400.4
trans-4-ethyl-2-hexene	175.7	176.6	223.3	265.1	302.0	334.1	361.4	383.8	401.3
cis-4-ethyl-2-hexene	170.1	171.0	218.8	261.6	299.4	332.1	359.8	382.5	400.2
3-ethyl-3-hexene	170.9	171.8	219.9	262.9	300.7	333.4	361.0	383.5	400.9
2,3(RS)-dimethyl-1-hexene	173.9	174.8	222.5	265.1	302.6	335.1	362.4	384.7	402.0
2,4(RS)-dimethyl-1-hexene	173.9	174.8	222.4	265.0	302.5	334.9	362.4	384.7	402.0
2,5-dimethyl-1-hexene	179.5	180.4	226.9	268.4	305.1	336.9	363.9	385.9	403.1
3,3-dimethyl-1-hexene	179.2	180.2	229.0	272.4	310.4	342.9	369.9	391.5	407.7
3(RS),4(RS)-dimethyl-1-hexene	175.8	176.8	224.7	267.4	305.0	337.3	364.5	386.5	403.3
3(RS),4(RS)-dimethyl-1-hexene	175.8	176.8	224.7	267.4	305.0	337.3	364.5	386.5	403.3
3(RS),5-dimethyl-1-hexene	175.8	176.8	224.7	267.4	305.0	337.3	364.5	386.5	403.3
4,4-dimethyl-1-hexene	179.2	180.2	229.1	272.5	310.4	342.9	369.9	391.4	407.4
4(RS),5-dimethyl-1-hexene	175.8	176.7	224.6	267.3	304.8	337.2	364.4	386.5	403.4
2,3-dimethyl-1-hexene	176.4	177.3	223.0	264.0	300.5	332.3	359.6	382.2	400.2
2,4(RS)-dimethyl-2-hexene	172.7	173.6	220.8	263.0	300.3	332.7	360.2	382.8	400.4
2,5-dimethyl-2-hexene	172.7	173.6	220.7	262.9	300.2	332.6	360.1	382.7	400.5
trans-3,4(RS)-dimethyl-2-hexene	172.7	173.6	220.8	263.0	300.3	332.7	360.2	382.8	400.4
cis-3,4(RS)-dimethyl-2-hexene	172.7	173.6	220.8	263.0	300.3	332.7	360.2	382.8	400.4
trans-3,5-dimethyl-2-hexene	172.7	173.6	220.7	262.9	300.2	332.6	360.1	382.7	400.5
cis-3,5-dimethyl-2-hexene	172.7	173.6	220.7	262.9	300.2	332.6	360.1	382.7	400.5
trans-4,4-dimethyl-2-hexene	178.1	179.0	227.3	270.3	308.1	340.5	367.7	389.6	406.2
cis-4,4-dimethyl-2-hexene	172.4	173.4	222.9	266.9	305.4	338.5	366.2	388.3	405.0
trans-4(RS),5-dimethyl-2-hexene	174.7	175.6	222.9	265.3	302.6	335.0	362.3	384.6	401.8
cis-4(RS),5-dimethyl-2-hexene	169.0	169.9	218.5	261.8	300.0	333.0	360.7	383.3	400.7
trans-5,5-dimethyl-2-hexene	178.0	179.0	227.3	270.4	308.1	340.5	367.6	389.4	405.9
cis-5,5-dimethyl-2-hexene	172.4	173.3	222.9	266.9	305.4	338.5	366.1	388.2	404.8
trans-2,2-dimethyl-1-hexene	178.0	179.0	227.3	270.4	308.1	340.5	367.6	389.4	405.9
cis-2,2-dimethyl-3-hexene	172.4	173.3	222.9	266.9	305.4	338.5	366.1	388.2	404.8
trans-2,3-dimethyl-3-hexene	171.3	172.2	220.2	263.1	300.9	333.5	361.1	383.6	400.9
cis-2,3-dimethyl-3-hexene	171.3	172.2	220.2	263.1	300.9	333.5	361.1	383.6	400.9
trans-2,4-dimethyl-3-hexene	171.3	172.2	220.2	263.1	300.9	333.5	361.1	383.6	400.9
cis-2,4-dimethyl-3-hexene	171.3	172.2	220.2	263.1	300.9	333.5	361.1	383.6	400.9
trans-2,5-dimethyl-3-hexene	173.3	174.2	222.5	265.5	303.3	335.9	363.3	385.4	402.2
cis-2,5-dimethyl-3-hexene	167.6	168.6	218.0	262.1	300.7	333.9	361.7	384.1	401.1
trans-3,4-dimethyl-3-hexene	175.0	175.9	222.4	264.1	301.1	333.2	360.5	383.0	400.7
cis-3,4-dimethyl-3-hexene	175.0	175.9	222.4	264.1	301.1	333.2	360.5	383.0	400.7
3-ethyl-2-methyl-1-pentene	179.6	180.5	227.0	268.6	305.3	337.1	364.0	386.0	403.1
3-ethyl-3-methyl-1-pentene	179.2	180.2	229.0	272.4	310.4	342.9	369.9	391.5	407.7
3(RS)-ethyl-4-methyl-1-pentene	175.8	176.8	224.7	267.4	305.0	337.3	364.5	386.5	403.3
2-propyl-1-pentene	179.2	180.1	226.7	268.3	305.1	337.0	363.9	385.9	403.0
3-ethyl-1-2-methyl-2-pentene	175.0	175.9	222.4	264.1	301.1	333.2	360.5	383.0	400.7
trans-3-ethyl-4-methyl-2-pentene	171.3	172.2	220.2	263.1	300.9	333.5	361.1	383.6	400.9
cis-3-ethyl-4-methyl-2-pentene	171.3	172.2	220.2	263.1	300.9	333.5	361.1	383.6	400.9
2,3,3-trimethyl-1-pentene	181.9	182.8	231.0	273.8	311.3	343.5	370.3	391.8	407.9
2,3(RS),4-trimethyl-1-pentene	178.5	179.4	226.6	268.8	305.9	337.9	364.9	386.8	403.6
2,4,4-trimethyl-1-pentene	181.9	182.8	231.0	273.8	311.3	343.4	370.2	391.6	407.7
2,3,4,4-trimethyl-1-pentene	175.4	176.3	222.7	264.4	301.2	333.3	360.5	383.0	400.7
2,4,4-trimethyl-2-pentene	175.1	176.0	224.8	268.2	306.3	339.1	366.5	388.6	405.3
trans-3,4,4-trimethyl-2-pentene	175.1	176.0	224.8	268.2	306.3	339.1	366.5	388.6	405.3
cis-3,4,4-trimethyl-2-pentene	175.1	176.0	224.8	268.2	306.3	339.1	366.5	388.6	405.3
2-ethyl-1-3,3-dimethyl-1-butene	180.5	181.4	230.4	273.9	311.9	344.3	371.2	392.6	408.4
2-ethyl-1-1-hexene	179.2	180.1	226.7	268.3	305.1	337.0	363.9	385.9	403.0
3-methyl-2-isopropyl-4-butene	177.1	178.1	226.2	269.0	306.6	338.9	365.9	387.6	404.0
2-isopropyl-1-pentene	178.1	179.1	226.4	268.7	305.8	337.9	364.9	386.8	403.5
2-ethyl-1-3(RS)-methyl-1-pentene	178.1	179.1	226.4	268.7	305.8	337.9	364.9	386.8	403.5
2-ethyl-1-4-methyl-1-pentene	178.1	179.0	226.3	268.6	305.7	337.8	364.8	386.7	403.6
3,3,4-trimethyl-1-pentene	178.2	179.2	228.7	272.7	311.0	343.7	370.8	392.3	408.2
3(RS),4,4-trimethyl-1-pentene	178.2	179.2	228.8	272.8	311.1	343.8	370.8	392.2	407.9
5,5-dimethyl-1-hexene	179.2	180.2	229.1	272.5	310.4	342.9	369.9	391.4	407.4

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Table 11. Standard entropy of alkenes in J/K mol

Table II. Standard entropy of alkenes in J/K mol--Continued

T/K	298.15	300	400	500	600	700	800	900	1000
C8H16									
3(RS)-methyl-1-heptene	460.3	461.4	519.1	573.9	626.0	675.4	722.2	766.3	807.9
4(RS)-methyl-1-heptene	460.3	461.4	519.1	573.9	626.0	675.3	722.1	766.2	807.8
5(RS)-methyl-1-heptene	460.3	461.4	519.1	573.9	626.0	675.3	722.1	766.2	807.8
6-methyl-1-heptene	454.5	455.6	513.3	568.1	620.2	669.6	716.3	760.5	802.0
2-methyl-1-2-heptene	454.5	455.6	513.7	568.5	620.3	669.3	715.7	759.5	800.8
trans-3-methyl-1-2-heptene	454.5	455.5	512.2	566.1	617.3	666.0	712.1	755.8	797.0
cis-3-methyl-1-2-heptene	454.5	455.5	512.2	566.1	617.3	666.0	712.1	755.8	797.0
trans-4(RS)-methyl-1-2-heptene	456.8	457.9	515.2	569.6	621.3	670.3	716.7	760.6	802.0
cis-4(RS)-methyl-1-2-heptene	456.8	457.8	513.7	567.2	618.3	667.0	713.2	757.0	798.2
trans-5(RS)-methyl-1-2-heptene	456.8	457.9	515.2	569.6	621.2	670.2	716.6	760.5	801.9
cis-5(RS)-methyl-1-2-heptene	456.8	457.8	513.7	567.2	618.3	666.9	713.1	756.9	798.1
trans-6-methyl-1-2-heptene	451.0	452.1	509.4	563.8	615.4	664.4	710.9	754.8	796.2
cis-6-methyl-1-2-heptene	451.0	452.1	507.9	561.4	612.5	661.2	707.4	751.1	792.4
trans-2-methyl-1-3-heptene	450.1	451.2	508.2	562.6	614.3	663.5	710.0	754.0	795.5
cis-2-methyl-1-3-heptene	450.1	451.1	506.7	560.2	611.4	660.2	706.5	750.3	791.7
trans-3-methyl-1-3-heptene	453.5	454.6	511.0	564.9	616.1	664.9	711.2	754.9	796.2
cis-3-methyl-1-3-heptene	453.5	454.6	511.0	564.9	616.1	664.9	711.2	754.9	796.2
trans-4-methyl-1-3-heptene	453.5	454.6	511.0	564.9	616.1	664.9	711.2	754.9	796.2
cis-4-methyl-1-3-heptene	453.5	454.6	511.0	564.9	616.1	664.9	711.2	754.9	796.2
trans-5(RS)-methyl-1-3-heptene	455.9	456.9	514.0	568.3	620.1	669.2	715.8	759.8	801.2
cis-5(RS)-methyl-1-3-heptene	455.9	456.9	512.5	566.0	617.1	665.9	712.3	756.1	797.4
trans-6-methyl-1-3-heptene	450.1	451.2	508.2	562.5	614.2	663.4	709.9	753.9	795.4
cis-6-methyl-1-3-heptene	450.1	451.1	506.7	560.2	611.3	660.1	706.4	750.2	791.6
3(RS)-ethyl-1-hexene	460.3	461.4	519.1	573.9	626.0	675.4	722.2	766.3	807.9
4-ethyl-1-hexene	454.5	455.6	513.3	568.1	620.2	669.6	716.3	760.5	802.0
trans-3-ethyl-1-hexene	456.0	457.1	513.5	567.4	618.7	667.4	713.7	757.5	798.7
cis-3-ethyl-1-hexene	456.0	457.1	513.5	567.4	618.7	667.4	713.7	757.5	798.7
trans-4-ethyl-1-hexene	451.0	452.1	509.4	563.8	615.5	664.5	711.0	754.9	796.3
cis-4-ethyl-1-hexene	451.0	452.1	507.9	561.5	612.6	661.2	707.5	751.2	792.5
3-ethyl-1-hexene	457.6	458.7	514.8	568.6	620.0	668.9	715.2	759.1	800.5
2,3(RS)-dimethyl-1-hexene	452.5	453.6	510.5	564.8	616.5	665.7	712.3	756.3	797.8
2,4(RS)-dimethyl-1-hexene	452.5	453.6	510.5	564.8	616.5	665.6	712.2	756.2	797.7
2,5-dimethyl-1-hexene	446.7	447.8	506.2	561.4	613.6	663.1	709.9	754.1	795.7
3,3-dimethyl-1-hexene	436.8	437.9	496.6	552.5	605.6	655.9	703.6	748.4	790.6
3(RS),4(RS)-dimethyl-1-hexene	449.0	450.1	507.7	562.5	614.7	664.2	711.0	755.3	796.9
3(RS),5-dimethyl-1-hexene	449.0	450.1	507.7	562.5	614.7	664.2	711.0	755.3	796.9
4,4-dimethyl-1-hexene	436.8	437.9	496.6	552.5	605.6	656.0	703.6	748.4	790.5
4(RS),5-dimethyl-1-hexene	449.0	450.1	507.7	562.5	614.6	664.1	710.9	755.2	796.8
2,3-dimethyl-1-2-hexene	446.7	447.8	505.1	559.4	610.8	659.6	705.8	749.5	790.7
2,4(RS)-dimethyl-1-2-hexene	449.0	450.1	506.6	560.5	611.8	660.6	706.9	750.6	791.9
2,5-dimethyl-1-2-hexene	443.2	444.3	500.8	554.7	606.0	654.7	701.0	744.8	786.1
trans-3,4(RS)-dimethyl-1-2-hexene	449.0	450.1	506.6	560.5	611.8	660.6	706.9	750.6	791.9
cis-3,4(RS)-dimethyl-1-2-hexene	449.0	450.1	506.6	560.5	611.8	660.6	706.9	750.6	791.9
trans-3,5-dimethyl-1-2-hexene	443.2	444.3	500.8	554.7	606.0	654.7	701.0	744.8	786.1
cis-3,5-dimethyl-1-2-hexene	443.2	444.3	500.8	554.7	606.0	654.7	701.0	744.8	786.1
trans-4,4-dimethyl-1-2-hexene	433.4	434.5	492.7	548.1	600.8	650.8	698.1	742.8	784.7
cis-4,4-dimethyl-1-2-hexene	433.4	434.4	491.2	545.8	597.9	647.5	694.6	739.1	780.9
trans-4(RS),5-dimethyl-1-2-hexene	445.6	446.6	503.8	558.2	609.9	659.0	705.6	749.6	791.1
cis-4(RS),5-dimethyl-1-2-hexene	445.6	446.6	502.3	558.5	607.0	655.8	702.1	745.9	787.3
trans-5,5-dimethyl-1-2-hexene	424.2	425.3	483.6	539.0	591.7	641.7	689.0	733.6	775.5
cis-5,5-dimethyl-1-2-hexene	424.2	425.3	482.1	536.6	588.8	638.4	685.5	729.9	771.7
trans-2,2-dimethyl-1-3-hexene	421.7	422.8	481.0	536.5	589.2	639.2	686.5	731.1	773.0
cis-2,2-dimethyl-1-3-hexene	421.7	422.8	479.6	534.1	586.3	635.9	683.0	727.4	769.2
trans-2,3-dimethyl-1-3-hexene	442.3	443.4	499.6	553.5	604.8	653.7	700.1	744.0	785.4
cis-2,3-dimethyl-1-3-hexene	442.3	443.4	499.6	553.5	604.8	653.7	700.1	744.0	785.4
trans-2,4-dimethyl-1-3-hexene	442.3	443.4	499.6	553.5	604.8	653.7	700.1	744.0	785.4
cis-2,4-dimethyl-1-3-hexene	442.3	443.4	499.6	553.5	604.8	653.7	700.1	744.0	785.4
trans-2,5-dimethyl-1-3-hexene	438.9	439.9	496.8	551.2	603.0	652.3	699.0	743.1	784.6
cis-2,5-dimethyl-1-3-hexene	433.1	434.2	489.6	543.0	594.3	643.2	689.7	733.7	775.1
trans-3,4-dimethyl-1-3-hexene	445.7	446.8	503.9	558.1	609.6	658.5	704.8	748.6	789.9
cis-3,4-dimethyl-1-3-hexene	440.0	441.1	498.1	552.3	603.8	652.7	699.0	742.9	784.2
3-ethyl-1-2-methyl-1-pentene	446.7	447.8	506.2	561.4	613.7	663.2	710.0	754.2	795.8
3-ethyl-1-3-methyl-1-pentene	436.8	437.9	496.6	552.5	605.6	655.9	703.6	748.4	790.6
3(RS)-ethyl-1-4-methyl-1-pentene	449.0	450.1	507.7	562.5	614.7	664.2	711.0	755.3	796.9
2-propyl-1-pentene	453.8	454.9	513.2	568.3	620.6	670.1	716.9	761.0	802.6
3-ethyl-1-2-methyl-1-2-pentene	442.5	443.6	500.7	554.9	606.4	655.2	701.6	745.4	786.7
trans-3-ethyl-1-4-methyl-1-2-pentene	444.8	445.9	502.1	556.0	607.4	656.3	702.6	746.5	787.9
cis-3-ethyl-1-4-methyl-1-2-pentene	444.8	445.9	502.1	556.0	607.4	656.3	702.6	746.5	787.9
2,3,3-trimethyl-1-pentene	429.0	430.2	489.5	545.7	599.1	649.5	697.2	742.1	784.3
2,3(RS),4-trimethyl-1-pentene	441.2	442.4	500.6	555.8	608.1	657.7	704.7	749.0	790.6
2,4,4-trimethyl-1-pentene	419.9	421.0	480.4	536.6	589.9	640.4	688.1	733.0	775.1
2,3,4-trimethyl-1-2-pentene	435.4	436.5	493.7	548.0	599.5	648.4	694.7	738.5	779.9
2,4,4-trimethyl-1-2-pentene	416.4	417.5	475.0	529.9	582.2	632.0	679.1	723.6	765.5
trans-3,4,4-trimethyl-1-2-pentene	416.4	417.5	475.0	529.9	582.2	632.0	679.1	723.6	765.5
cis-3,4,4-trimethyl-1-2-pentene	413.9	415.0	472.4	527.4	579.7	629.5	676.6	721.1	763.0
2-ethyl-1-3,3-dimethyl-1-butene	421.5	422.6	481.7	537.9	591.2	641.8	689.6	734.6	776.8
2-ethyl-1-hexene	459.5	460.6	518.9	574.1	626.3	675.8	722.6	766.8	808.4
3-methyl-1-2-isopropyl-1-butene	431.3	432.4	490.4	545.5	598.0	647.7	694.8	739.2	780.9
2-isopropyl-1-pentene	448.3	449.4	507.5	562.7	615.0	664.7	711.6	755.9	797.5
2-ethyl-1-3(RS)-methyl-1-pentene	454.1	455.2	513.3	568.4	620.8	670.4	717.4	761.6	803.3
2-ethyl-1-4-methyl-1-pentene	448.3	449.4	507.5	562.6	615.0	664.6	711.5	755.8	797.4
3,3,4-trimethyl-1-pentene	425.6	426.7	485.2	541.0	594.2	644.7	692.4	737.4	779.6
3(RS),4,4-trimethyl-1-pentene	422.2	423.3	481.8	537.7	590.9	641.4	689.2	734.1	776.3
5,5-dimethyl-1-hexene	427.7	428.8	487.5	543.4	596.5	646.8	694.4	739.3	781.4

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

T/K		298.15	300	400	500	600	700	800	900	1000
C2H4										
ethylene		52.30	52.26	49.25	46.61	44.35	42.47	40.88	39.54	38.53
C3H6										
propene		20.42	20.33	15.73	11.72	8.28	5.48	3.22	1.46	.17
C4H8										
1-butene		-.13	-.25	-6.23	-11.30	-15.52	-18.87	-21.51	-23.51	-24.85
cis-2-butene		-6.99	-7.11	-13.81	-19.58	-24.35	-28.24	-31.34	-33.68	-35.31
trans-2-butene		-11.17	-11.30	-17.20	-22.30	-26.65	-30.12	-32.93	-35.06	-36.53
2-methyl-1-propene		-16.90	-17.03	-22.72	-27.61	-31.71	-35.02	-37.66	-39.62	-40.96
C5H10										
1-pentene		-20.92	-21.09	-28.33	-34.43	-39.41	-43.35	-46.36	-48.58	-49.96
cis-2-pentene		-28.07	-28.24	-36.19	-42.84	-48.28	-52.59	-55.94	-58.37	-60.00
trans-2-pentene		-31.76	-31.92	-39.29	-45.61	-50.79	-54.98	-58.20	-60.58	-62.17
2-methyl-1-butene		-36.32	-36.48	-43.68	-49.71	-54.64	-58.49	-61.46	-63.55	-64.85
2-methyl-2-butene		-42.55	-42.72	-50.42	-57.03	-62.51	-66.90	-70.33	-72.84	-74.56
3-methyl-1-butene		-28.95	-29.08	-35.40	-40.71	-45.06	-48.49	-51.09	-52.97	-54.10
C6H12										
1-hexene		-41.67	-41.84	-50.42	-57.61	-63.43	-67.95	-71.42	-73.85	-75.31
trans-2-hexene		-53.89	-54.06	-62.72	-70.04	-76.07	-80.79	-84.39	-87.03	-88.66
cis-2-hexene		-52.34	-52.55	-61.76	-69.45	-75.69	-80.54	-84.27	-86.94	-88.58
trans-3-hexene		-54.43	-54.60	-63.14	-70.25	-76.02	-80.58	-84.10	-86.61	-88.16
cis-3-hexene		-47.61	-47.82	-57.15	-64.85	-71.04	-75.86	-79.54	-82.17	-83.81
2-methyl-1-pentene		-59.37	-59.58	-67.82	-74.73	-80.29	-84.60	-87.91	-90.17	-91.50
3(RS)-methyl-1-pentene		-49.45	-49.62	-57.20	-63.39	-68.41	-72.30	-75.23	-77.19	-78.32
4-methyl-1-pentene		-51.21	-51.42	-60.50	-68.16	-74.43	-79.33	-83.18	-85.98	-87.86
2-methyl-2-pentene		-66.86	-67.07	-76.15	-84.10	-89.87	-94.68	-98.41	-101.09	-102.80
trans-3-methyl-2-pentene		-63.09	-63.30	-72.38	-79.96	-86.11	-90.92	-94.64	-97.32	-99.04
cis-3-methyl-2-pentene		-62.17	-62.38	-71.46	-79.04	-85.19	-90.00	-93.72	-96.40	-98.11
trans-4-methyl-2-pentene		-61.46	-61.63	-69.37	-75.90	-81.25	-85.44	-88.66	-90.92	-92.26
cis-4-methyl-2-pentene		-57.45	-57.66	-66.19	-73.26	-78.99	-83.47	-86.90	-89.33	-90.83
3,3-dimethyl-1-butene		-61.50	-61.71	-70.84	-78.41	-84.47	-89.20	-92.80	-95.52	-97.28
2,3-dimethyl-1-butene		-66.32	-66.48	-73.97	-80.21	-85.27	-89.24	-92.26	-94.31	-95.52
2,3-dimethyl-2-butene		-69.79	-70.00	-79.58	-87.82	-94.60	-99.91	-103.97	-106.82	-108.53
2-ethyl-1-butene		-55.98	-56.19	-64.56	-71.42	-75.48	-81.30	-84.56	-86.82	-88.16
C7H14										
1-heptene		-62.3	-62.6	-72.4	-80.7	-87.3	-92.4	-96.1	-98.6	-100.1
trans-2-heptene		-74.6	-74.9	-84.8	-93.3	-100.2	-105.5	-109.4	-112.1	-113.8
trans-3-heptene		-73.9	-74.1	-84.2	-92.7	-99.6	-104.8	-108.6	-111.2	-112.9
2-methyl-1-hexene		-75.0	-75.2	-84.8	-92.9	-99.5	-104.5	-108.1	-110.5	-112.0
3(RS)-methyl-1-hexene		-70.7	-70.9	-80.8	-89.1	-95.7	-100.7	-104.2	-106.6	-108.1
4(RS)-methyl-1-hexene		-71.7	-71.9	-81.8	-90.1	-96.7	-101.8	-105.3	-107.7	-109.2
5-methyl-1-hexene		-71.7	-71.9	-81.8	-90.1	-96.7	-101.8	-105.3	-107.7	-109.2
2-methyl-2-hexene		-83.1	-83.3	-93.6	-102.3	-109.4	-114.8	-118.9	-121.7	-123.4
cis-3-methyl-2-hexene		-83.1	-83.3	-93.6	-102.3	-109.4	-114.8	-118.9	-121.7	-123.4
trans-3-methyl-2-hexene		-83.1	-83.3	-93.6	-102.3	-109.4	-114.8	-118.9	-121.7	-123.4
cis-4(RS)-methyl-2-hexene		-78.8	-79.0	-89.6	-98.4	-105.6	-111.0	-115.0	-117.7	-119.5
trans-4(RS)-methyl-2-hexene		-83.0	-83.2	-93.2	-101.7	-108.5	-113.8	-117.6	-120.2	-121.8
cis-5-methyl-2-hexene		-79.8	-80.1	-90.6	-99.5	-106.6	-112.1	-116.1	-118.8	-120.6
trans-5-methyl-2-hexene		-84.0	-84.2	-94.3	-102.8	-109.6	-114.9	-118.7	-121.3	-122.9
cis-2-methyl-3-hexene		-78.1	-78.3	-88.9	-97.8	-104.9	-110.3	-114.2	-116.9	-118.5
trans-2-methyl-3-hexene		-78.1	-78.3	-88.9	-97.8	-104.9	-110.3	-114.2	-116.9	-118.5
cis-3-methyl-3-hexene		-80.3	-80.5	-90.9	-99.6	-106.6	-112.0	-116.0	-118.7	-120.4
trans-3-methyl-3-hexene		-84.5	-84.7	-94.5	-102.9	-109.6	-114.8	-118.5	-121.1	-122.7
2,3(RS)-dimethyl-1-pentene		-81.2	-81.4	-91.1	-99.2	-105.7	-110.6	-114.1	-116.5	-117.9
2,4-dimethyl-1-pentene		-84.3	-84.6	-94.2	-102.4	-108.9	-113.8	-117.3	-119.7	-121.1
3(RS)-4-dimethyl-1-pentene		-80.0	-80.3	-90.2	-98.5	-105.1	-110.0	-113.5	-115.8	-117.2
2,3-dimethyl-2-pentene		-91.5	-91.8	-102.3	-111.2	-118.5	-124.2	-128.3	-131.2	-133.1
2,4-dimethyl-2-pentene		-89.3	-89.5	-99.9	-108.6	-115.6	-121.0	-124.9	-127.6	-129.3
cis-3,4-dimethyl-2-pentene		-89.3	-89.5	-99.9	-108.6	-115.6	-121.0	-124.9	-127.6	-129.3
trans-3,4-dimethyl-2-pentene		-78.4	-78.6	-88.4	-96.5	-103.0	-107.8	-111.3	-113.5	-114.9
2-ethyl-3-methyl-1-butene		-79.5	-79.7	-89.3	-97.1	-102.1	-107.5	-110.4	-112.2	-113.1
3,3-dimethyl-1-pentene		-83.7	-83.9	-93.5	-101.3	-107.3	-111.7	-114.7	-116.4	-117.4
4,4-dimethyl-1-pentene		-75.1	-75.3	-85.5	-93.9	-100.5	-105.3	-108.7	-110.8	-112.0
cis-4,4-dimethyl-2-pentene		-79.2	-79.5	-89.2	-97.2	-103.4	-108.1	-111.2	-113.2	-114.3
trans-4,4-dimethyl-2-pentene		-77.5	-77.7	-87.0	-94.7	-100.6	-104.9	-107.8	-109.5	-110.4
2,3,3-trimethyl-1-butene		-72.2	-72.4	-82.1	-90.2	-96.7	-101.7	-105.2	-107.6	-109.0
2-ethyl-1-pentene		-70.7	-70.9	-80.8	-89.1	-95.7	-100.7	-104.2	-106.6	-108.1
3-ethyl-1-pentene		-80.3	-80.5	-90.9	-99.6	-106.6	-112.0	-116.0	-118.7	-120.4
cis-2-heptene		-70.5	-70.7	-81.2	-90.0	-97.2	-102.8	-106.9	-109.7	-111.5
cis-3-heptene		-69.7	-70.0	-80.6	-89.5	-96.6	-102.1	-106.1	-108.8	-110.6
C8H16										
1-octene		-83.0	-83.2	-94.4	-103.7	-111.2	-116.9	-120.9	-123.6	-125.2
trans-2-octene		-95.3	-95.5	-106.8	-116.4	-124.1	-130.0	-134.3	-137.2	-139.0
cis-2-octene		-91.1	-91.3	-103.1	-113.1	-121.1	-127.3	-131.7	-134.7	-136.6
trans-3-octene		-94.6	-94.8	-106.2	-115.8	-123.4	-129.3	-133.5	-136.3	-138.0
trans-4-octene		-90.4	-90.6	-102.5	-112.5	-120.5	-126.6	-130.9	-133.9	-135.7
cis-4-octene		-94.6	-94.8	-106.2	-115.8	-123.4	-129.3	-133.5	-136.3	-138.0
2-methyl-1-heptene		-90.4	-90.6	-102.5	-112.5	-120.5	-126.6	-130.9	-133.9	-135.7
2-methyl-1-octene		-95.6	-95.8	-106.8	-116.0	-123.3	-129.0	-133.0	-135.6	-137.2

Table 12. Standard enthalpy of formation for alkenes in kJ/mol--Continued

T/K	298.15	300	400	500	600	700	800	900	1000
C8H16									
3(RS)-methyl-1-heptene	-91.3	-91.5	-102.7	-112.1	-119.5	-125.1	-129.1	-131.7	-133.2
4(RS)-methyl-1-heptene	-92.3	-92.6	-103.8	-113.2	-120.6	-126.2	-130.2	-132.8	-134.3
5(RS)-methyl-1-heptene	-92.3	-92.6	-103.8	-113.2	-120.6	-126.2	-130.2	-132.8	-134.3
6-methyl-1-heptene	-92.3	-92.6	-103.8	-113.2	-120.6	-126.2	-130.2	-132.8	-134.3
2-methyl-2-heptene	-107.9	-108.1	-119.2	-128.6	-136.2	-142.1	-146.3	-149.2	-150.9
trans-3-methyl-1-heptene	-103.7	-104.0	-115.5	-125.3	-133.2	-139.3	-143.7	-146.7	-148.6
cis-3-methyl-1-heptene	-103.7	-104.0	-115.5	-125.3	-133.2	-139.3	-143.7	-146.7	-148.6
trans-4(RS)-methyl-2-heptene	-103.6	-103.8	-115.2	-124.7	-132.4	-138.2	-142.4	-145.2	-146.9
cis-4(RS)-methyl-2-heptene	-99.4	-99.7	-111.5	-121.5	-129.4	-135.5	-139.9	-142.8	-144.6
trans-5(RS)-methyl-2-heptene	-104.6	-104.9	-116.3	-125.8	-133.5	-139.3	-143.5	-146.3	-148.0
cis-5(RS)-methyl-2-heptene	-100.5	-100.7	-112.6	-125.5	-130.5	-136.6	-141.0	-143.9	-145.7
trans-6-methyl-1-heptene	-104.6	-104.9	-116.3	-125.8	-133.5	-139.3	-143.5	-146.3	-148.0
cis-6-methyl-1-heptene	-100.5	-100.7	-112.6	-122.5	-130.5	-136.6	-141.0	-143.9	-145.7
trans-2-methyl-1-heptene	-102.9	-103.1	-114.6	-124.2	-131.8	-137.5	-141.6	-144.3	-146.0
cis-2-methyl-1-heptene	-98.7	-99.0	-110.9	-120.9	-128.8	-134.8	-139.1	-141.9	-143.7
trans-3-methyl-1-heptene	-100.9	-101.2	-112.8	-122.6	-130.5	-136.5	-140.8	-143.8	-145.6
cis-3-methyl-1-heptene	-100.9	-101.2	-112.8	-122.6	-130.5	-136.5	-140.8	-143.8	-145.6
trans-4-methyl-1-heptene	-100.9	-101.2	-112.8	-122.6	-130.5	-136.5	-140.8	-143.8	-145.6
cis-4-methyl-1-heptene	-100.9	-101.2	-112.8	-122.6	-130.5	-136.5	-140.8	-143.8	-145.6
trans-5(RS)-methyl-1-heptene	-102.9	-103.1	-114.6	-124.2	-131.8	-137.5	-141.6	-144.3	-146.0
cis-5(RS)-methyl-1-heptene	-98.7	-99.0	-110.9	-120.9	-128.8	-134.8	-139.1	-141.9	-143.7
trans-6-methyl-1-heptene	-103.9	-104.2	-115.6	-125.2	-132.8	-138.6	-142.7	-145.5	-147.1
cis-6-methyl-1-heptene	-99.7	-100.0	-112.0	-121.9	-129.9	-135.9	-140.2	-143.0	-144.8
3(RS)-ethyl-1-hexene	-91.3	-91.5	-102.7	-112.1	-119.5	-125.1	-129.1	-131.7	-133.2
4-ethyl-1-hexene	-92.3	-92.6	-103.8	-113.2	-120.6	-126.2	-130.2	-132.8	-134.3
trans-3-ethyl-1-hexene	-100.9	-101.2	-112.8	-122.6	-130.5	-136.5	-140.8	-143.8	-145.6
cis-3-ethyl-1-hexene	-103.6	-103.8	-115.2	-124.7	-132.4	-138.2	-142.4	-145.2	-146.9
trans-4-ethyl-1-hexene	-99.4	-99.7	-111.5	-121.5	-129.4	-135.5	-139.9	-142.8	-144.6
3-ethyl-1-hexene	-98.1	-98.4	-110.1	-120.0	-127.8	-133.7	-137.9	-140.8	-142.5
2,3(RS)-dimethyl-1-hexene	-97.7	-97.9	-109.4	-119.0	-126.6	-132.4	-136.4	-139.1	-140.8
2,4(RS)-dimethyl-1-hexene	-100.8	-101.0	-112.5	-122.1	-129.8	-135.5	-139.6	-142.3	-144.0
2,5-dimethyl-1-hexene	-105.0	-105.2	-116.2	-125.4	-132.7	-138.3	-142.2	-144.8	-146.3
3,3-dimethyl-1-hexene	-100.1	-100.4	-111.2	-120.1	-127.0	-132.0	-135.3	-137.3	-138.3
3(RS),4(RS)-dimethyl-1-hexene	-100.7	-100.9	-112.2	-121.5	-128.9	-134.5	-138.3	-140.8	-142.3
3(RS),5-dimethyl-1-hexene	-100.7	-100.9	-112.2	-121.5	-128.9	-134.5	-138.3	-140.8	-142.3
4,4-dimethyl-1-hexene	-104.3	-104.6	-115.5	-124.4	-131.2	-136.2	-139.5	-141.5	-142.5
4(RS),5-dimethyl-1-hexene	-101.7	-102.0	-113.2	-122.6	-130.0	-135.6	-139.4	-141.9	-143.4
2,3-dimethyl-2-hexene	-108.0	-108.2	-119.6	-129.2	-137.0	-143.0	-147.4	-150.3	-152.2
2,4(RS)-dimethyl-2-hexene	-110.0	-110.2	-121.8	-131.6	-139.5	-145.5	-149.8	-152.7	-154.5
2,5-dimethyl-2-hexene	-113.1	-113.3	-125.0	-134.8	-142.6	-148.6	-153.0	-155.9	-157.7
trans-3,4(RS)-dimethyl-2-hexene	-110.0	-110.2	-121.8	-131.6	-139.5	-145.5	-149.8	-152.7	-154.5
cis-3,4(RS)-dimethyl-2-hexene	-110.0	-110.2	-121.8	-131.6	-139.5	-145.5	-149.8	-152.7	-154.5
trans-3,6-dimethyl-2-hexene	-110.1	-113.3	-125.0	-134.8	-142.6	-140.6	-153.0	-155.9	-157.7
cis-3,5-dimethyl-2-hexene	-113.1	-113.3	-125.0	-134.8	-142.6	-148.6	-153.0	-155.9	-157.7
trans-4,4-dimethyl-2-hexene	-112.4	-112.7	-123.7	-132.8	-139.9	-145.1	-148.6	-150.8	-152.0
cis-4,4-dimethyl-2-hexene	-108.2	-108.5	-120.0	-129.5	-136.9	-142.3	-146.1	-148.4	-149.7
trans-4(RS),5-dimethyl-2-hexene	-113.0	-113.2	-124.6	-134.2	-141.8	-147.6	-151.7	-154.4	-156.0
cis-4(RS),5-dimethyl-2-hexene	-108.8	-109.0	-121.1	-130.9	-138.8	-144.8	-149.1	-152.0	-153.7
trans-5,5-dimethyl-2-hexene	-104.1	-104.3	-115.4	-124.5	-131.5	-136.8	-140.3	-142.5	-143.7
cis-5,5-dimethyl-2-hexene	-99.9	-100.2	-111.7	-121.2	-128.6	-134.0	-137.7	-140.1	-141.4
trans-2,2-dimethyl-1-hexene	-104.1	-104.3	-115.4	-124.5	-131.5	-136.8	-140.3	-142.5	-143.7
cis-2,2-dimethyl-3-hexene	-99.9	-100.2	-111.7	-121.2	-128.6	-134.0	-137.7	-140.1	-141.4
trans-2,3-dimethyl-1-hexene	-107.2	-107.4	-119.1	-128.9	-136.7	-142.7	-146.9	-149.7	-151.4
cis-2,3-dimethyl-1-hexene	-107.2	-107.4	-119.1	-128.9	-136.7	-142.7	-146.9	-149.7	-151.4
trans-2,4-dimethyl-1-hexene	-107.2	-107.4	-119.1	-128.9	-136.7	-142.7	-146.9	-149.7	-151.4
cis-2,4-dimethyl-1-hexene	-107.2	-107.4	-119.1	-128.9	-136.7	-142.7	-146.9	-149.7	-151.4
trans-2,5-dimethyl-1-hexene	-111.2	-111.5	-123.0	-132.5	-140.1	-145.8	-149.8	-152.4	-154.0
cis-2,5-dimethyl-1-hexene	-107.0	-107.3	-119.3	-129.3	-137.1	-143.0	-147.2	-150.0	-151.7
trans-3,4-dimethyl-1-hexene	-103.1	-103.3	-114.8	-124.4	-132.2	-138.1	-142.4	-145.3	-147.0
cis-3,4-dimethyl-1-hexene	-103.1	-103.3	-114.8	-124.4	-132.2	-138.1	-142.4	-145.3	-147.0
3-ethyl-2-methyl-1-pentene	-101.8	-102.1	-113.1	-122.2	-129.6	-135.1	-139.0	-141.6	-143.1
3-ethyl-1-3-methyl-1-pentene	-100.1	-100.4	-111.2	-120.1	-127.0	-132.0	-135.3	-137.3	-138.3
3(RS)-ethyl-1-4-methyl-1-pentene	-100.7	-100.9	-112.2	-121.5	-128.9	-134.5	-138.3	-140.8	-142.3
2-propyl-1-pentene	-92.8	-93.0	-104.1	-113.3	-120.6	-126.2	-130.1	-132.6	-134.1
3-ethyl-1-2-methyl-2-pentene	-103.1	-103.3	-114.8	-124.4	-132.2	-138.1	-142.4	-145.3	-147.0
trans-3-ethyl-1-4-methyl-2-pentene	-107.2	-107.4	-119.1	-128.9	-136.7	-142.7	-146.9	-149.7	-151.4
cis-3-ethyl-4-methyl-1-pentene	-107.2	-107.4	-119.1	-128.9	-136.7	-142.7	-146.9	-149.7	-151.4
2,3,3-trimethyl-1-pentene	-108.6	-108.8	-119.5	-128.2	-134.9	-139.8	-143.1	-145.1	-146.0
2,3(RS),4-trimethyl-1-pentene	-111.2	-111.4	-122.5	-131.7	-139.0	-144.4	-148.2	-150.7	-152.2
2,4,4-trimethyl-1-pentene	-102.3	-102.6	-113.2	-122.0	-128.7	-133.6	-136.9	-138.8	-139.8
2,3,4-trimethyl-2-pentene	-112.1	-112.4	-123.8	-133.4	-141.1	-147.1	-151.3	-154.2	-156.0
2,4,4-trimethyl-2-pentene	-106.2	-106.5	-117.8	-127.1	-134.4	-139.7	-143.4	-145.7	-147.0
trans-3,4,4-trimethyl-2-pentene	-106.2	-106.5	-117.8	-127.1	-134.4	-139.7	-143.4	-145.7	-147.0
cis-3,4,4-trimethyl-2-pentene	-95.3	-95.5	-106.3	-115.0	-121.8	-126.6	-129.8	-131.6	-132.5
2-ethyl-1-3,3-dimethyl-1-butene	-92.8	-93.0	-104.1	-113.3	-120.6	-126.2	-130.1	-132.6	-134.1
3-methyl-1-2-isopropyl-4-butene	-105.3	-105.5	-116.7	-125.9	-133.1	-138.5	-142.2	-144.6	-145.9
2-isopropyl-1-pentene	-99.0	-99.3	-110.4	-119.6	-126.8	-132.3	-136.1	-138.6	-140.0
2-ethyl-1-3(RS)-methyl-1-pentene	-99.0	-99.3	-110.4	-119.6	-126.8	-132.3	-136.1	-138.6	-140.0
2-ethyl-1-4-methyl-1-pentene	-102.2	-102.4	-113.5	-122.7	-130.0	-135.5	-139.3	-141.8	-143.2
3,3,4-trimethyl-1-pentene	-109.5	-109.7	-120.7	-129.6	-136.4	-141.3	-144.5	-146.4	-147.4
3(RS),4,4-trimethyl-1-pentene	-100.1	-100.4	-111.3	-120.2	-127.0	-131.9	-135.1	-137.0	-138.0
5,5-dimethyl-1-hexene	-91.8	-92.0	-102.9	-111.8	-118.7	-123.6	-127.0	-129.0	-130.0

CHEMICAL THERMODYNAMIC PROPERTIES OF ALKENE ISOMER GROUPS

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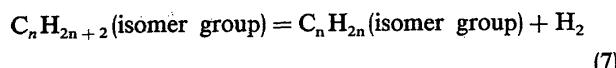
Table 13. Standard Gibbs energy of formation for alkenes in kJ/mol

Table 13. Standard Gibbs energy of formation for alkenes in kJ/mol--Continued

T/K	298.15	300	400	500	600	700	800	900	1000
C8H16									
3(RS)-methyl-1-heptene	96.9	98.0	163.0	230.5	299.8	370.1	441.2	512.6	584.2
4(RS)-methyl-1-heptene	95.8	97.0	161.9	229.5	298.8	369.1	440.2	511.6	583.3
5(RS)-methyl-1-heptene	95.8	97.0	161.9	229.5	298.8	369.1	440.2	511.6	583.3
6-methyl-1-heptene	97.5	98.7	164.2	232.4	302.2	373.1	444.8	516.8	589.0
2-methyl-2-heptene	82.0	83.2	148.7	216.7	286.6	357.5	429.2	501.3	573.6
trans-3-methyl-2-heptene	86.2	87.3	152.9	221.2	291.3	362.5	434.6	507.0	579.7
cis-3-methyl-2-heptene	86.2	87.3	152.9	221.2	291.3	362.5	434.6	507.0	579.7
trans-4(RS)-methyl-2-heptene	85.6	86.8	152.1	220.0	289.8	360.6	432.2	504.1	576.4
cis-4(RS)-methyl-2-heptene	89.8	91.0	156.4	224.5	294.5	365.6	437.6	509.9	582.5
trans-5(RS)-methyl-2-heptene	84.6	85.7	151.1	219.0	288.7	359.6	431.2	503.1	575.4
cis-5(RS)-methyl-2-heptene	88.7	89.9	155.3	223.5	293.5	364.6	436.6	508.9	581.5
trans-6-methyl-2-heptene	86.3	87.5	153.4	221.9	292.2	363.6	435.8	508.3	581.2
cis-6-methyl-2-heptene	90.5	91.6	157.6	226.3	296.9	368.6	441.2	514.1	587.3
trans-2-methyl-3-heptene	88.3	89.5	155.5	224.1	294.6	366.1	438.4	511.0	583.9
cis-2-methyl-3-heptene	92.5	93.7	159.8	228.6	299.3	371.1	443.7	516.7	590.0
trans-3-methyl-3-heptene	89.2	90.4	156.1	224.5	294.7	366.1	438.2	510.8	583.6
cis-3-methyl-3-heptene	89.2	90.4	156.1	224.5	294.7	366.1	438.2	510.8	583.6
trans-4-methyl-3-heptene	89.2	90.4	156.1	224.5	294.7	366.1	438.2	510.8	583.6
cis-4-methyl-3-heptene	89.2	90.4	156.1	224.5	294.7	366.1	438.2	510.8	583.6
trans-5(RS)-methyl-3-heptene	86.6	87.8	153.2	221.3	291.1	362.1	433.8	505.8	578.1
cis-5(RS)-methyl-3-heptene	90.8	91.9	157.5	225.7	295.8	367.1	439.1	511.5	584.2
trans-6-methyl-3-heptene	87.3	88.4	154.5	223.1	293.5	365.1	437.3	510.0	582.9
cis-6-methyl-3-heptene	91.4	92.6	158.7	227.6	298.3	370.1	442.7	515.7	589.0
3(RS)-ethyl-1-hexene	96.9	98.0	163.0	230.5	299.8	370.1	441.2	512.6	584.2
4-ethyl-1-hexene	97.5	98.7	164.2	232.4	302.2	373.1	444.8	516.8	589.0
trans-3-ethyl-2-hexene	88.5	89.7	155.1	223.3	293.2	364.3	436.2	508.5	581.1
cis-3-ethyl-2-hexene	88.5	89.7	155.1	223.3	293.2	364.3	436.2	508.5	581.1
trans-4-ethyl-2-hexene	87.3	88.5	154.4	222.9	293.2	364.6	436.8	509.3	582.2
cis-4-ethyl-2-hexene	91.5	92.7	158.7	227.4	298.0	369.7	442.2	515.1	588.3
3-ethyl-3-hexene	90.8	92.0	157.3	225.3	295.2	366.1	437.9	510.0	582.4
2,3(RS)-dimethyl-1-hexene	92.8	94.0	159.8	228.2	298.4	369.7	441.7	514.1	586.8
2,4(RS)-dimethyl-1-hexene	89.7	90.9	156.6	225.1	295.3	366.6	438.6	511.0	583.7
2,5-dimethyl-1-hexene	87.2	88.4	154.7	223.5	294.0	365.6	437.9	510.5	583.4
3,3-dimethyl-1-hexene	95.0	96.2	163.5	233.2	304.6	376.9	449.9	523.1	596.5
3(RS),4(RS)-dimethyl-1-hexene	90.8	92.0	158.1	226.8	297.2	368.7	440.9	513.4	586.1
3(RS),4(RS)-dimethyl-1-hexene	90.8	92.0	158.1	226.8	297.2	368.7	440.9	513.4	586.1
3(RS),5-dimethyl-1-hexene	90.8	92.0	158.1	226.8	297.2	368.7	440.9	513.4	586.1
4,4-dimethyl-1-hexene	90.8	92.0	159.3	229.0	300.4	372.7	445.6	518.9	592.3
4(RS),5-dimethyl-1-hexene	89.8	91.0	157.1	225.8	296.2	367.6	439.8	512.4	585.1
2,3-dimethyl-2-hexene	84.2	85.4	151.8	220.7	291.5	363.4	436.0	509.1	582.5
2,4(RS)-dimethyl-2-hexene	81.6	82.7	148.9	217.7	288.4	360.2	432.8	505.7	579.0
2,5-dimethyl-2-hexene	80.1	81.3	148.1	217.5	288.7	361.1	434.3	507.8	581.6
trans-3,4(RS)-dimethyl-2-hexene	81.6	82.7	148.9	217.7	288.4	360.2	432.8	505.7	579.0
cis-3,4(RS)-dimethyl-2-hexene	81.6	82.7	148.9	217.7	288.4	360.2	432.8	505.7	579.0
trans-3,5-dimethyl-2-hexene	80.1	81.3	148.1	217.5	288.7	361.1	434.3	507.8	581.6
cis-3,5-dimethyl-2-hexene	80.1	81.3	148.1	217.5	288.7	361.1	434.3	507.8	581.6
trans-4,4-dimethyl-2-hexene	83.8	85.0	152.6	222.7	294.6	367.4	440.9	514.7	588.7
cis-4,4-dimethyl-2-hexene	87.9	89.2	156.9	227.2	299.3	372.4	446.3	520.4	594.8
trans-4(RS),5-dimethyl-2-hexene	79.6	80.8	147.2	216.3	287.2	359.1	431.9	504.9	578.3
cis-4(RS),5-dimethyl-2-hexene	83.8	84.9	151.5	220.8	291.9	364.2	437.2	510.7	584.4
trans-5,5-dimethyl-2-hexene	94.8	96.0	164.6	235.6	308.4	382.1	456.5	531.2	606.1
cis-5,5-dimethyl-2-hexene	99.0	100.2	168.8	240.1	313.1	387.1	461.9	536.9	612.2
trans-2,2-dimethyl-3-hexene	95.6	96.8	165.6	236.9	309.9	383.9	458.5	533.5	608.6
cis-2,2-dimethyl-3-hexene	99.7	101.0	169.8	241.4	314.6	388.9	463.9	539.2	614.7
trans-2,3-dimethyl-3-hexene	86.4	87.6	154.4	223.9	295.3	367.8	441.0	514.6	588.5
cis-2,3-dimethyl-3-hexene	86.4	87.6	154.4	223.9	295.3	367.8	441.0	514.6	588.5
trans-2,4-dimethyl-3-hexene	86.4	87.6	154.4	223.9	295.3	367.8	441.0	514.6	588.5
cis-2,4-dimethyl-3-hexene	86.4	87.6	154.4	223.9	295.3	367.8	441.0	514.6	588.5
trans-2,5-dimethyl-3-hexene	83.3	84.5	151.7	221.5	293.0	365.7	439.1	512.8	586.8
cis-2,5-dimethyl-3-hexene	89.2	90.4	158.2	228.8	301.2	374.7	449.0	523.7	598.6
trans-3,4-dimethyl-3-hexene	89.4	90.6	157.0	226.1	297.0	369.0	441.8	514.9	580.4
cis-3,4-dimethyl-3-hexene	91.1	92.3	159.3	229.0	300.5	373.0	446.4	520.1	594.1
3-ethyl-2-methyl-1-pentene	90.4	91.5	157.8	226.6	297.1	368.7	441.0	513.6	586.5
3-ethyl-3-methyl-1-pentene	95.0	96.2	163.5	233.2	304.6	376.9	449.9	523.1	596.5
3(RS)-ethyl-1-4-methyl-1-pentene	90.8	92.0	158.1	226.8	297.2	368.7	440.9	513.4	586.1
2-propyl-1-pentene	97.3	98.5	164.0	232.2	302.0	372.9	444.5	516.4	588.6
3-ethyl-1-2-methyl-2-pentene	90.4	91.6	158.3	227.7	299.0	371.3	444.4	517.9	591.6
trans-3-ethyl-1-4-methyl-2-pentene	85.6	86.8	153.4	222.7	293.8	366.0	439.0	512.4	586.0
cis-3-ethyl-1-4-methyl-2-pentene	85.6	86.8	153.4	222.7	293.8	366.0	439.0	512.4	586.0
2,3,3-trimethyl-1-pentene	88.9	90.1	158.1	228.5	300.6	373.5	447.1	521.0	595.1
2,3(RS),4-trimethyl-1-pentene	82.6	83.8	150.7	220.0	291.1	363.2	436.0	509.2	582.6
2,4,4-trimethyl-1-pentene	97.9	99.1	168.0	239.3	312.3	386.2	460.7	535.5	610.4
2,3,4-trimethyl-1-pentene	83.4	84.6	152.1	222.2	294.1	367.1	440.9	515.1	589.5
2,4,4-trimethyl-2-pentene	95.0	96.2	165.6	237.6	311.2	385.9	461.3	537.0	612.9
trans-3,4,4-trimethyl-2-pentene	95.0	96.2	165.6	237.6	311.2	385.9	461.3	537.0	612.9
cis-3,4,4-trimethyl-2-pentene	95.7	97.0	166.6	238.8	312.7	387.7	463.3	539.2	615.4
2-ethyl-1-3,3-dimethyl-1-butene	104.4	105.6	174.4	245.6	318.4	392.2	466.6	541.2	616.0
2-ethyl-1-hexene	95.6	96.7	161.7	229.3	298.5	368.8	439.8	511.2	582.8
3-methyl-2-isopropyl-4-butene	91.5	92.7	160.6	231.0	303.1	376.2	450.0	524.1	598.5
2-isopropyl-1-pentene	92.7	93.9	160.0	228.7	299.1	370.5	442.6	515.1	587.8
2-ethyl-1-3(RS)-methyl-1-pentene	91.0	92.1	157.7	225.8	295.6	366.5	438.0	509.9	582.0
2-ethyl-1-4-methyl-1-pentene	89.6	90.7	156.9	225.6	295.9	367.4	439.5	512.0	584.7
3,3,4-trimethyl-1-pentene	89.0	90.2	158.6	229.5	302.0	375.5	449.5	523.9	598.4
3(RS),4,4-trimethyl-1-pentene	99.4	100.6	169.3	240.5	313.4	387.2	461.6	536.2	611.1
5,5-dimethyl-1-hexene	106.1	107.3	175.5	246.1	318.4	391.6	465.5	539.6	614.0

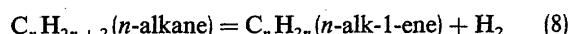
7. Discussion

The values of standard thermodynamic properties of isomer groups given here may be used in predicting equilibrium compositions of organic systems at temperature-catalyst conditions where species in an isomer group are in equilibrium. The values of the standard Gibbs energies of formation of the alkene isomer groups calculated here and the values for the alkanes published earlier² can be used to calculate the equilibrium constants for the reaction



in the ideal gas state. This equilibrium constant can be interpreted as the partial pressure of hydrogen in bars at which the ratio of the mole fractions of alkenes and alkanes is unity.

The values for $\Delta_f G^\circ(\text{I})$ for C_9H_{18} and $\text{C}_{10}\text{H}_{20}$ have been obtained using the increment in the last column of Table 6. The dependence of $\log K$ on carbon number and temperature is given in Table 14. As the carbon number increases the equilibrium constant continues to increase, partly because there are more alkene isomers than alkane isomers at a given carbon number. To contrast the behavior of the isomer groups with the behavior of the linear chains, Table 15 gives the dependence of $\log K$ on carbon number and temperature for the reaction



in the ideal gas state. The equilibrium constant for this reaction tends to level off at higher carbon numbers.

Table 14. LogK for reaction 7 for various carbon numbers

T/K	C2	C3	C4	C5	C6	C7	C8	C9	C10
298	-17.49	-15.28	-13.83	-13.55	-12.43	-12.33	-11.95	-11.80	-11.61
300	-17.36	-15.14	-13.71	-13.44	-12.30	-12.21	-11.83	-11.68	-11.48
400	-11.39	-9.65	-8.58	-8.10	-7.37	-7.35	-7.03	-6.79	-6.54
500	-7.78	-6.32	-5.46	-5.00	-4.41	-4.41	-4.13	-3.89	-3.65
600	-5.35	-4.09	-3.37	-2.96	-2.43	-2.43	-2.18	-1.97	-1.73
700	-3.61	-2.46	-1.84	-1.49	-1.01	-1.03	-0.78	-0.58	-0.36
800	-2.29	-1.26	-0.72	-0.38	0.06	0.04	0.26	0.46	0.67
900	-1.24	-0.31	0.16	0.46	0.88	0.88	1.09	1.28	1.47
1000	-0.44	0.44	0.86	1.15	1.56	1.55	1.75	1.93	2.12

Table 15. LogK for reaction 8 for various carbon numbers

T/K	C2	C3	C4	C5	C6	C7	C8	C9	C10
298	-17.49	-15.28	-15.43	-15.34	-15.35	-15.22	-15.22	-15.18	-15.15
300	-17.36	-15.14	-15.29	-15.20	-15.21	-15.09	-15.09	-15.05	-15.01
400	-11.39	-9.65	-9.79	-9.71	-9.72	-9.60	-9.60	-9.56	-9.52
500	-7.78	-6.32	-6.45	-6.37	-6.39	-6.27	-6.26	-6.22	-6.19
600	-5.35	-4.09	-4.22	-4.12	-4.15	-4.01	-4.01	-3.99	-3.96
700	-3.61	-2.46	-2.58	-2.52	-2.52	-2.42	-2.40	-2.38	-2.36
800	-2.29	-1.26	-1.37	-1.30	-1.31	-1.22	-1.21	-1.17	-1.13
900	-1.24	-0.31	0.43	0.37	0.39	0.25	0.25	0.22	0.19
1000	-0.44	0.44	0.32	0.39	0.38	0.51	0.50	0.54	0.58

8. Nomenclature

C_p°	= standard heat capacity at constant pressure of isomer i , $\text{J K}^{-1} \text{mol}^{-1}$
$C_p^\circ(\text{I})$	= standard heat capacity at constant pressure of isomer group I, $\text{J K}^{-1} \text{mol}^{-1}$
$\Delta_f G_i^\circ$	= standard Gibbs energy of formation of isomer i , kJ mol^{-1}
$\Delta_f G^\circ(\text{I})$	= standard Gibbs energy of formation of isomer group I, kJ mol^{-1}
$H^\circ(\text{I}, T) - H^\circ(\text{I}, 298.15 \text{ K})$	= standard enthalpy for isomer groups relative to isomer groups at 298.15 K, kJ mol^{-1}
$H^\circ(\text{I}, T) - H^\circ(\text{I}, 298.15 \text{ K}) + \Delta_f H^\circ(\text{I}, 298.16 \text{ K})$	= 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}
$\Delta_f H^\circ(\text{I})$	= 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 , $\text{J K}^{-1} \text{mol}^{-1}$
$S^\circ(\text{I})$	= standard entropy of isomer group I, $\text{J K}^{-1} \text{mol}^{-1}$
TSN	= total symmetry number
y_i	= mole fraction of isomer i within the isomer group
y_{I}	= mole fraction of isomer group I in a mixture

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