Standard Chemical Thermodynamic Properties of Alkylnaphthalene Isomer Groups

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The chemical thermodynamic properties of alkylnaphthalene isomer groups for $C_{10}H_8$ and $C_{11}H_{10}$ 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 $C_{12}H_{12}$ to $C_{14}H_{16}$ have been calculated using Benson group values. A new Benson group value for the 1,8-dimethyl steric hindrance has been calculated from recent experimental data. The increments in isomer group properties per carbon atom have been calculated to show the extent to which thermodynamic properties of higher isomer groups may be obtained by linear extrapolation. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 298.15 to 1000 K. Values of C_p°, S°, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ are given for all species from $C_{10}H_8$ to $C_{14}H_{16}$ with energy units of joules for a standard state pressure of 1 bar.

Key words: alkylnaphthalenes; 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

Since the number of isomers of alkylnaphthalenes increases rapidly with carbon number, it is convenient to use isomer group thermodynamic properties for cases in which all isomers in the isomer group are in equilibrium. The tables presented here are of the same type as those published for the alkanes,[1] alkylbenzenes,[2] and alkenes.[3]

Milligan, Becker, and Pitzer[4] calculated the standard thermodynamic properties of the alkylnaphthalenes in the ideal gas state through $C_{12}H_{12}$, except for 1,8-dimethylnaphthalene, using the method of increments. Some further

small changes were made by Stull, Westrum, and Sinke[5] in publishing their book in 1969. We have added tables to include all isomers through $C_{14}H_{16}$ using the Benson method.[6,7] Stein, Golden, and Benson[8] have extended this method to the prediction of standard gas-phase thermodynamic properties for polycyclic aromatic hydrocarbons consisting of six-membered rings. They showed that the group additivity method reproduced the measured $\Delta_f H°(298.15\ K)$ values for substituted naphthalenes within 5 kJ mol^{-1}.

2. Standard Thermodynamic Properties of Alkylnaphthalene Isomer Groups

When isomers are in equilibrium, the standard Gibbs energy of formation $\Delta_f G°(I)$ of the isomer group is defined by[9,10]

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

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

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

where y_I is the sum of the mole fractions of the individual isomers. The corresponding equations for the other standard thermodynamic properties $C_P^\circ(I)$, $S°(I)$, and $\Delta_f H°(I)$ can be derived by differentiating Eq. (1) with respect to temperature.[11] 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 alkylnaphthalenes, the standard chemical thermodynamic properties for an isomer group are interrelated by

$$\Delta_f G°(I) = \Delta_f H°(I) - T [S°(I) - nS°_{graphite} - (n-6)S°_{H_2(g)}], \quad (3)$$

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. The numbers of chiral centers and isomers of the alkylnaphthalenes 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. The 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. Table 1 also summarizes the numbers of lines in the tables in this article.

Table 1. Numbers of isomers of alkylnaphthalenes

	Number of lines	One Chiral Center	Total isomers
C10H8	1	0	1
C11H10	2	0	2
C12H12	12	0	12
C13H14	32	0	32
C14H16	110	2	112

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

Since the literature values are incomplete on the $C_{12}H_{12}$ alkylnaphthalenes, the isomer group properties for $C_{12}H_{12}$ have been calculated using the Benson method. Since the increments per carbon atom in isomer group properties are still changing at $C_{12}H_{12}$, this method has also been used to calculate properties for all isomers of $C_{13}H_{14}$ and $C_{14}H_{16}$.

In order to make these calculations the structure of each alkylnaphthalene species was divided into $C(H)_3(C)$, $C(H)_2(C)_2$, $C(H)(C)_3$, $C(C)_4$, $C(C_B)(C)(H)_2$, $C(C_B)(C)_2(H)$, $C(C_B)(C)_3$, $C_B(H)$, $C_B(C)$, and $C_{BF}(C_B)_2(C_{BF})$; the group contributions from Ref. 7 were used. In addition the total symmetry number (TSN), number of optical isomers (OPT), and *ortho* corrections were identified. Gauche corrections were made for sec- and isobutylnaphthalene. Naphthalene has a symmetry number of 4; 2,3,6,7-tetramethylnaphthalene has a symmetry number of 4×3^4; and 1,5-dimethylnaphthalene has a symmetry number of 2×3^2. The report by Davies, Syverud, and Steiner[12] was very helpful in calculating symmetry numbers.

We made the first estimates of the thermodynamic properties of the various species of $C_{12}H_{12}$, $C_{13}H_{14}$, and $C_{14}H_{16}$ using Benson group values published in 1976.[7] Gammon pointed out to the authors that there is steric hindrance in 1,8-dimethylnaphthalene that is not provided for in the 1976 Benson values. The enthalpies of combustion of 1,8-dimethylnaphthalene, 2,3-dimethylnaphthalene, 2,6-dimethylnaphthalene, and 2,7-dimethylnaphthalene were measured by Good,[13] who pointed out that the enthalpy of formation of the crystalline 1,8-dimethylnaphthalene is about 7.5 kcal mol^{-1} more positive than those for 2,6-dimethylnaphthalene and 2,7-dimethylnaphthalene. The enthalpies of vaporization of these substances were measured by Osborn and Douslin,[14] and their heat capacities and enthalpies of transition were measured by Finke, Messerly, Lee, Osborn, and Douslin.[15] To remedy this deficiency in our estimates, an additional Benson group was introduced to provide for the 1,8 steric hindrance. The group value for $\Delta_f H°_{298}$ for this group was taken to be 5.88 kcal mol^{-1} because this is the difference between the extrapolated value for the 1,8-dimethylnaphthalene and the prediction by the Benson method without this correction. The Benson method gives the correct values for $\Delta_f H°$ for 2,6-dimethylnaphthalene and 2,7-dimethylnaphthalene within their uncertainties. The experimental entropies of the 2,6- and 2,7-dimethylnaphthalenes from 340 to 410 K agree within experimental error and extrapolate linearly to the $S°$ estimated by the Benson method. The experimental entropies of the 1,8-dimethylnaphthalene are definitely lower and extrapolate linearly to an $S°$ value about 9.3 J K^{-1} mol^{-1} lower than that estimated by the Benson method. Therefore the entropy assigned to the 1,8 repulsion was taken to be –2.22 cal K^{-1} mol^{-1}. The experimental data do not indicate any heat ca-

Table 2. Root mean square deviations between alkylnaphthalene 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								
C10H8	1.66	1.63	.80	1.70	.57	1.24	2.32	1.67	1.51
C11H10	2.36	2.40	5.66	7.05	5.91	4.01	2.56	2.47	4.99
C12H12	4.31	4.36	7.91	9.71	8.67	6.80	5.25	4.68	6.77
C13H14	4.59	4.63	6.98	7.63	6.22	3.96	6.35	2.81	5.56
C14H16	2.93	2.99	5.97	7.23	5.59	3.28	1.52	1.87	5.69
	Standard entropy in J/K mol								
C10H8	3.07	3.08	2.97	3.29	3.54	3.48	3.19	2.92	2.90
C11H10	3.31	3.28	2.20	1.15	1.22	1.74	2.06	2.27	2.62
C12H12	8.13	8.09	6.56	4.91	3.72	3.07	2.76	2.64	2.73
C13H14	3.42	3.41	2.87	3.31	4.06	4.62	4.45	4.36	4.70
C14H16	1.77	1.74	1.29	2.01	3.00	3.61	3.86	3.99	4.32
	Standard enthalpy of formation in kJ/mol								
C10H8	.33	.35	.18	.29	.36	.35	.11	.13	.07
C11H10	.80	.81	.57	.50	.97	1.47	1.73	1.94	2.36
C12H12	1.71	1.69	1.39	1.02	1.28	1.90	2.39	2.82	3.40
C13H14	1.85	1.85	1.43	.81	.49	.81	.65	.69	1.06
C14H16	2.95	2.96	2.66	2.06	1.55	1.15	1.10	1.07	.92
	Standard Gibbs energy of formation in kJ/mol								
C10H8	.71	.70	1.04	1.30	1.72	2.00	2.37	2.62	2.84
C11H10	.78	.76	.93	1.10	1.16	1.23	1.26	1.32	1.40
C12H12	1.66	1.67	2.22	2.73	3.12	3.46	3.66	3.88	4.06
C13H14	1.76	1.77	1.90	2.12	2.56	2.89	3.40	3.74	4.11
C14H16	2.83	2.84	2.84	2.96	3.27	3.50	3.97	4.24	4.54

pacity corrections for the 1,8 interaction. In the revised calculations given here these values were also applied to 4,5 methyl groups in trimethyl and tetramethyl naphthalenes. In the absence of any experimental data on 1,8 methyl–ethyl or other interactions, this group value was also applied whenever there were 1,8 or 4,5 alkyl groups in $C_{13}H_{14}$ and $C_{14}H_{16}$.

The matrix of numbers of contributions was matrix multiplied by a matrix of the Benson values to obtain for each isomer the sum of the contributions to $\Delta_f H^\circ_{298}$, $S^\circ_{\text{int}298}$, C°_{P300}, C°_{P400}, C°_{P500}, C°_{P600}, C°_{P800}, and C°_{P1000}. In further steps in the calculation the heat capacity values were fit to the equation

$$C^\circ_P = \alpha + \beta T + \gamma T^2, \tag{4}$$

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,

$$S^\circ = S^\circ_0 + \alpha \ln T + \beta T + (\gamma/2)T^2 - R \ln (\text{TSN/OPT}), \tag{5}$$

$$\Delta_f H^\circ = \Delta_f H^\circ_0 + \alpha T + (\beta/2)T^2 + (\gamma/3)T^3 - n(H^\circ - H^\circ_{298})_{\text{graph}} - (n-6)(H^\circ - H^\circ_{298})_{H_2}. \tag{6}$$

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 values from Stull, Westrum, and Sinke[7] for $C_{10}H_8$, $C_{11}H_{10}$, 11 of the 12 isomers of $C_{12}H_{12}$, five of the 32 isomers of $C_{13}H_{14}$ and two of the 112 isomers of $C_{14}H_{16}$. 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 $C_{10}H_8$ this yields the magnitude of the deviations, and for the higher isomer groups it yields the root-mean-square deviations as a function of temperature.

4. Tables of Standard Thermodynamic Properties of Alkylnaphthalene 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 (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 $R \ln(1.013\,25) = 0.109$ J K^{-1} 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 $(7 - n)$ in moles of gas in the formation reaction.[16]

In Tables 3–8, the Stull, Westrum, and Sinke tables have been used to calculate the isomer group properties for $C_{10}H_8$ and $C_{11}H_{10}$, and the Benson method has been used to calculate the isomer group properties for $C_{12}H_{12}$ to $C_{14}H_{16}$. For each property the increments in going from one carbon number to the next are provided. Thus, of the four increments per carbon atom, the last two have been calculated using the Benson alone. These increments provide a basis for a linear extrapolation of standard thermodynamic properties of alkane isomer groups to higher carbon numbers.

Table 7 gives $H^\circ(\text{I},T) - H^\circ(\text{I},298.15\text{ K})$, the standard enthalpy for an isomer group relative to the isomer group at 298.15 K. Table 8 gives values for $H^\circ(\text{I},T) - H^\circ(\text{I},298.15\text{ K}) + \Delta_f H^\circ(\text{I},298.15\text{ K})$, 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.

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

T/K	C10H8	C11H10	C12H12	C13H14	C14H16
298.15	132.55	159.87	181.5	208.7	244.7
300.00	133.43	160.85	182.6	209.8	246.1
400.00	179.20	211.78	235.8	269.9	313.8
500.00	218.11	255.38	283.1	323.1	370.2
600.00	249.66	290.88	324.4	369.2	417.9
700.00	275.18	320.06	359.7	408.3	458.4
800.00	296.10	344.08	388.9	440.6	492.1
900.00	313.42	363.97	412.1	466.1	518.9
1000.00	327.94	380.87	429.1	484.9	538.7

Table 3a. Increments per carbon atom

T/K	C11-C10	C12-C11	C13-C12	C14-C13
298.15	27.32	21.7	27.1	36.1
300.00	27.42	21.7	27.3	36.3
400.00	32.57	24.0	34.1	43.9
500.00	37.27	27.7	40.0	47.1
600.00	41.22	33.5	44.8	48.7
700.00	44.87	39.6	48.7	50.1
800.00	47.98	44.8	51.7	51.4
900.00	50.55	48.1	54.1	52.7
1000.00	52.93	48.3	55.8	53.8

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

T/K	C10H8	C11H10	C12H12	C13H14	C14H16
298.15	335.75	384.61	433.9	473.1	506.8
300.00	336.59	385.63	435.0	474.4	508.3
400.00	381.40	439.06	494.9	543.1	588.6
500.00	425.71	491.16	552.7	609.2	664.9
600.00	468.38	540.92	608.1	672.3	736.7
700.00	508.84	588.04	660.8	732.2	804.3
800.00	546.96	632.38	710.8	788.9	867.7
900.00	582.86	674.08	758.0	842.3	927.3
1000.00	616.66	713.35	802.4	892.5	983.1

Table 4a. Increments per carbon atom

T/K	C11-C10	C12-C11	C13-C12	C14-C13
298.15	48.86	49.3	39.2	33.7
300.00	49.04	49.4	39.4	33.9
400.00	57.66	55.9	48.2	45.5
500.00	65.45	61.6	56.4	55.7
600.00	72.54	67.2	64.2	64.5
700.00	79.20	72.8	71.4	72.1
800.00	85.42	78.5	78.1	78.8
900.00	91.23	84.0	84.3	85.0
1000.00	96.69	89.0	90.1	90.6

TABLE 5. Standard enthalpy of formation for alkylnaphthalene isomer groups

T/K	C10H8	C11H10	C12H12	C13H14	C14H16
298.15	150.96	116.37	83.9	51.0	19.4
300.00	150.83	116.20	83.7	50.8	19.2
400.00	144.56	109.04	75.0	41.2	9.8
500.00	139.49	103.19	67.5	33.2	2.1
600.00	135.39	98.51	61.5	26.9	-4.0
700.00	132.21	94.95	56.8	22.2	-8.4
800.00	129.75	92.24	53.5	19.1	-11.4
900.00	127.95	90.35	51.3	17.1	-13.1
1000.00	126.90	89.34	49.9	16.1	-13.9

Table 5a. Increments per carbon atom

T/K	C11-C10	C12-C11	C13-C12	C14-C13
298.15	-34.59	-32.5	-32.9	-31.6
300.00	-34.63	-32.5	-32.9	-31.6
400.00	-35.52	-34.0	-33.8	-31.5
500.00	-36.30	-35.7	-34.3	-31.1
600.00	-36.88	-37.1	-34.6	-30.8
700.00	-37.26	-38.1	-34.6	-30.6
800.00	-37.50	-38.7	-34.5	-30.4
900.00	-37.59	-39.0	-34.2	-30.2
1000.00	-37.56	-39.4	-33.8	-30.0

TABLE 6. Standard Gibbs energy of formation for alkylnaphthalene isomer groups in kJ/mol

T/K	C10H8	C11H10	C12H12	C13H14	C14H16
298.15	223.69	215.21	208.9	204.9	204.0
300.00	224.15	215.82	209.6	205.9	205.1
400.00	249.58	250.18	253.0	259.1	268.6
500.00	276.47	286.16	298.3	314.5	334.2
600.00	304.21	323.14	345.1	371.4	401.3
700.00	332.65	360.93	392.8	429.2	469.2
800.00	361.42	399.08	441.0	487.6	537.6
900.00	390.49	437.57	489.5	546.2	606.3
1000.00	419.77	476.26	538.3	605.1	675.2

Table 6a. Increments per carbon atom

T/K	C11-C10	C12-C11	C13-C12	C14-C13
298.15	-8.48	-6.4	-3.9	-.9
300.00	-8.34	-6.2	-3.7	-.8
400.00	.59	2.8	6.1	9.5
500.00	9.69	12.2	16.2	19.7
600.00	18.93	22.0	26.3	29.9
700.00	28.28	31.8	36.5	39.9
800.00	37.66	41.9	46.6	50.0
900.00	47.07	52.0	56.7	60.1
1000.00	56.49	62.0	66.8	70.1

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

T/K	C10H8	C11H10	C12H12	C13H14	C14H16
298.15	.00	.00	.0	.0	.0
300.00	.26	.29	.3	.4	.5
400.00	15.81	18.88	21.3	24.4	28.6
500.00	35.71	42.24	47.3	54.1	62.8
600.00	59.09	69.56	77.7	88.8	102.3
700.00	85.40	100.19	112.0	127.7	146.2
800.00	113.96	133.38	149.5	170.2	193.7
900.00	144.43	168.77	189.5	215.6	244.3
1000.00	176.62	206.13	231.7	263.3	297.3

Table 7a. Increments per carbon atom

T/K	C11-C10	C12-C11	C13-C12	C14-C13
298.15	.00	.0	.0	.0
300.00	.03	.0	.1	.1
400.00	3.07	2.4	3.1	4.1
500.00	6.54	5.1	6.8	8.7
600.00	10.46	8.2	11.1	13.5
700.00	14.79	11.8	15.8	18.4
800.00	19.43	16.1	20.8	23.5
900.00	24.35	20.8	26.1	28.7
1000.00	29.51	25.5	31.6	34.0

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

T/K	C10H8	C11H10	C12H12	C13H14	C14H16
298.15	150.96	116.37	83.9	51.0	19.4
300.00	151.22	116.66	84.2	51.4	19.9
400.00	166.77	135.25	105.2	75.4	48.0
500.00	186.67	158.61	131.2	105.1	82.3
600.00	210.05	185.93	161.6	139.8	121.7
700.00	236.36	216.56	195.9	178.7	165.6
800.00	264.92	249.75	233.4	221.2	213.2
900.00	295.38	285.14	273.5	266.6	263.8
1000.00	327.58	322.50	315.6	314.3	316.7

Table 8a. Increments per carbon atom

T/K	C11-C10	C12-C11	C13-C12	C14-C13
298.15	-34.59	-32.5	-32.9	-31.6
300.00	-34.56	-32.4	-32.9	-31.5
400.00	-31.52	-30.0	-29.8	-27.5
500.00	-28.05	-27.4	-26.1	-22.9
600.00	-24.13	-24.3	-21.8	-18.1
700.00	-19.80	-20.7	-17.1	-13.2
800.00	-15.16	-16.4	-12.1	-8.1
900.00	-10.24	-11.7	-6.8	-2.9
1000.00	-5.08	-6.9	-1.3	2.5

5. Equilibrium Mole Fractions Within Alkylnaphthalene 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 $\Delta_f G°(I)$ and $\Delta_f G_i^\circ$ are about the same, the uncertainty in the difference is nearly independent of the relative values of the two parameters, but the absolute uncertainty does increase with temperature. Since the nearly constant uncertainty is in the exponent in the calculation, the equilibrium mole fractions of the isomers at a given temperature are uncertain by the same factor, whether they are large or small. The usual equation for the propagation of variance indicates that the equilibrium mole fractions are uncertain by abou 15% at the lower temperature and 10% at the higher tem peratures. 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.[17] In naming species with two or more ring hydrogens substituted, the name of the largest substituent is given first to clarify the relationships between the various structural isomers. Naphthalene has four possible starting positions, each one being the carbon adjacent to the fused ring carbons. Because of the many possible combinations for names, the group appearing first in the alphabetically arranged name has priority if two groups are in equilivalent positions. For example, 1-ethyl-8-methyl is used. However, names were made to yield the lowest possible numbers when there were more than two substituents. For example, 8-ethyl-1,2-dimethylnaphthalene is used.

Table 9 shows that in general alkylnaphthalenes with branched side chains have very low equilibrium mole fractions, especially at low temperatures. At higher temperatures there is in general a more even distribution of the mole fractions between the less branched isomers, reflecting the fact that entropies are more similar than the enthalpies of formation.

Table 9. Equilibrium mole fractions within alkylnaphthalene isomer groups

T/K	298.15	300	400	500	600	700	800	900	1000
C11H10									
1-methylnaphthalene	.3488	.3535	.3709	.3815	.3907	.3990	.4068	.4128	.4177
2-methylnaphthalene	.6512	.6465	.6291	.6185	.6093	.6010	.5932	.5872	.5823
C12H12									
1,2-dimethylnaphthalene	.0323	.0324	.0413	.0488	.0551	.0604	.0649	.0686	.0717
1,3-dimethylnaphthalene	.1899	.1898	.1859	.1815	.1769	.1721	.1673	.1627	.1582
1,4-dimethylnaphthalene	.0949	.0949	.0929	.0908	.0884	.0860	.0837	.0813	.0791
1,5-dimethylnaphthalene	.0949	.0949	.0929	.0908	.0884	.0860	.0837	.0813	.0791
1,6-dimethylnaphthalene	.1899	.1898	.1859	.1815	.1769	.1721	.1673	.1627	.1582
1,7-dimethylnaphthalene	.1899	.1898	.1859	.1815	.1769	.1721	.1673	.1627	.1582
1,8-dimethylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0004	.0007	.0010	.0013
2,3-dimethylnaphthalene	.0161	.0162	.0207	.0244	.0275	.0302	.0324	.0343	.0359
2,6-dimethylnaphthalene	.0949	.0949	.0929	.0908	.0884	.0860	.0837	.0813	.0791
2,7-dimethylnaphthalene	.0949	.0949	.0929	.0908	.0884	.0860	.0837	.0813	.0791
1-ethylnaphthalene	.0011	.0012	.0043	.0096	.0164	.0242	.0327	.0414	.0500
2-ethylnaphthalene	.0011	.0012	.0043	.0096	.0164	.0242	.0327	.0414	.0500
C13H14									
1,2,3-trimethylnaphthalene	.0057	.0057	.0088	.0115	.0138	.0157	.0171	.0182	.0190
1,2,4-trimethylnaphthalene	.0332	.0334	.0395	.0429	.0444	.0446	.0441	.0430	.0418
1,2,5-trimethylnaphthalene	.0332	.0334	.0395	.0429	.0444	.0446	.0441	.0430	.0418
1,2,6-trimethylnaphthalene	.0332	.0334	.0395	.0429	.0444	.0446	.0441	.0430	.0418
1,2,7-trimethylnaphthalene	.0332	.0334	.0395	.0429	.0444	.0446	.0441	.0430	.0418
1,2,8-trimethylnaphthalene	.0000	.0000	.0000	.0000	.0001	.0002	.0004	.0005	.0007
1,3,5-trimethylnaphthalene	.1956	.1953	.1774	.1595	.1425	.1271	.1136	.1020	.0922
1,3,6-trimethylnaphthalene	.1956	.1953	.1774	.1595	.1425	.1271	.1136	.1020	.0922
1,3,7-trimethylnaphthalene	.1956	.1953	.1774	.1595	.1425	.1271	.1136	.1020	.0922
1,3,8-trimethylnaphthalene	.0000	.0000	.0000	.0001	.0003	.0006	.0009	.0012	.0016
1,4,5-trimethylnaphthalene	.0000	.0000	.0000	.0001	.0003	.0006	.0009	.0012	.0016
1,4,6-trimethylnaphthalene	.1956	.1953	.1774	.1595	.1425	.1271	.1136	.1020	.0922
1,6,7-trimethylnaphthalene	.0332	.0334	.0395	.0429	.0444	.0446	.0441	.0430	.0418
2,3,6-trimethylnaphthalene	.0332	.0334	.0395	.0429	.0444	.0446	.0441	.0430	.0418
1-ethyl-2-methylnaphthalene	.0002	.0002	.0009	.0023	.0041	.0063	.0086	.0109	.0132
1-ethyl-3-methylnaphthalene	.0012	.0012	.0041	.0084	.0132	.0179	.0222	.0260	.0291
1-ethyl-4-methylnaphthalene	.0012	.0012	.0041	.0084	.0132	.0179	.0222	.0260	.0291
1-ethyl-5-methylnaphthalene	.0012	.0012	.0041	.0084	.0132	.0179	.0222	.0260	.0291
1-ethyl-6-methylnaphthalene	.0012	.0012	.0041	.0084	.0132	.0179	.0222	.0260	.0291
1-ethyl-7-methylnaphthalene	.0012	.0012	.0041	.0084	.0132	.0179	.0222	.0260	.0291
1-ethyl-8-methylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0001	.0002	.0003	.0005
2-ethyl-1-methylnaphthalene	.0002	.0002	.0009	.0023	.0041	.0063	.0086	.0109	.0132
2-ethyl-3-methylnaphthalene	.0002	.0002	.0009	.0023	.0041	.0063	.0086	.0109	.0132
2-ethyl-6-methylnaphthalene	.0012	.0012	.0041	.0084	.0132	.0179	.0222	.0260	.0291
2-ethyl-7-methylnaphthalene	.0012	.0012	.0041	.0084	.0132	.0179	.0222	.0260	.0291
3-ethyl-1-methylnaphthalene	.0012	.0012	.0041	.0084	.0132	.0179	.0222	.0260	.0291
6-ethyl-1-methylnaphthalene	.0012	.0012	.0041	.0084	.0132	.0179	.0222	.0260	.0291
7-ethyl-1-methylnaphthalene	.0012	.0012	.0041	.0084	.0132	.0179	.0222	.0260	.0291
1-propylnaphthalene	.0000	.0000	.0001	.0005	.0013	.0026	.0043	.0063	.0086
2-propylnaphthalene	.0000	.0000	.0001	.0005	.0013	.0026	.0043	.0063	.0086
1-isopropylnaphthalene	.0000	.0000	.0002	.0005	.0011	.0018	.0026	.0035	.0045
2-isopropylnaphthalene	.0000	.0000	.0002	.0005	.0011	.0018	.0026	.0035	.0045
C14H16									
1,2,3,4-tetramethylnaphthalene	.0016	.0017	.0026	.0032	.0035	.0037	.0038	.0038	.0037
1,2,3,5-tetramethylnaphthalene	.0193	.0194	.0231	.0237	.0227	.0211	.0194	.0178	.0164
1,2,3,6-tetramethylnaphthalene	.0193	.0194	.0231	.0237	.0227	.0211	.0194	.0178	.0164
1,2,3,7-tetramethylnaphthalene	.0193	.0194	.0231	.0237	.0227	.0211	.0194	.0178	.0164
1,2,3,8-tetramethylnaphthalene	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0002	.0003
1,2,4,5-tetramethylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0003	.0004	.0005	.0006
1,2,4,6-tetramethylnaphthalene	.1135	.1135	.1041	.0882	.0729	.0601	.0500	.0422	.0362
1,2,4,7-tetramethylnaphthalene	.1135	.1135	.1041	.0882	.0729	.0601	.0500	.0422	.0362
1,2,4,8-tetramethylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0003	.0004	.0005	.0006
1,2,5,6-tetramethylnaphthalene	.0096	.0097	.0116	.0119	.0113	.0105	.0097	.0089	.0082
1,2,5,7-tetramethylnaphthalene	.1135	.1135	.1041	.0882	.0729	.0601	.0500	.0422	.0362
1,2,5,8-tetramethylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0003	.0004	.0005	.0006
1,2,6,7-tetramethylnaphthalene	.0193	.0194	.0231	.0237	.0227	.0211	.0194	.0178	.0164
1,2,6,8-tetramethylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0003	.0004	.0005	.0006
1,2,7,8-tetramethylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0001	.0001	.0001	.0001
1,3,5,7-tetramethylnaphthalene	.3339	.3318	.2339	.1641	.1170	.0856	.0645	.0501	.0399
1,3,5,8-tetramethylnaphthalene	.0000	.0000	.0001	.0003	.0006	.0008	.0010	.0012	.0014
1,3,6,7-tetramethylnaphthalene	.1135	.1135	.1041	.0882	.0729	.0601	.0500	.0422	.0362
1,3,6,8-tetramethylnaphthalene	.0000	.0000	.0000	.0001	.0003	.0004	.0005	.0006	.0007
1,4,5,8-tetramethylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
1,4,6,7-tetramethylnaphthalene	.0568	.0567	.0520	.0441	.0364	.0300	.0250	.0211	.0181
2,3,6,7-tetramethylnaphthalene	.0048	.0048	.0058	.0059	.0057	.0053	.0049	.0045	.0041
1-ethyl-2,3-dimethylnaphthalene	.0001	.0001	.0005	.0013	.0021	.0030	.0038	.0045	.0052
1-ethyl-2,4-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
1-ethyl-2,5-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
1-ethyl-2,6-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
1-ethyl-2,7-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
1-ethyl-2,8-dimethylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0000	.0001	.0001	.0002
1-ethyl-3,5-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
1-ethyl-3,6-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252

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

T/K	298.15	300	400	500	600	700	800	900	1000
C14H16									
1-ethyl-3,7-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
1-ethyl-3,8-dimethylnaphthalene	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0004
1-ethyl-4,5-dimethylnaphthalene	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0004
1-ethyl-4,6-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
1-ethyl-6,7-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
2-ethyl-1,3-dimethylnaphthalene	.0001	.0001	.0005	.0013	.0021	.0030	.0038	.0045	.0052
2-ethyl-1,4-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
2-ethyl-1,5-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
2-ethyl-1,6-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
2-ethyl-1,7-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
2-ethyl-1,8-dimethylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0000	.0001	.0001	.0002
2-ethyl-3,6-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
3-ethyl-1,2-dimethylnaphthalene	.0001	.0001	.0005	.0013	.0021	.0030	.0038	.0045	.0052
3-ethyl-1,5-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
3-ethyl-1,6-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
3-ethyl-1,7-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
3-ethyl-1,8-dimethylnaphthalene	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0004
3-ethyl-2,6-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
4-ethyl-1,2-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
4-ethyl-1,5-dimethylnaphthalene	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0004
4-ethyl-1,6-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
5-ethyl-1,2-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
5-ethyl-1,3-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
5-ethyl-1,4-dimethylnaphthalene	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0004
6-ethyl-1,2-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
6-ethyl-1,3-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
6-ethyl-1,4-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
6-ethyl-1,7-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
6-ethyl-2,3-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
7-ethyl-1,2-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
7-ethyl-1,3-dimethylnaphthalene	.0040	.0041	.0109	.0173	.0217	.0241	.0252	.0255	.0252
7-ethyl-1,6-dimethylnaphthalene	.0007	.0007	.0024	.0047	.0068	.0085	.0098	.0107	.0114
8-ethyl-1,2-dimethylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0000	.0001	.0001	.0002
8-ethyl-1,3-dimethylnaphthalene	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0004
1-methyl-2-propylnaphthalene	.0000	.0000	.0001	.0003	.0007	.0012	.0019	.0026	.0034
1-methyl-3-propylnaphthalene	.0000	.0000	.0003	.0010	.0021	.0034	.0048	.0062	.0074
1-methyl-4-propylnaphthalene	.0000	.0000	.0003	.0010	.0021	.0034	.0048	.0062	.0074
1-methyl-5-propylnaphthalene	.0000	.0000	.0003	.0010	.0021	.0034	.0048	.0062	.0074
1-methyl-6-propylnaphthalene	.0000	.0000	.0003	.0010	.0021	.0034	.0048	.0062	.0074
1-methyl-7-propylnaphthalene	.0000	.0000	.0003	.0010	.0021	.0034	.0048	.0062	.0074
1-methyl-8-propylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0001	.0001
2-methyl-1-propylnaphthalene	.0000	.0000	.0001	.0003	.0007	.0012	.0019	.0026	.0034
2-methyl-3-propylnaphthalene	.0000	.0000	.0001	.0003	.0007	.0012	.0019	.0026	.0034
2-methyl-6-propylnaphthalene	.0000	.0000	.0003	.0010	.0021	.0034	.0048	.0062	.0074
2-methyl-7-propylnaphthalene	.0000	.0000	.0003	.0010	.0021	.0034	.0048	.0062	.0074
3-methyl-1-propylnaphthalene	.0000	.0000	.0003	.0010	.0021	.0034	.0048	.0062	.0074
6-methyl-1-propylnaphthalene	.0000	.0000	.0003	.0010	.0021	.0034	.0048	.0062	.0074
7-methyl-1-propylnaphthalene	.0000	.0000	.0003	.0010	.0021	.0034	.0048	.0062	.0074
1-butylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0005	.0009	.0015	.0022
2-butylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0005	.0009	.0015	.0022
1,2-diethylnaphthalene	.0000	.0000	.0001	.0002	.0006	.0012	.0019	.0027	.0036
1,3-diethylnaphthalene	.0000	.0000	.0003	.0009	.0020	.0034	.0049	.0065	.0080
1,4-diethylnaphthalene	.0000	.0000	.0001	.0005	.0010	.0017	.0025	.0032	.0040
1,5-diethylnaphthalene	.0000	.0000	.0001	.0005	.0010	.0017	.0025	.0032	.0040
1,6-diethylnaphthalene	.0000	.0000	.0003	.0009	.0020	.0034	.0049	.0065	.0080
1,7-diethylnaphthalene	.0000	.0000	.0003	.0009	.0020	.0034	.0049	.0065	.0080
1,8-diethylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0001
2,3-diethylnaphthalene	.0000	.0000	.0000	.0001	.0003	.0006	.0010	.0014	.0018
2,6-diethylnaphthalene	.0000	.0000	.0001	.0005	.0010	.0017	.0025	.0032	.0040
2,7-diethylnaphthalene	.0000	.0000	.0001	.0005	.0010	.0017	.0025	.0032	.0040
1-t-butylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0000	.0001	.0001	.0001
2-t-butylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0000	.0001	.0001	.0001
1-isopropyl-2-methylnaphthalene	.0000	.0000	.0001	.0003	.0005	.0008	.0012	.0015	.0018
1-isopropyl-3-methylnaphthalene	.0001	.0001	.0004	.0010	.0017	.0024	.0030	.0035	.0039
1-isopropyl-4-methylnaphthalene	.0001	.0001	.0004	.0010	.0017	.0024	.0030	.0035	.0039
1-isopropyl-5-methylnaphthalene	.0001	.0001	.0004	.0010	.0017	.0024	.0030	.0035	.0039
1-isopropyl-6-methylnaphthalene	.0001	.0001	.0004	.0010	.0017	.0024	.0030	.0035	.0039
1-isopropyl-7-methylnaphthalene	.0001	.0001	.0004	.0010	.0017	.0024	.0030	.0035	.0039
1-isopropyl-8-methylnaphthalene	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0001
2-isopropyl-1-methylnaphthalene	.0000	.0000	.0001	.0003	.0005	.0008	.0012	.0015	.0018
2-isopropyl-3-methylnaphthalene	.0000	.0000	.0001	.0003	.0005	.0008	.0012	.0015	.0018
2-isopropyl-6-methylnaphthalene	.0001	.0001	.0004	.0010	.0017	.0024	.0030	.0035	.0039
2-isopropyl-7-methylnaphthalene	.0001	.0001	.0004	.0010	.0017	.0024	.0030	.0035	.0039
3-isopropyl-1-methylnaphthalene	.0001	.0001	.0004	.0010	.0017	.0024	.0030	.0035	.0039
6-isopropyl-1-methylnaphthalene	.0001	.0001	.0004	.0010	.0017	.0024	.0030	.0035	.0039
7-isopropyl-1-methylnaphthalene	.0001	.0001	.0004	.0010	.0017	.0024	.0030	.0035	.0039
1-secbutylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0004	.0007	.0011	.0015
2-secbutylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0004	.0007	.0011	.0015
1-isobutylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0004	.0006	.0009	.0012
2-isobutylnaphthalene	.0000	.0000	.0000	.0001	.0002	.0004	.0006	.0009	.0012

6. Standard Thermodynamic Properties of Individual Alkylnaphthalene Species

The values of C_P°, S°, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ for all the alkylnaphthalene species through $C_{14}H_{16}$ are given in Tables 10–13 in joules for a standard state pressure of 1 bar. The values for $C_{10}H_8$ and $C_{11}H_{10}$ have been converted from the tables of Stull, Westrum, and Sinke[5] and the values for $C_{12}H_{12}$ through $C_{14}H_{16}$ have been calculated using the Benson method.[7] The values for chiral forms are for the racemates.

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

T/K	298.15	300	400	500	600	700	800	900	1000
C10H8									
naphthalene	132.55	133.43	179.20	218.11	249.66	275.18	296.10	313.42	327.94
C11H10									
1-methylnaphthalene	159.54	160.54	212.30	256.27	292.00	321.16	345.10	364.80	381.62
2-methylnaphthalene	159.79	160.75	211.29	254.68	289.99	319.16	343.21	363.21	380.16
C12H12									
1,2-dimethylnaphthalene	185.5	186.5	239.1	285.7	326.2	360.7	389.2	411.7	428.1
1,3-dimethylnaphthalene	180.4	181.4	233.9	280.5	321.3	356.1	385.1	408.2	425.5
1,4-dimethylnaphthalene	180.4	181.4	233.9	280.5	321.3	356.1	385.1	408.2	425.5
1,5-dimethylnaphthalene	180.4	181.4	233.9	280.5	321.3	356.1	385.1	408.2	425.5
1,6-dimethylnaphthalene	180.4	181.4	233.9	280.5	321.3	356.1	385.1	408.2	425.5
1,7-dimethylnaphthalene	180.4	181.4	233.9	280.5	321.3	356.1	385.1	408.2	425.5
1,8-dimethylnaphthalene	180.4	181.4	233.9	280.5	321.3	356.1	385.1	408.2	425.5
2,3-dimethylnaphthalene	185.5	186.5	239.1	285.7	326.2	360.7	389.2	411.7	428.1
2,6-dimethylnaphthalene	180.4	181.4	233.9	280.5	321.3	356.1	385.1	408.2	425.5
2,7-dimethylnaphthalene	180.4	181.4	233.9	280.5	321.3	356.1	385.1	408.2	425.5
1-ethylnaphthalene	182.1	183.2	237.6	285.6	327.1	362.0	390.6	412.6	428.1
2-ethylnaphthalene	182.1	183.2	237.6	285.6	327.1	362.0	390.6	412.6	428.1
C13H14									
1,2,3-trimethylnaphthalene	213.7	214.8	272.1	322.9	367.3	405.2	436.7	461.6	480.1
1,2,4-trimethylnaphthalene	208.6	209.7	266.9	317.8	362.3	400.6	432.6	458.2	477.6
1,2,5-trimethylnaphthalene	208.6	209.7	266.9	317.8	362.3	400.6	432.6	458.2	477.6
1,2,6-trimethylnaphthalene	208.6	209.7	266.9	317.8	362.3	400.6	432.6	458.2	477.6
1,2,7-trimethylnaphthalene	208.6	209.7	266.9	317.8	362.3	400.6	432.6	458.2	477.6
1,2,8-trimethylnaphthalene	208.6	209.7	266.9	317.8	362.3	400.6	432.6	458.2	477.6
1,3,5-trimethylnaphthalene	203.5	204.6	261.7	312.6	357.3	396.0	428.5	454.8	475.0
1,3,6-trimethylnaphthalene	203.5	204.6	261.7	312.6	357.3	396.0	428.5	454.8	475.0
1,3,7-trimethylnaphthalene	203.5	204.6	261.7	312.6	357.3	396.0	428.5	454.8	475.0
1,3,8-trimethylnaphthalene	203.5	204.6	261.7	312.6	357.3	396.0	428.5	454.8	475.0
1,4,5-trimethylnaphthalene	203.5	204.6	261.7	312.6	357.3	396.0	428.5	454.8	475.0
1,4,6-trimethylnaphthalene	203.5	204.6	261.7	312.6	357.3	396.0	428.5	454.8	475.0
1,6,7-trimethylnaphthalene	208.6	209.7	266.9	317.8	362.3	400.6	432.6	458.2	477.6
2,3,6-trimethylnaphthalene	208.6	209.7	266.9	317.8	362.3	400.6	432.6	458.2	477.6
1-ethyl-2-methylnaphthalene	210.3	211.4	270.6	322.8	368.1	406.5	438.0	462.6	480.2
1-ethyl-3-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
1-ethyl-4-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
1-ethyl-5-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
1-ethyl-6-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
1-ethyl-7-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
1-ethyl-8-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
2-ethyl-1-methylnaphthalene	210.3	211.4	270.6	322.8	368.1	406.5	438.0	462.6	480.2
2-ethyl-3-methylnaphthalene	210.3	211.4	270.6	322.8	368.1	406.5	438.0	462.6	480.2
2-ethyl-6-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
2-ethyl-7-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
3-ethyl-1-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
6-ethyl-1-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
7-ethyl-1-methylnaphthalene	205.2	206.3	265.4	317.6	363.1	401.9	433.9	459.1	477.6
1-propylnaphthalene	205.1	206.3	266.7	319.9	366.1	405.2	437.1	461.9	479.6
2-propylnaphthalene	205.1	206.3	266.7	319.9	366.1	405.2	437.1	461.9	479.6
1-isopropylnaphthalene	204.0	205.2	266.3	320.2	366.8	406.1	438.1	462.8	480.2
2-isopropylnaphthalene	204.0	205.2	266.3	320.2	366.8	406.1	438.1	462.8	480.2
C14H16									
1,2,3,4-tetramethylnaphthalene	241.8	243.0	305.1	360.2	408.4	449.7	484.1	511.6	532.2
1,2,3,5-tetramethylnaphthalene	236.8	238.0	299.8	355.0	403.4	445.1	480.0	508.2	529.7
1,2,3,6-tetramethylnaphthalene	236.8	238.0	299.8	355.0	403.4	445.1	480.0	508.2	529.7
1,2,3,7-tetramethylnaphthalene	236.8	238.0	299.8	355.0	403.4	445.1	480.0	508.2	529.7
1,2,3,8-tetramethylnaphthalene	236.8	238.0	299.8	355.0	403.4	445.1	480.0	508.2	529.7
1,2,4,5-tetramethylnaphthalene	231.7	232.9	294.6	349.8	398.4	440.5	475.9	504.8	527.1
1,2,4,6-tetramethylnaphthalene	231.7	232.9	294.6	349.8	398.4	440.5	475.9	504.8	527.1
1,2,4,7-tetramethylnaphthalene	231.7	232.9	294.6	349.8	398.4	440.5	475.9	504.8	527.1
1,2,4,8-tetramethylnaphthalene	231.7	232.9	294.6	349.8	398.4	440.5	475.9	504.8	527.1
1,2,5,6-tetramethylnaphthalene	236.8	238.0	299.8	355.0	403.4	445.1	480.0	508.2	529.7
1,2,5,7-tetramethylnaphthalene	231.7	232.9	294.6	349.8	398.4	440.5	475.9	504.8	527.1
1,2,5,8-tetramethylnaphthalene	231.7	232.9	294.6	349.8	398.4	440.5	475.9	504.8	527.1
1,2,6,7-tetramethylnaphthalene	236.8	238.0	299.8	355.0	403.4	445.1	480.0	508.2	529.7
1,2,6,8-tetramethylnaphthalene	231.7	232.9	294.6	349.8	398.4	440.5	475.9	504.8	527.1
1,2,7,8-tetramethylnaphthalene	236.8	238.0	299.8	355.0	403.4	445.1	480.0	508.2	529.7
1,3,5,7-tetramethylnaphthalene	226.6	227.8	289.4	344.6	393.4	435.8	471.8	501.4	524.6
1,3,5,8-tetramethylnaphthalene	226.6	227.8	289.4	344.6	393.4	435.8	471.8	501.4	524.6
1,3,6,7-tetramethylnaphthalene	231.7	232.9	294.6	349.8	398.4	440.5	475.9	504.8	527.1
1,3,6,8-tetramethylnaphthalene	226.6	227.8	289.4	344.6	393.4	435.8	471.8	501.4	524.6
1,4,5,8-tetramethylnaphthalene	226.6	227.8	289.4	344.6	393.4	435.8	471.8	501.4	524.6
1,4,6,7-tetramethylnaphthalene	231.7	232.9	294.6	349.8	398.4	440.5	475.9	504.8	527.1
2,3,6,7-tetramethylnaphthalene	236.8	238.0	299.8	355.0	403.4	445.1	480.0	508.2	529.7
1-ethyl-2,3-dimethylnaphthalene	238.4	239.7	303.5	360.0	409.2	451.0	485.4	512.5	532.3
1-ethyl-2,4-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
1-ethyl-2,5-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
1-ethyl-2,6-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
1-ethyl-2,7-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
1-ethyl-2,8-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7

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

T/K	298.15	300	400	500	600	700	800	900	1000
C14H16									
1-ethyl-3,5-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
1-ethyl-3,6-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
1-ethyl-3,7-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
1-ethyl-3,8-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
1-ethyl-4,5-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
1-ethyl-4,6-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
1-ethyl-6,7-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
2-ethyl-1,3-dimethylnaphthalene	238.4	239.7	303.5	360.0	409.2	451.0	485.4	512.5	532.3
2-ethyl-1,4-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
2-ethyl-1,5-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
2-ethyl-1,6-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
2-ethyl-1,7-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
2-ethyl-1,8-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
2-ethyl-3,6-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
3-ethyl-1,2-dimethylnaphthalene	238.4	239.7	303.5	360.0	409.2	451.0	485.4	512.5	532.3
3-ethyl-1,5-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
3-ethyl-1,6-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
3-ethyl-1,7-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
3-ethyl-1,8-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
3-ethyl-2,6-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
4-ethyl-1,2-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
4-ethyl-1,5-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
4-ethyl-1,6-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
5-ethyl-1,2-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
5-ethyl-1,3-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
5-ethyl-1,4-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
6-ethyl-1,2-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
6-ethyl-1,3-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
6-ethyl-1,4-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
6-ethyl-1,7-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
6-ethyl-2,3-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
7-ethyl-1,2-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
7-ethyl-1,3-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
7-ethyl-1,6-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
8-ethyl-1,2-dimethylnaphthalene	233.4	234.6	298.3	354.9	404.2	446.4	481.3	509.1	529.7
8-ethyl-1,3-dimethylnaphthalene	228.3	229.5	293.1	349.7	399.2	441.7	477.2	505.7	527.2
1-methyl-2-propylnaphthalene	233.2	234.5	299.6	357.2	407.2	449.6	484.6	511.9	531.7
1-methyl-3-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
1-methyl-4-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
1-methyl-5-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
1-methyl-6-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
1-methyl-7-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
1-methyl-8-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
2-methyl-1-propylnaphthalene	233.2	234.5	299.6	357.2	407.2	449.6	484.6	511.9	531.7
2-methyl-3-propylnaphthalene	233.2	234.5	299.6	357.2	407.2	449.6	484.6	511.9	531.7
2-methyl-6-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
2-methyl-7-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
3-methyl-1-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
6-methyl-1-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
7-methyl-1-propylnaphthalene	228.2	229.4	294.4	352.0	402.2	445.0	480.5	508.5	529.2
1-butylnaphthalene	228.1	229.4	295.7	354.3	405.2	448.3	483.7	511.3	531.2
2-butylnaphthalene	228.1	229.4	295.7	354.3	405.2	448.3	483.7	511.3	531.2
1,2-diethylnaphthalene	235.0	236.3	302.0	359.9	410.0	452.3	486.8	513.5	532.4
1,3-diethylnaphthalene	230.0	231.2	296.8	354.7	405.0	447.7	482.7	510.1	529.8
1,4-diethylnaphthalene	230.0	231.2	296.8	354.7	405.0	447.7	482.7	510.1	529.8
1,5-diethylnaphthalene	230.0	231.2	296.8	354.7	405.0	447.7	482.7	510.1	529.8
1,6-diethylnaphthalene	230.0	231.2	296.8	354.7	405.0	447.7	482.7	510.1	529.8
1,7-diethylnaphthalene	230.0	231.2	296.8	354.7	405.0	447.7	482.7	510.1	529.8
1,8-diethylnaphthalene	230.0	231.2	296.8	354.7	405.0	447.7	482.7	510.1	529.8
2,3-diethylnaphthalene	235.0	236.3	302.0	359.9	410.0	452.3	486.8	513.5	532.4
2,6-diethylnaphthalene	230.0	231.2	296.8	354.7	405.0	447.7	482.7	510.1	529.8
2,7-diethylnaphthalene	230.0	231.2	296.8	354.7	405.0	447.7	482.7	510.1	529.8
1-t-butylnaphthalene	228.3	229.7	299.0	359.8	412.1	455.9	491.2	517.9	536.2
2-t-butylnaphthalene	228.3	229.7	299.0	359.8	412.1	455.9	491.2	517.9	536.2
1-isopropyl-2-methylnaphthalene	232.2	233.5	299.3	357.4	407.9	450.5	485.5	512.7	532.3
1-isopropyl-3-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
1-isopropyl-4-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
1-isopropyl-5-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
1-isopropyl-6-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
1-isopropyl-7-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
1-isopropyl-8-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
2-isopropyl-1-methylnaphthalene	232.2	233.5	299.3	357.4	407.9	450.5	485.5	512.7	532.3
2-isopropyl-3-methylnaphthalene	232.2	233.5	299.3	357.4	407.9	450.5	485.5	512.7	532.3
2-isopropyl-6-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
2-isopropyl-7-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
3-isopropyl-1-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
6-isopropyl-1-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
7-isopropyl-1-methylnaphthalene	227.1	228.4	294.1	352.3	402.9	445.9	481.4	509.3	529.7
1-secbutylnaphthalene	227.0	228.3	295.4	354.6	405.8	449.2	484.6	512.1	531.7
2-secbutylnaphthalene	227.0	228.3	295.4	354.6	405.8	449.2	484.6	512.1	531.7
1-isobutylnaphthalene	227.0	228.3	295.4	354.5	405.8	449.1	484.6	512.1	531.7
2-isobutylnaphthalene	227.0	228.3	295.4	354.5	405.8	449.1	484.6	512.1	531.7

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

T/K	298.15	300	400	500	600	700	800	900	1000
C10H8									
naphthalene	335.75	336.59	381.40	425.71	468.38	508.84	546.96	582.86	616.66
C11H10									
1-methylnaphthalene	377.55	378.55	432.02	484.28	534.24	581.52	625.99	667.83	707.16
2-methylnaphthalene	380.14	381.15	434.49	486.46	536.08	583.07	627.29	668.88	708.08
C12H12									
1,2-dimethylnaphthalene	412.8	414.0	475.0	533.5	589.2	642.2	692.3	739.5	783.8
1,3-dimethylnaphthalene	419.6	420.7	480.2	537.5	592.4	644.6	694.1	740.8	784.8
1,4-dimethylnaphthalene	413.8	414.9	474.5	531.8	586.6	638.8	688.3	735.1	779.0
1,5-dimethylnaphthalene	413.8	414.9	474.5	531.8	586.6	638.8	688.3	735.1	779.0
1,6-dimethylnaphthalene	419.6	420.7	480.2	537.5	592.4	644.6	694.1	740.8	784.8
1,7-dimethylnaphthalene	419.6	420.7	480.2	537.5	592.4	644.6	694.1	740.8	784.8
1,8-dimethylnaphthalene	404.5	405.6	465.2	522.5	577.3	629.5	679.0	725.8	769.7
2,3-dimethylnaphthalene	407.1	408.2	469.2	527.7	583.5	636.4	686.5	733.7	778.0
2,6-dimethylnaphthalene	413.8	414.9	474.5	531.8	586.6	638.8	688.3	735.1	779.0
2,7-dimethylnaphthalene	413.8	414.9	474.5	531.8	586.6	638.8	688.3	735.1	779.0
1-ethylnaphthalene	421.0	422.1	482.4	540.7	596.5	649.6	699.9	747.3	791.6
2-ethylnaphthalene	421.0	422.1	482.4	540.7	596.5	649.6	699.9	747.3	791.6
C13H14									
1,2,3-trimethylnaphthalene	443.8	445.1	514.9	581.2	644.1	703.6	759.9	812.8	862.5
1,2,4-trimethylnaphthalene	450.5	451.8	520.1	585.3	647.2	706.0	761.7	814.2	863.5
1,2,5-trimethylnaphthalene	450.5	451.8	520.1	585.3	647.2	706.0	761.7	814.2	863.5
1,2,6-trimethylnaphthalene	450.5	451.8	520.1	585.3	647.2	706.0	761.7	814.2	863.5
1,2,7-trimethylnaphthalene	450.5	451.8	520.1	585.3	647.2	706.0	761.7	814.2	863.5
1,2,8-trimethylnaphthalene	441.2	442.5	510.8	576.0	637.9	696.7	752.4	804.9	854.2
1,3,5-trimethylnaphthalene	457.3	458.5	525.3	589.3	650.4	708.4	763.5	815.5	864.6
1,3,6-trimethylnaphthalene	457.3	458.5	525.3	589.3	650.4	708.4	763.5	815.5	864.6
1,3,7-trimethylnaphthalene	457.3	458.5	525.3	589.3	650.4	708.4	763.5	815.5	864.6
1,3,8-trimethylnaphthalene	448.0	449.2	516.1	580.0	641.1	699.1	754.2	806.2	855.3
1,4,5-trimethylnaphthalene	448.0	449.2	516.1	580.0	641.1	699.1	754.2	806.2	855.3
1,4,6-trimethylnaphthalene	457.3	458.5	525.3	589.3	650.4	708.4	763.5	815.5	864.6
1,6,7-trimethylnaphthalene	450.5	451.8	520.1	585.3	647.2	706.0	761.7	814.2	863.5
2,3,6-trimethylnaphthalene	450.5	451.8	520.1	585.3	647.2	706.0	761.7	814.2	863.5
1-ethyl-2-methylnaphthalene	451.9	453.2	522.3	588.4	651.4	711.1	767.5	820.6	870.3
1-ethyl-3-methylnaphthalene	458.6	459.9	527.5	592.5	654.5	713.5	769.3	822.0	871.3
1-ethyl-4-methylnaphthalene	458.6	459.9	527.5	592.5	654.5	713.5	769.3	822.0	871.3
1-ethyl-5-methylnaphthalene	458.6	459.9	527.5	592.5	654.5	713.5	769.3	822.0	871.3
1-ethyl-6-methylnaphthalene	458.6	459.9	527.5	592.5	654.5	713.5	769.3	822.0	871.3
1-ethyl-7-methylnaphthalene	458.6	459.9	527.5	592.5	654.5	713.5	769.3	822.0	871.3
1-ethyl-8-methylnaphthalene	449.4	450.6	518.2	583.2	645.2	704.2	760.0	812.7	862.1
2-ethyl-1-methylnaphthalene	451.9	453.2	522.3	588.4	651.4	711.1	767.5	820.6	870.3
2-ethyl-3-methylnaphthalene	451.9	453.2	522.3	588.4	651.4	711.1	767.5	820.6	870.3
2-ethyl-6-methylnaphthalene	458.6	459.9	527.5	592.5	654.5	713.5	769.3	822.0	871.3
2-ethyl-7-methylnaphthalene	458.6	459.9	527.5	592.5	654.5	713.5	769.3	822.0	871.3
3-ethyl-1-methylnaphthalene	458.6	459.9	527.5	592.5	654.5	713.5	769.3	822.0	871.3
6-ethyl-1-methylnaphthalene	458.6	459.9	527.5	592.5	654.5	713.5	769.3	822.0	871.3
7-ethyl-1-methylnaphthalene	458.6	459.9	527.5	592.5	654.5	713.5	769.3	822.0	871.3
1-propylnaphthalene	460.4	461.7	529.4	594.8	657.3	716.8	773.0	826.0	875.7
2-propylnaphthalene	460.4	461.7	529.4	594.8	657.3	716.8	773.0	826.0	875.7
1-isopropylnaphthalene	449.2	450.4	518.0	583.4	646.0	705.5	761.9	815.0	864.8
2-isopropylnaphthalene	449.2	450.4	518.0	583.4	646.0	705.5	761.9	815.0	864.8
C14H16									
1,2,3,4-tetramethylnaphthalene	469.0	470.5	549.0	623.2	693.2	759.3	821.7	880.4	935.4
1,2,3,5-tetramethylnaphthalene	481.5	482.9	560.0	633.0	702.1	767.5	829.3	887.5	942.2
1,2,3,6-tetramethylnaphthalene	481.5	482.9	560.0	633.0	702.1	767.5	829.3	887.5	942.2
1,2,3,7-tetramethylnaphthalene	481.5	482.9	560.0	633.0	702.1	767.5	829.3	887.5	942.2
1,2,3,8-tetramethylnaphthalene	472.2	473.6	550.7	623.7	692.8	758.2	820.0	878.2	932.9
1,2,4,5-tetramethylnaphthalene	478.9	480.4	556.0	627.8	695.9	760.6	821.8	879.6	934.0
1,2,4,6-tetramethylnaphthalene	488.2	489.6	565.3	637.0	705.2	769.9	831.1	888.9	943.3
1,2,4,7-tetramethylnaphthalene	488.2	489.6	565.3	637.0	705.2	769.9	831.1	888.9	943.3
1,2,4,8-tetramethylnaphthalene	478.9	480.4	556.0	627.8	695.9	760.6	821.8	879.6	934.0
1,2,5,6-tetramethylnaphthalene	475.7	477.2	554.3	627.2	696.3	761.7	823.5	881.7	936.5
1,2,5,7-tetramethylnaphthalene	488.2	489.6	565.3	637.0	705.2	769.9	831.1	888.9	943.3
1,2,5,8-tetramethylnaphthalene	478.9	480.4	556.0	627.8	695.9	760.6	821.8	879.6	934.0
1,2,6,7-tetramethylnaphthalene	481.5	482.9	560.0	633.0	702.1	767.5	829.3	887.5	942.2
1,2,6,8-tetramethylnaphthalene	478.9	480.4	556.0	627.8	695.9	760.6	821.8	879.6	934.0
1,2,7,8-tetramethylnaphthalene	466.4	467.9	545.0	617.9	687.0	752.4	814.2	872.5	927.2
1,3,5,7-tetramethylnaphthalene	489.2	490.6	564.7	635.3	702.6	766.5	827.1	884.5	938.5
1,3,5,8-tetramethylnaphthalene	485.7	487.1	561.2	631.8	699.1	763.0	823.6	880.9	935.0
1,3,6,7-tetramethylnaphthalene	488.2	489.6	565.3	637.0	705.2	769.9	831.1	888.9	943.3
1,3,6,8-tetramethylnaphthalene	479.9	481.3	555.4	626.1	693.3	757.2	817.8	875.2	929.3
1,4,5,8-tetramethylnaphthalene	464.8	466.2	540.4	611.0	678.2	742.2	802.8	860.1	914.2
1,4,6,7-tetramethylnaphthalene	482.4	483.9	559.5	631.3	699.5	764.1	825.3	883.1	937.5
2,3,6,7-tetramethylnaphthalene	469.9	471.4	548.5	621.5	690.6	756.0	817.8	876.0	930.7
1-ethyl-2,3-dimethylnaphthalene	482.9	484.3	562.2	636.2	706.3	772.6	835.1	893.9	949.0
1-ethyl-2,4-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
1-ethyl-2,5-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
1-ethyl-2,6-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
1-ethyl-2,7-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
1-ethyl-2,8-dimethylnaphthalene	480.3	481.8	558.1	630.9	700.1	765.7	827.6	886.0	940.8

Table 11. Standard entropy of alkylnaphthalenes in J/K mol--Continued

T/K	298.15	300	400	500	600	700	800	900	1000
C14H16									
1-ethyl-3,5-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
1-ethyl-3,6-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
1-ethyl-3,7-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
1-ethyl-3,8-dimethylnaphthalene	487.0	488.5	563.4	635.0	703.2	768.0	829.4	887.4	941.8
1-ethyl-4,5-dimethylnaphthalene	487.0	488.5	563.4	635.0	703.2	768.0	829.4	887.4	941.8
1-ethyl-4,6-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
1-ethyl-6,7-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
2-ethyl-1,3-dimethylnaphthalene	482.9	484.3	562.2	636.2	706.3	772.6	835.1	893.9	949.0
2-ethyl-1,4-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
2-ethyl-1,5-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
2-ethyl-1,6-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
2-ethyl-1,7-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
2-ethyl-1,8-dimethylnaphthalene	480.3	481.8	558.1	630.9	700.1	765.7	827.6	886.0	940.8
2-ethyl-3,6-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
3-ethyl-1,2-dimethylnaphthalene	482.9	484.3	562.2	636.2	706.3	772.6	835.1	893.9	949.0
3-ethyl-1,5-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
3-ethyl-1,6-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
3-ethyl-1,7-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
3-ethyl-1,8-dimethylnaphthalene	487.0	488.5	563.4	635.0	703.2	768.0	829.4	887.4	941.8
3-ethyl-2,6-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
4-ethyl-1,2-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
4-ethyl-1,5-dimethylnaphthalene	487.0	488.5	563.4	635.0	703.2	768.0	829.4	887.4	941.8
4-ethyl-1,6-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
5-ethyl-1,2-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
5-ethyl-1,3-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
5-ethyl-1,4-dimethylnaphthalene	487.0	488.5	563.4	635.0	703.2	768.0	829.4	887.4	941.8
6-ethyl-1,2-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
6-ethyl-1,3-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
6-ethyl-1,4-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
6-ethyl-1,7-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
6-ethyl-2,3-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
7-ethyl-1,2-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
7-ethyl-1,3-dimethylnaphthalene	496.3	497.8	572.7	644.3	712.5	777.3	838.7	896.6	951.1
7-ethyl-1,6-dimethylnaphthalene	489.6	491.0	567.4	640.2	709.4	774.9	836.9	895.3	950.1
8-ethyl-1,2-dimethylnaphthalene	480.3	481.8	558.1	630.9	700.1	765.7	827.6	886.0	940.8
8-ethyl-1,3-dimethylnaphthalene	487.0	488.5	563.4	635.0	703.2	768.0	829.4	887.4	941.8
1-methyl-2-propylnaphthalene	491.3	492.8	569.3	642.5	712.2	778.2	840.6	899.4	954.4
1-methyl-3-propylnaphthalene	498.1	499.5	574.6	646.6	715.3	780.6	842.4	900.7	955.4
1-methyl-4-propylnaphthalene	498.1	499.5	574.6	646.6	715.3	780.6	842.4	900.7	955.4
1-methyl-5-propylnaphthalene	498.1	499.5	574.6	646.6	715.3	780.6	842.4	900.7	955.4
1-methyl-6-propylnaphthalene	498.1	499.5	574.6	646.6	715.3	780.6	842.4	900.7	955.4
1-methyl-7-propylnaphthalene	498.1	499.5	574.6	646.6	715.3	780.6	842.4	900.7	955.4
1-methyl-8-propylnaphthalene	488.8	490.2	565.3	637.3	706.0	771.3	833.1	891.4	946.1
2-methyl-1-propylnaphthalene	491.3	492.8	569.3	642.5	712.2	778.2	840.6	899.4	954.4
2-methyl-3-propylnaphthalene	491.3	492.8	569.3	642.5	712.2	778.2	840.6	899.4	954.4
2-methyl-6-propylnaphthalene	498.1	499.5	574.6	646.6	715.3	780.6	842.4	900.7	955.4
2-methyl-7-propylnaphthalene	498.1	499.5	574.6	646.6	715.3	780.6	842.4	900.7	955.4
3-methyl-1-propylnaphthalene	498.1	499.5	574.6	646.6	715.3	780.6	842.4	900.7	955.4
6-methyl-1-propylnaphthalene	498.1	499.5	574.6	646.6	715.3	780.6	842.4	900.7	955.4
7-methyl-1-propylnaphthalene	498.1	499.5	574.6	646.6	715.3	780.6	842.4	900.7	955.4
1-butylnaphthalene	499.8	501.2	576.5	648.9	718.1	783.9	846.1	904.8	959.8
2-butylnaphthalene	499.8	501.2	576.5	648.9	718.1	783.9	846.1	904.8	959.8
1,2-diethylnaphthalene	491.0	492.5	569.6	643.4	713.5	780.0	842.8	901.7	956.9
1,3-diethylnaphthalene	497.7	499.2	574.8	647.4	716.7	782.4	844.6	903.1	957.9
1,4-diethylnaphthalene	492.0	493.4	569.1	641.7	710.9	776.6	838.8	897.3	952.1
1,5-diethylnaphthalene	492.0	493.4	569.1	641.7	710.9	776.6	838.8	897.3	952.1
1,6-diethylnaphthalene	497.7	499.2	574.8	647.4	716.7	782.4	844.6	903.1	957.9
1,7-diethylnaphthalene	497.7	499.2	574.8	647.4	716.7	782.4	844.6	903.1	957.9
1,8-diethylnaphthalene	482.7	484.1	559.8	632.4	701.6	767.4	829.5	888.0	942.8
2,3-diethylnaphthalene	485.2	486.7	563.9	637.6	707.8	774.3	837.0	895.9	951.1
2,6-diethylnaphthalene	492.0	493.4	569.1	641.7	710.9	776.6	838.8	897.3	952.1
2,7-diethylnaphthalene	492.0	493.4	569.1	641.7	710.9	776.6	838.8	897.3	952.1
1-t-butylnaphthalene	461.8	463.2	538.9	612.4	682.7	749.6	812.9	872.4	928.0
2-t-butylnaphthalene	461.8	463.2	538.9	612.4	682.7	749.6	812.9	872.4	928.0
1-isopropyl-2-methylnaphthalene	480.1	481.5	557.9	631.1	700.8	767.0	829.5	888.4	943.5
1-isopropyl-3-methylnaphthalene	486.8	488.2	563.1	635.1	704.0	769.4	831.3	889.7	944.5
1-isopropyl-4-methylnaphthalene	486.8	488.2	563.1	635.1	704.0	769.4	831.3	889.7	944.5
1-isopropyl-5-methylnaphthalene	486.8	488.2	563.1	635.1	704.0	769.4	831.3	889.7	944.5
1-isopropyl-6-methylnaphthalene	486.8	488.2	563.1	635.1	704.0	769.4	831.3	889.7	944.5
1-isopropyl-7-methylnaphthalene	486.8	488.2	563.1	635.1	704.0	769.4	831.3	889.7	944.5
1-isopropyl-8-methylnaphthalene	477.5	479.0	553.8	625.9	694.7	760.1	822.0	880.4	935.2
2-isopropyl-1-methylnaphthalene	480.1	481.5	557.9	631.1	700.8	767.0	829.5	888.4	943.5
2-isopropyl-3-methylnaphthalene	480.1	481.5	557.9	631.1	700.8	767.0	829.5	888.4	943.5
2-isopropyl-6-methylnaphthalene	486.8	488.2	563.1	635.1	704.0	769.4	831.3	889.7	944.5
2-isopropyl-7-methylnaphthalene	486.8	488.2	563.1	635.1	704.0	769.4	831.3	889.7	944.5
3-isopropyl-1-methylnaphthalene	486.8	488.2	563.1	635.1	704.0	769.4	831.3	889.7	944.5
6-isopropyl-1-methylnaphthalene	486.8	488.2	563.1	635.1	704.0	769.4	831.3	889.7	944.5
7-isopropyl-1-methylnaphthalene	486.8	488.2	563.1	635.1	704.0	769.4	831.3	889.7	944.5
1-secbutylnaphthalene	494.3	495.7	570.8	643.2	712.5	778.4	840.8	899.6	954.6
2-secbutylnaphthalene	494.3	495.7	570.8	643.2	712.5	778.4	840.8	899.6	954.6
1-isobutylnaphthalene	488.6	490.0	565.0	637.4	706.7	772.6	835.0	893.8	948.8
2-isobutylnaphthalene	488.6	490.0	565.0	637.4	706.7	772.6	835.0	893.8	948.8

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

T/K	298.15	300	400	500	600	700	800	900	1000
C10H8									
naphthalene	150.96	150.83	144.56	139.49	135.39	132.21	129.75	127.95	126.90
C11H10									
1-methylnaphthalene	116.86	116.69	109.54	103.76	99.20	95.73	93.14	91.34	90.42
2-methylnaphthalene	116.11	115.94	108.74	102.84	98.07	94.43	91.63	89.66	88.58
C12H12									
1,2-dimethylnaphthalene	86.1	86.0	77.6	70.5	64.6	60.1	56.9	54.7	53.2
1,3-dimethylnaphthalene	83.8	83.6	74.7	67.0	60.7	55.7	52.0	49.4	47.7
1,4-dimethylnaphthalene	83.8	83.6	74.7	67.0	60.7	55.7	52.0	49.4	47.7
1,5-dimethylnaphthalene	83.8	83.6	74.7	67.0	60.7	55.7	52.0	49.4	47.7
1,6-dimethylnaphthalene	83.8	83.6	74.7	67.0	60.7	55.7	52.0	49.4	47.7
1,7-dimethylnaphthalene	83.8	83.6	74.7	67.0	60.7	55.7	52.0	49.4	47.7
1,8-dimethylnaphthalene	108.4	108.2	99.3	91.6	85.3	80.3	76.6	74.0	72.3
2,3-dimethylnaphthalene	86.1	86.0	77.6	70.5	64.6	60.1	56.9	54.7	53.2
2,6-dimethylnaphthalene	83.8	83.6	74.7	67.0	60.7	55.7	52.0	49.4	47.7
2,7-dimethylnaphthalene	83.8	83.6	74.7	67.0	60.7	55.7	52.0	49.4	47.7
1-ethylnaphthalene	96.9	96.7	88.1	80.8	75.0	70.6	67.5	65.4	64.1
2-ethylnaphthalene	96.9	96.7	88.1	80.8	75.0	70.6	67.5	65.4	64.1
C13H14									
1,2,3-trimethylnaphthalene	55.1	54.9	45.7	37.8	31.4	26.4	22.9	20.6	19.1
1,2,4-trimethylnaphthalene	52.7	52.5	42.8	34.4	27.4	22.0	18.1	15.3	13.6
1,2,5-trimethylnaphthalene	52.7	52.5	42.8	34.4	27.4	22.0	18.1	15.3	13.6
1,2,6-trimethylnaphthalene	52.7	52.5	42.8	34.4	27.4	22.0	18.1	15.3	13.6
1,2,7-trimethylnaphthalene	52.7	52.5	42.8	34.4	27.4	22.0	18.1	15.3	13.6
1,2,8-trimethylnaphthalene	77.3	77.1	67.4	59.0	52.0	46.6	42.7	39.9	38.2
1,3,5-trimethylnaphthalene	50.3	50.1	39.9	30.9	23.5	17.6	13.2	10.1	8.0
1,3,6-trimethylnaphthalene	50.3	50.1	39.9	30.9	23.5	17.6	13.2	10.1	8.0
1,3,7-trimethylnaphthalene	50.3	50.1	39.9	30.9	23.5	17.6	13.2	10.1	8.0
1,3,8-trimethylnaphthalene	74.9	74.7	64.5	55.5	48.1	42.2	37.8	34.7	32.6
1,4,5-trimethylnaphthalene	74.9	74.7	64.5	55.5	48.1	42.2	37.8	34.7	32.6
1,4,6-trimethylnaphthalene	50.3	50.1	39.9	30.9	23.5	17.6	13.2	10.1	8.0
1,6,7-trimethylnaphthalene	52.7	52.5	42.8	34.4	27.4	22.0	18.1	15.3	13.6
2,3,6-trimethylnaphthalene	52.7	52.5	42.8	34.4	27.4	22.0	18.1	15.3	13.6
1-ethyl-2-methylnaphthalene	65.8	65.6	56.2	48.2	41.8	36.9	33.6	31.4	29.9
1-ethyl-3-methylnaphthalene	63.4	63.2	53.3	44.7	37.8	32.5	28.7	26.1	24.4
1-ethyl-4-methylnaphthalene	63.4	63.2	53.3	44.7	37.8	32.5	28.7	26.1	24.4
1-ethyl-5-methylnaphthalene	63.4	63.2	53.3	44.7	37.8	32.5	28.7	26.1	24.4
1-ethyl-6-methylnaphthalene	63.4	63.2	53.3	44.7	37.8	32.5	28.7	26.1	24.4
1-ethyl-7-methylnaphthalene	63.4	63.2	53.3	44.7	37.8	32.5	28.7	26.1	24.4
1-ethyl-8-methylnaphthalene	88.0	87.8	77.9	69.3	62.4	57.1	53.3	50.7	49.0
2-ethyl-1-methylnaphthalene	65.8	65.6	56.2	48.2	41.8	36.9	33.6	31.4	29.9
2-ethyl-3-methylnaphthalene	65.8	65.6	56.2	48.2	41.8	36.9	33.6	31.4	29.9
2-ethyl-6-methylnaphthalene	63.4	63.2	53.3	44.7	37.8	32.5	28.7	26.1	24.4
2-ethyl-7-methylnaphthalene	63.4	63.2	53.3	44.7	37.8	32.5	28.7	26.1	24.4
3-ethyl-1-methylnaphthalene	63.4	63.2	53.3	44.7	37.8	32.5	28.7	26.1	24.4
6-ethyl-1-methylnaphthalene	63.4	63.2	53.3	44.7	37.8	32.5	28.7	26.1	24.4
7-ethyl-1-methylnaphthalene	63.4	63.2	53.3	44.7	37.8	32.5	28.7	26.1	24.4
1-propylnaphthalene	76.2	76.0	66.1	57.8	51.2	46.2	42.7	40.4	38.9
2-propylnaphthalene	76.2	76.0	66.1	57.8	51.2	46.2	42.7	40.4	38.9
1-isopropylnaphthalene	70.4	70.2	60.2	51.9	45.3	40.4	37.0	34.8	33.4
2-isopropylnaphthalene	70.4	70.2	60.2	51.9	45.3	40.4	37.0	34.8	33.4
C14H16									
1,2,3,4-tetramethylnaphthalene	24.1	23.8	13.8	5.1	-1.9	-7.3	-11.0	-13.5	-15.0
1,2,3,5-tetramethylnaphthalene	21.7	21.4	10.9	1.7	-5.8	-11.7	-15.9	-18.8	-20.5
1,2,3,6-tetramethylnaphthalene	21.7	21.4	10.9	1.7	-5.8	-11.7	-15.9	-18.8	-20.5
1,2,3,7-tetramethylnaphthalene	21.7	21.4	10.9	1.7	-5.8	-11.7	-15.9	-18.8	-20.5
1,2,3,8-tetramethylnaphthalene	46.3	46.0	35.5	26.3	18.8	12.9	8.7	5.8	4.1
1,2,4,5-tetramethylnaphthalene	43.9	43.7	32.6	22.9	14.8	8.5	3.8	.6	-1.5
1,2,4,6-tetramethylnaphthalene	19.3	19.0	8.0	-1.7	-9.8	-16.1	-20.8	-24.0	-26.1
1,2,4,7-tetramethylnaphthalene	19.3	19.0	8.0	-1.7	-9.8	-16.1	-20.8	-24.0	-26.1
1,2,4,8-tetramethylnaphthalene	43.9	43.7	32.6	22.9	14.8	8.5	3.8	.6	-1.5
1,2,5,6-tetramethylnaphthalene	21.7	21.4	10.9	1.7	-5.8	-11.7	-15.9	-18.8	-20.5
1,2,5,7-tetramethylnaphthalene	19.3	19.0	8.0	-1.7	-9.8	-16.1	-20.8	-24.0	-26.1
1,2,5,8-tetramethylnaphthalene	43.9	43.7	32.6	22.9	14.8	8.5	3.8	.6	-1.5
1,2,6,7-tetramethylnaphthalene	21.7	21.4	10.9	1.7	-5.8	-11.7	-15.9	-18.8	-20.5
1,2,6,8-tetramethylnaphthalene	43.9	43.7	32.6	22.9	14.8	8.5	3.8	.6	-1.5
1,2,7,8-tetramethylnaphthalene	46.3	46.0	35.5	26.3	18.8	12.9	8.7	5.8	4.1
1,3,5,7-tetramethylnaphthalene	16.9	16.7	5.0	-5.2	-13.7	-20.5	-25.6	-29.2	-31.6
1,3,5,8-tetramethylnaphthalene	41.5	41.3	29.6	19.4	10.9	4.1	-1.0	-4.6	-7.0
1,3,6,7-tetramethylnaphthalene	19.3	19.0	8.0	-1.7	-9.8	-16.1	-20.8	-24.0	-26.1
1,3,6,8-tetramethylnaphthalene	41.5	41.3	29.6	19.4	10.9	4.1	-1.0	-4.6	-7.0
1,4,5,8-tetramethylnaphthalene	66.1	65.9	54.3	44.0	35.5	28.7	23.6	20.0	17.6
1,4,6,7-tetramethylnaphthalene	19.3	19.0	8.0	-1.7	-9.8	-16.1	-20.8	-24.0	-26.1
2,3,6,7-tetramethylnaphthalene	21.7	21.4	10.9	1.7	-5.8	-11.7	-15.9	-18.8	-20.5
1-ethyl-2,3-dimethylnaphthalene	34.8	34.5	24.2	15.5	8.5	3.3	-.4	-2.7	-4.2
1-ethyl-2,4-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
1-ethyl-2,5-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
1-ethyl-2,6-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
1-ethyl-2,7-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
1-ethyl-2,8-dimethylnaphthalene	57.0	56.7	45.9	36.7	29.2	23.4	19.4	16.6	14.9

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

T/K	298.15	300	400	500	600	700	800	900	1000
C14H16									
1-ethyl-3,5-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
1-ethyl-3,6-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
1-ethyl-3,7-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
1-ethyl-3,8-dimethylnaphthalene	54.6	54.4	43.0	33.3	25.2	19.0	14.5	11.4	9.4
1-ethyl-4,5-dimethylnaphthalene	54.6	54.4	43.0	33.3	25.2	19.0	14.5	11.4	9.4
1-ethyl-4,6-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
1-ethyl-6,7-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
2-ethyl-1,3-dimethylnaphthalene	34.8	34.5	24.2	15.5	8.5	3.3	-.4	-2.7	-4.2
2-ethyl-1,4-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
2-ethyl-1,5-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
2-ethyl-1,6-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
2-ethyl-1,7-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
2-ethyl-1,8-dimethylnaphthalene	57.0	56.7	45.9	36.7	29.2	23.4	19.4	16.6	14.9
2-ethyl-3,6-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
3-ethyl-1,2-dimethylnaphthalene	34.8	34.5	24.2	15.5	8.5	3.3	-.4	-2.7	-4.2
3-ethyl-1,5-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
3-ethyl-1,6-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
3-ethyl-1,7-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
3-ethyl-1,8-dimethylnaphthalene	54.6	54.4	43.0	33.3	25.2	19.0	14.5	11.4	9.4
3-ethyl-2,6-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
4-ethyl-1,2-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
4-ethyl-1,5-dimethylnaphthalene	54.6	54.4	43.0	33.3	25.2	19.0	14.5	11.4	9.4
4-ethyl-1,6-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
5-ethyl-1,2-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
5-ethyl-1,3-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
5-ethyl-1,4-dimethylnaphthalene	54.6	54.4	43.0	33.3	25.2	19.0	14.5	11.4	9.4
6-ethyl-1,2-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
6-ethyl-1,3-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
6-ethyl-1,4-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
6-ethyl-1,7-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
6-ethyl-2,3-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
7-ethyl-1,2-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
7-ethyl-1,3-dimethylnaphthalene	30.0	29.8	18.4	8.7	.6	-5.6	-10.1	-13.2	-15.2
7-ethyl-1,6-dimethylnaphthalene	32.4	32.1	21.3	12.1	4.6	-1.2	-5.2	-8.0	-9.7
8-ethyl-1,2-dimethylnaphthalene	57.0	56.7	45.9	36.7	29.2	23.4	19.4	16.6	14.9
8-ethyl-1,3-dimethylnaphthalene	54.6	54.4	43.0	33.3	25.2	19.0	14.5	11.4	9.4
1-methyl-2-propylnaphthalene	45.2	45.0	34.2	25.1	17.9	12.5	8.7	6.3	4.8
1-methyl-3-propylnaphthalene	42.8	42.6	31.3	21.7	14.0	8.1	3.9	1.1	-.7
1-methyl-4-propylnaphthalene	42.8	42.6	31.3	21.7	14.0	8.1	3.9	1.1	-.7
1-methyl-5-propylnaphthalene	42.8	42.6	31.3	21.7	14.0	8.1	3.9	1.1	-.7
1-methyl-6-propylnaphthalene	42.8	42.6	31.3	21.7	14.0	8.1	3.9	1.1	-.7
1-methyl-7-propylnaphthalene	42.8	42.6	31.3	21.7	14.0	8.1	3.9	1.1	-.7
1-methyl-8-propylnaphthalene	67.4	67.2	55.9	46.3	38.6	32.7	28.5	25.7	23.9
2-methyl-1-propylnaphthalene	45.2	45.0	34.2	25.1	17.9	12.5	8.7	6.3	4.8
2-methyl-3-propylnaphthalene	45.2	45.0	34.2	25.1	17.9	12.5	8.7	6.3	4.8
2-methyl-6-propylnaphthalene	42.8	42.6	31.3	21.7	14.0	8.1	3.9	1.1	-.7
2-methyl-7-propylnaphthalene	42.8	42.6	31.3	21.7	14.0	8.1	3.9	1.1	-.7
3-methyl-1-propylnaphthalene	42.8	42.6	31.3	21.7	14.0	8.1	3.9	1.1	-.7
6-methyl-1-propylnaphthalene	42.8	42.6	31.3	21.7	14.0	8.1	3.9	1.1	-.7
7-methyl-1-propylnaphthalene	42.8	42.6	31.3	21.7	14.0	8.1	3.9	1.1	-.7
1-butylnaphthalene	55.6	55.4	44.2	34.8	27.3	21.7	17.8	15.3	13.8
2-butylnaphthalene	55.6	55.4	44.2	34.8	27.3	21.7	17.8	15.3	13.8
1,2-diethylnaphthalene	45.5	45.2	34.7	25.9	18.9	13.8	10.3	8.0	6.7
1,3-diethylnaphthalene	43.1	42.9	31.8	22.5	15.0	9.4	5.4	2.8	1.1
1,4-diethylnaphthalene	43.1	42.9	31.8	22.5	15.0	9.4	5.4	2.8	1.1
1,5-diethylnaphthalene	43.1	42.9	31.8	22.5	15.0	9.4	5.4	2.8	1.1
1,6-diethylnaphthalene	43.1	42.9	31.8	22.5	15.0	9.4	5.4	2.8	1.1
1,7-diethylnaphthalene	43.1	42.9	31.8	22.5	15.0	9.4	5.4	2.8	1.1
1,8-diethylnaphthalene	67.7	67.5	56.4	47.1	39.6	34.0	30.0	27.4	25.7
2,3-diethylnaphthalene	45.5	45.2	34.7	25.9	18.9	13.8	10.3	8.0	6.7
2,6-diethylnaphthalene	43.1	42.9	31.8	22.5	15.0	9.4	5.4	2.8	1.1
2,7-diethylnaphthalene	43.1	42.9	31.8	22.5	15.0	9.4	5.4	2.8	1.1
1-t-butylnaphthalene	43.6	43.4	32.3	23.4	16.5	11.7	8.6	6.8	5.8
2-t-butylnaphthalene	43.6	43.4	32.3	23.4	16.5	11.7	8.6	6.8	5.8
1-isopropyl-2-methylnaphthalene	39.4	39.1	28.3	19.3	12.1	6.7	3.1	.7	-.7
1-isopropyl-3-methylnaphthalene	37.0	36.7	25.4	15.8	8.1	2.3	-1.8	-4.5	-6.2
1-isopropyl-4-methylnaphthalene	37.0	36.7	25.4	15.8	8.1	2.3	-1.8	-4.5	-6.2
1-isopropyl-5-methylnaphthalene	37.0	36.7	25.4	15.8	8.1	2.3	-1.8	-4.5	-6.2
1-isopropyl-6-methylnaphthalene	37.0	36.7	25.4	15.8	8.1	2.3	-1.8	-4.5	-6.2
1-isopropyl-7-methylnaphthalene	37.0	36.7	25.4	15.8	8.1	2.3	-1.8	-4.5	-6.2
1-isopropyl-8-methylnaphthalene	61.6	61.3	50.0	40.4	32.7	26.9	22.8	20.1	18.4
2-isopropyl-1-methylnaphthalene	39.4	39.1	28.3	19.3	12.1	6.7	3.1	.7	-.7
2-isopropyl-3-methylnaphthalene	39.4	39.1	28.3	19.3	12.1	6.7	3.1	.7	-.7
2-isopropyl-6-methylnaphthalene	37.0	36.7	25.4	15.8	8.1	2.3	-1.8	-4.5	-6.2
2-isopropyl-7-methylnaphthalene	37.0	36.7	25.4	15.8	8.1	2.3	-1.8	-4.5	-6.2
3-isopropyl-1-methylnaphthalene	37.0	36.7	25.4	15.8	8.1	2.3	-1.8	-4.5	-6.2
6-isopropyl-1-methylnaphthalene	37.0	36.7	25.4	15.8	8.1	2.3	-1.8	-4.5	-6.2
7-isopropyl-1-methylnaphthalene	37.0	36.7	25.4	15.8	8.1	2.3	-1.8	-4.5	-6.2
1-secbutylnaphthalene	53.1	52.9	41.6	32.2	24.8	19.3	15.5	13.1	11.6
2-secbutylnaphthalene	53.1	52.9	41.6	32.2	24.8	19.3	15.5	13.1	11.6
1-isobutylnaphthalene	49.6	49.3	38.1	28.7	21.2	15.7	11.9	9.5	8.0
2-isobutylnaphthalene	49.6	49.3	38.1	28.7	21.2	15.7	11.9	9.5	8.0

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

T/K	298.15	300	400	500	600	700	800	900	1000
C10H8									
naphthalene	223.69	224.15	249.58	276.47	304.21	332.65	361.42	390.49	419.77
C11H10									
1-methylnaphthalene	217.82	218.41	253.47	290.17	327.83	366.28	405.07	444.19	483.52
2-methylnaphthalene	216.28	216.90	251.72	288.16	325.61	363.89	402.56	441.55	480.76
C12H12									
1,2-dimethylnaphthalene	217.4	218.2	263.6	310.9	359.6	409.1	459.2	509.6	560.2
1,3-dimethylnaphthalene	213.0	213.8	258.6	305.4	353.8	403.0	452.9	503.1	553.6
1,4-dimethylnaphthalene	214.7	215.5	260.9	308.3	357.2	407.0	457.5	508.3	559.4
1,5-dimethylnaphthalene	214.7	215.5	260.9	308.3	357.2	407.0	457.5	508.3	559.4
1,6-dimethylnaphthalene	213.0	213.8	258.6	305.4	353.8	403.0	452.9	503.1	553.6
1,7-dimethylnaphthalene	213.0	213.8	258.6	305.4	353.8	403.0	452.9	503.1	553.6
1,8-dimethylnaphthalene	242.1	242.9	289.2	337.6	387.4	438.1	489.6	541.3	593.3
2,3-dimethylnaphthalene	219.1	219.9	265.9	313.8	363.0	413.1	463.8	514.8	566.0
2,6-dimethylnaphthalene	214.7	215.5	260.9	308.3	357.2	407.0	457.5	508.3	559.4
2,7-dimethylnaphthalene	214.7	215.5	260.9	308.3	357.2	407.0	457.5	508.3	559.4
1-ethylnaphthalene	225.7	226.4	271.1	317.7	365.6	414.4	463.8	513.4	563.2
2-ethylnaphthalene	225.7	226.4	271.1	317.7	365.6	414.4	463.8	513.4	563.2
C13H14									
1,2,3-trimethylnaphthalene	217.8	218.8	274.9	333.1	392.8	453.4	514.7	576.2	638.1
1,2,4-trimethylnaphthalene	213.4	214.4	269.9	327.6	387.0	447.3	508.4	569.8	631.5
1,2,5-trimethylnaphthalene	213.4	214.4	269.9	327.6	387.0	447.3	508.4	569.8	631.5
1,2,6-trimethylnaphthalene	213.4	214.4	269.9	327.6	387.0	447.3	508.4	569.8	631.5
1,2,7-trimethylnaphthalene	213.4	214.4	269.9	327.6	387.0	447.3	508.4	569.8	631.5
1,2,8-trimethylnaphthalene	240.8	241.8	298.2	356.9	417.1	478.4	540.4	602.7	665.4
1,3,5-trimethylnaphthalene	209.0	210.0	264.9	322.1	381.2	441.2	502.1	563.3	624.9
1,3,6-trimethylnaphthalene	209.0	210.0	264.9	322.1	381.2	441.2	502.1	563.3	624.9
1,3,7-trimethylnaphthalene	209.0	210.0	264.9	322.1	381.2	441.2	502.1	563.3	624.9
1,3,8-trimethylnaphthalene	236.4	237.3	293.2	351.4	411.3	472.3	534.1	596.3	658.8
1,4,5-trimethylnaphthalene	236.4	237.3	293.2	351.4	411.3	472.3	534.1	596.3	658.8
1,4,6-trimethylnaphthalene	209.0	210.0	264.9	322.1	381.2	441.2	502.1	563.3	624.9
1,6,7-trimethylnaphthalene	213.4	214.4	269.9	327.6	387.0	447.3	508.4	569.8	631.5
2,3,6-trimethylnaphthalene	213.4	214.4	269.9	327.6	387.0	447.3	508.4	569.8	631.5
1-ethyl-2-methylnaphthalene	226.1	227.0	282.4	339.8	398.8	458.7	519.3	580.0	641.1
1-ethyl-3-methylnaphthalene	221.7	222.6	277.4	334.4	393.0	452.6	512.9	573.6	634.5
1-ethyl-4-methylnaphthalene	221.7	222.6	277.4	334.4	393.0	452.6	512.9	573.6	634.5
1-ethyl-5-methylnaphthalene	221.7	222.6	277.4	334.4	393.0	452.6	512.9	573.6	634.5
1-ethyl-6-methylnaphthalene	221.7	222.6	277.4	334.4	393.0	452.6	512.9	573.6	634.5
1-ethyl-7-methylnaphthalene	221.7	222.6	277.4	334.4	393.0	452.6	512.9	573.6	634.5
1-ethyl-8-methylnaphthalene	249.0	250.0	305.7	363.6	423.2	483.7	545.0	606.5	668.4
2-ethyl-1-methylnaphthalene	226.1	227.0	282.4	339.8	398.8	458.7	519.3	580.0	641.1
2-ethyl-3-methylnaphthalene	226.1	227.0	282.4	339.8	398.8	458.7	519.3	580.0	641.1
2-ethyl-6-methylnaphthalene	221.7	222.6	277.4	334.4	393.0	452.6	512.9	573.6	634.5
2-ethyl-7-methylnaphthalene	221.7	222.6	277.4	334.4	393.0	452.6	512.9	573.6	634.5
3-ethyl-1-methylnaphthalene	221.7	222.6	277.4	334.4	393.0	452.6	512.9	573.6	634.5
6-ethyl-1-methylnaphthalene	221.7	222.6	277.4	334.4	393.0	452.6	512.9	573.6	634.5
7-ethyl-1-methylnaphthalene	221.7	222.6	277.4	334.4	393.0	452.6	512.9	573.6	634.5
1-propylnaphthalene	234.0	234.9	289.5	346.3	404.7	464.0	523.9	584.2	644.7
2-propylnaphthalene	234.0	234.9	289.5	346.3	404.7	464.0	523.9	584.2	644.7
1-isopropylnaphthalene	231.5	232.5	288.2	346.1	405.6	466.1	527.2	588.5	650.1
2-isopropylnaphthalene	231.5	232.5	288.2	346.1	405.6	466.1	527.2	588.5	650.1
C14H16									
1,2,3,4-tetramethylnaphthalene	219.9	221.1	288.5	358.1	429.4	501.7	574.8	648.1	721.7
1,2,3,5-tetramethylnaphthalene	213.8	215.0	281.1	349.8	420.2	491.6	563.9	636.4	709.3
1,2,3,6-tetramethylnaphthalene	213.8	215.0	281.1	349.8	420.2	491.6	563.9	636.4	709.3
1,2,3,7-tetramethylnaphthalene	213.8	215.0	281.1	349.8	420.2	491.6	563.9	636.4	709.3
1,2,3,8-tetramethylnaphthalene	241.2	242.4	309.5	379.0	450.3	522.7	595.9	669.4	743.2
1,2,4,5-tetramethylnaphthalene	236.8	237.9	304.5	373.6	444.5	516.6	589.6	662.9	736.6
1,2,4,6-tetramethylnaphthalene	209.4	210.6	276.1	344.3	414.4	485.5	557.6	630.0	702.7
1,2,4,7-tetramethylnaphthalene	209.4	210.6	276.1	344.3	414.4	485.5	557.6	630.0	702.7
1,2,4,8-tetramethylnaphthalene	236.8	237.9	304.5	373.6	444.5	516.6	589.6	662.9	736.6
1,2,5,6-tetramethylnaphthalene	215.5	216.7	283.5	352.7	423.6	495.7	568.5	641.6	715.1
1,2,5,7-tetramethylnaphthalene	209.4	210.6	276.1	344.3	414.4	485.5	557.6	630.0	702.7
1,2,5,8-tetramethylnaphthalene	236.8	237.9	304.5	373.6	444.5	516.6	589.6	662.9	736.6
1,2,6,7-tetramethylnaphthalene	213.8	215.0	281.1	349.8	420.2	491.6	563.9	636.4	709.3
1,2,6,8-tetramethylnaphthalene	236.8	237.9	304.5	373.6	444.5	516.6	589.6	662.9	736.6
1,2,7,8-tetramethylnaphthalene	242.9	244.1	311.8	381.9	453.8	526.8	600.5	674.6	749.0
1,3,5,7-tetramethylnaphthalene	206.7	207.9	273.5	341.7	412.0	483.5	555.9	628.7	701.9
1,3,5,8-tetramethylnaphthalene	232.4	233.5	299.5	368.1	438.7	510.5	583.3	656.5	730.1
1,3,6,7-tetramethylnaphthalene	209.4	210.6	276.1	344.3	414.4	485.5	557.6	630.0	702.7
1,3,6,8-tetramethylnaphthalene	234.1	235.3	301.8	371.0	442.2	514.6	587.9	661.7	735.8
1,4,5,8-tetramethylnaphthalene	263.2	264.4	332.4	403.1	475.8	549.7	624.5	699.8	775.5
1,4,6,7-tetramethylnaphthalene	211.1	212.3	278.5	347.2	417.8	489.6	562.2	635.2	708.5
2,3,6,7-tetramethylnaphthalene	217.2	218.4	285.8	355.5	427.1	499.7	573.1	646.8	720.9
1-ethyl-2,3-dimethylnaphthalene	226.5	227.6	293.6	362.0	432.0	503.0	574.7	646.7	718.9
1-ethyl-2,4-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
1-ethyl-2,5-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
1-ethyl-2,6-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
1-ethyl-2,7-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
1-ethyl-2,8-dimethylnaphthalene	249.4	250.6	317.0	385.8	456.4	528.0	600.5	673.2	746.2

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

T/K	298.15	300	400	500	600	700	800	900	1000
C14H16									
1-ethyl-3,5-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
1-ethyl-3,6-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
1-ethyl-3,7-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
1-ethyl-3,8-dimethylnaphthalene	245.0	246.2	312.0	380.3	450.6	521.9	594.2	666.7	739.6
1-ethyl-4,5-dimethylnaphthalene	245.0	246.2	312.0	380.3	450.6	521.9	594.2	666.7	739.6
1-ethyl-4,6-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
1-ethyl-6,7-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
2-ethyl-1,3-dimethylnaphthalene	226.5	227.6	293.6	362.0	432.0	503.0	574.7	646.7	718.9
2-ethyl-1,4-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
2-ethyl-1,5-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
2-ethyl-1,6-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
2-ethyl-1,7-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
2-ethyl-1,8-dimethylnaphthalene	249.4	250.6	317.0	385.8	456.4	528.0	600.5	673.2	746.2
2-ethyl-3,6-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
3-ethyl-1,2-dimethylnaphthalene	226.5	227.6	293.6	362.0	432.0	503.0	574.7	646.7	718.9
3-ethyl-1,5-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
3-ethyl-1,6-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
3-ethyl-1,7-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
3-ethyl-1,8-dimethylnaphthalene	245.0	246.2	312.0	380.3	450.6	521.9	594.2	666.7	739.6
3-ethyl-2,6-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
4-ethyl-1,2-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
4-ethyl-1,5-dimethylnaphthalene	245.0	246.2	312.0	380.3	450.6	521.9	594.2	666.7	739.6
4-ethyl-1,6-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
5-ethyl-1,2-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
5-ethyl-1,3-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
5-ethyl-1,4-dimethylnaphthalene	245.0	246.2	312.0	380.3	450.6	521.9	594.2	666.7	739.6
6-ethyl-1,2-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
6-ethyl-1,3-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
6-ethyl-1,4-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
6-ethyl-1,7-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
6-ethyl-2,3-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
7-ethyl-1,2-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
7-ethyl-1,3-dimethylnaphthalene	217.7	218.8	283.7	351.1	420.4	490.8	562.1	633.8	705.8
7-ethyl-1,6-dimethylnaphthalene	222.1	223.2	288.6	356.6	426.2	496.9	568.4	640.2	712.3
8-ethyl-1,2-dimethylnaphthalene	249.4	250.6	317.0	385.8	456.4	528.0	600.5	673.2	746.2
8-ethyl-1,3-dimethylnaphthalene	245.0	246.2	312.0	380.3	450.6	521.9	594.2	666.7	739.6
1-methyl-2-propylnaphthalene	234.4	235.5	300.8	368.5	437.9	508.3	579.4	650.8	722.5
1-methyl-3-propylnaphthalene	230.0	231.1	295.8	363.0	432.0	502.2	573.1	644.4	715.9
1-methyl-4-propylnaphthalene	230.0	231.1	295.8	363.0	432.0	502.2	573.1	644.4	715.9
1-methyl-5-propylnaphthalene	230.0	231.1	295.8	363.0	432.0	502.2	573.1	644.4	715.9
1-methyl-6-propylnaphthalene	230.0	231.1	295.8	363.0	432.0	502.2	573.1	644.4	715.9
1-methyl-7-propylnaphthalene	230.0	231.1	295.8	363.0	432.0	502.2	573.1	644.4	715.9
1-methyl-8-propylnaphthalene	257.3	258.5	324.1	392.2	462.2	533.3	605.1	677.3	749.8
2-methyl-1-propylnaphthalene	234.4	235.5	300.8	368.5	437.9	508.3	579.4	650.8	722.5
2-methyl-3-propylnaphthalene	234.4	235.5	300.8	368.5	437.9	508.3	579.4	650.8	722.5
2-methyl-6-propylnaphthalene	230.0	231.1	295.8	363.0	432.0	502.2	573.1	644.4	715.9
2-methyl-7-propylnaphthalene	230.0	231.1	295.8	363.0	432.0	502.2	573.1	644.4	715.9
3-methyl-1-propylnaphthalene	230.0	231.1	295.8	363.0	432.0	502.2	573.1	644.4	715.9
6-methyl-1-propylnaphthalene	230.0	231.1	295.8	363.0	432.0	502.2	573.1	644.4	715.9
7-methyl-1-propylnaphthalene	230.0	231.1	295.8	363.0	432.0	502.2	573.1	644.4	715.9
1-butylnaphthalene	242.2	243.4	307.9	374.9	443.7	513.5	584.1	655.0	726.1
2-butylnaphthalene	242.2	243.4	307.9	374.9	443.7	513.5	584.1	655.0	726.1
1,2-diethylnaphthalene	234.7	235.9	301.2	368.8	438.1	508.3	579.3	650.5	721.9
1,3-diethylnaphthalene	230.4	231.5	296.2	363.3	432.3	502.2	573.0	644.0	715.3
1,4-diethylnaphthalene	232.1	233.2	298.5	366.2	435.7	506.3	577.6	649.2	721.1
1,5-diethylnaphthalene	232.1	233.2	298.5	366.2	435.7	506.3	577.6	649.2	721.1
1,6-diethylnaphthalene	230.4	231.5	296.2	363.3	432.3	502.2	573.0	644.0	715.3
1,7-diethylnaphthalene	230.4	231.5	296.2	363.3	432.3	502.2	573.0	644.0	715.3
1,8-diethylnaphthalene	259.4	260.6	326.8	395.5	465.9	537.4	609.6	682.2	755.0
2,3-diethylnaphthalene	236.5	237.6	303.5	371.7	441.5	512.4	583.9	655.7	727.7
2,6-diethylnaphthalene	232.1	233.2	298.5	366.2	435.7	506.3	577.6	649.2	721.1
2,7-diethylnaphthalene	232.1	233.2	298.5	366.2	435.7	506.3	577.6	649.2	721.1
1-t-butylnaphthalene	241.6	242.8	311.0	381.8	454.2	527.5	601.4	675.6	749.9
2-t-butylnaphthalene	241.6	242.8	311.0	381.8	454.2	527.5	601.4	675.6	749.9
1-isopropyl-2-methylnaphthalene	231.9	233.1	299.4	368.3	438.8	510.4	582.6	655.1	727.9
1-isopropyl-3-methylnaphthalene	227.5	228.7	294.4	362.8	433.0	504.3	576.3	648.7	721.3
1-isopropyl-4-methylnaphthalene	227.5	228.7	294.4	362.8	433.0	504.3	576.3	648.7	721.3
1-isopropyl-5-methylnaphthalene	227.5	228.7	294.4	362.8	433.0	504.3	576.3	648.7	721.3
1-isopropyl-6-methylnaphthalene	227.5	228.7	294.4	362.8	433.0	504.3	576.3	648.7	721.3
1-isopropyl-7-methylnaphthalene	227.5	228.7	294.4	362.8	433.0	504.3	576.3	648.7	721.3
1-isopropyl-8-methylnaphthalene	254.9	256.1	322.8	392.1	463.2	535.4	608.4	681.6	755.2
2-isopropyl-1-methylnaphthalene	231.9	233.1	299.4	368.3	438.8	510.4	582.6	655.1	727.9
2-isopropyl-3-methylnaphthalene	231.9	233.1	299.4	368.3	438.8	510.4	582.6	655.1	727.9
2-isopropyl-6-methylnaphthalene	227.5	228.7	294.4	362.8	433.0	504.3	576.3	648.7	721.3
2-isopropyl-7-methylnaphthalene	227.5	228.7	294.4	362.8	433.0	504.3	576.3	648.7	721.3
3-isopropyl-1-methylnaphthalene	227.5	228.7	294.4	362.8	433.0	504.3	576.3	648.7	721.3
6-isopropyl-1-methylnaphthalene	227.5	228.7	294.4	362.8	433.0	504.3	576.3	648.7	721.3
7-isopropyl-1-methylnaphthalene	227.5	228.7	294.4	362.8	433.0	504.3	576.3	648.7	721.3
1-secbutylnaphthalene	241.4	242.6	307.6	375.2	444.5	514.9	586.0	657.4	729.1
2-secbutylnaphthalene	241.4	242.6	307.6	375.2	444.5	514.9	586.0	657.4	729.1
1-isobutylnaphthalene	239.6	240.7	306.3	374.5	444.4	515.4	587.1	659.1	731.3
2-isobutylnaphthalene	239.6	240.7	306.3	374.5	444.4	515.4	587.1	659.1	731.3

7. Discussion

The chemical thermodynamic properties of the polycyclic aromatic hydrocarbons are of interest in connection with soot formation, carcinogenesis, and coal conversion processes. Enthalpies of formation of large polycyclic aromatic hydrocarbons have been estimated by Stein, Golden, and Benson.[8] Shaw, Golden, and Benson[18] have summarized thermodynamic properties of dihydronaphthalenes, tetrahydronaphthalenes, hexahydronaphthalenes, and other polycyclic compounds related to coal. Stein[19] has used existing and new predictive methods to discuss high temperature chemical equilibria of polycyclic aromatic hydrocarbons.

8. Nomenclature

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

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

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

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

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

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

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

$\Delta_f H^\circ(\mathrm{I})$ = 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}

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

TSN = total symmetry number

y_i = mole fraction of isomer i within the isomer group

y_I = mole fraction of isomer group I in a mixture

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