Standard Chemical Thermodynamic Properties of Alkylbenzene Isomer Groups

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Robert A. Alberty

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Robert A. Alberty

Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

The chemical thermodynamic properties of alkylbenzene isomer groups from C_8H_{10} to C_9H_{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 $C_{10}H_{14}$ to $C_{12}H_{18}$ have been calculated using Benson group values. 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. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 298.15 to 1000 K. Values of $C^\circ_p, S^\circ, \Delta_f H^\circ$, and $\Delta_f G^\circ$ are given for all species from C_6H_6 to $C_{12}H_{18}$ in joules for a standard state pressure of 1 bar.

Key words: alkylbenzenes; 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

When chemical equilibrium calculations are made on organic systems involving alkylbenzenes larger than toluene, the number of isomeric species increases very rapidly with carbon number. It is therefore convenient to calculate chemical thermodynamic properties for alkylbenzene isomer groups and use these properties in equilibrium calculations, as recommended by Smith.[1] The mole fractions of individual species may then be calculated in a second step since their mole fractions in their isomer groups are functions of temperature only for ideal gases.

The preceding article[2] in this series has presented chemical thermodynamic properties of alkane isomer groups through $C_{10}H_{22}$ for the ideal gas state from 200 to 1500 K. These tables provide a basis for extrapolation to higher carbon numbers.

The first statistical-mechanical correlations of the chemical thermodynamic properties of the alkylbenzenes were made by Pitzer and Scott.[3] Prosen, Johnson, and Rossini[4] computed a number of enthalpies of formation of alkylbenzenes and developed an extrapolation formula. Taylor, Wagman, Williams, Pitzer, and Rossini[5] made statistical mechanical correlations for the four C_8H_{10} and the eight C_9H_{12} alkylbenzenes. Further work was done by Rossini, Pitzer, Arnett, Braun, and Pimentel,[6] who published tables in 1953. Some further small changes were made by Stull, Westrum, and Sinke[7] in publishing their book in 1969. The enthalpies of formation of alkylbenzenes at 298.15 K have been evaluated by Cox and Pilcher,[8] and the thermodynamic properties of the $C_{10}H_{14}$ alkylbenzenes at 298.15 K have been presented by Somayajulu.[9]

2. Standard Thermodynamic Properties of Isomer Groups

When isomers are in chemical equilibrium, it has been know for some time[1,10-16] that they can be aggregated in calculations of equilibrium mole fractions by use of the standard Gibbs energy of formation $\Delta_f G°(\mathrm{I})$ of the isomer group defined by

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

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

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

where y_I is the sum of the mole fractions of the individual isomers. The corresponding equations for the other standard thermodynamic properties $C_P°(\mathrm{I})$, $S°(\mathrm{I})$, and $\Delta_f H°(\mathrm{I})$ can be derived by differentiating Eq. (1) with respect to temperature.[16] 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 alkylbenzenes the standard chemical thermodynamic properties for an isomer group are interrelated by

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

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 alkylbenzenes 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 and of isomers are compared in Table 1.

Table 1. Numbers of isomers of alkylbenzenes

	Number of lines	Chiral Centers One	Chiral Centers Two	Total isomers
C6H6	1	0	0	1
C7H8	1	0	0	1
C8H10	4	0	0	4
C9H12	8	0	0	8
C10H14	22	1	0	23
C11H16	40	6	0	46
C12H18	87	20	2	109

Stull, Westrum, and Sinke[7] give data on all the isomers through C_9H_{12} and on 7 of the 23 isomers of $C_{10}H_{14}$. In order to compare the properties expected for the remaining isomers of $C_{10}H_{14}$ and to examine the relationship between isomer group properties and carbon number, the Benson group method was used.

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

In view of the rapid increase in the number of isomers with carbon number, we are dependent on various estimation and extrapolation methods for thermodynamic properties of higher isomers. Calculations using the Benson method[17,18] were useful in considerations of the properties of the higher alkanes,[2] and they are needed for the alkylbenzenes because the increments in isomer group thermodynamic properties are still increasing with carbon number at C_9H_{12}. Therefore the Benson method was used to estimate $C_P°$, $S°$, $\Delta_f H°$, and $\Delta_f G°$ for all the individual isomers of the alkylbenzenes up to $C_{12}H_{18}$ in the ideal gas state using computer programs written in APL.[2]

In order to make these calculations, the structure of each alkylbenzene species was divided into the following Benson groups: $C(H)_3(C)$, $C(H)_2(C)_2$, $C(H)(C)_3$, $C(C)_4$, $C(C_B)(C)(H)_2$, $C(C_B)(C)_2(H)$, $C(C_B)(C)_3$, $C_B(H)$, and $C_B(C)$. In addition the total symmetry number (TSN), number of optical isomers (OPT), and ortho corrections were identified. In view of some of the uncertainties in some of the alkylbenzene group values indicated by Benson, the gauche and 1,5-H repulsions, which affect only several of the most highly branched species were omitted. In calculating symmetry numbers a report by Davies, Syverud, and Steiner[19] was very helpful. The group assignments were checked by matrix multiplication to be sure they accounted for the correct numbers of carbon and hydrogen atoms.

The matrix of numbers of contributions was then matrix multiplied by a matrix of the Benson values to obtain for each isomer the sum of the contributions to $\Delta_f H°_{298}$, $S°_{\mathrm{int}\,298}$,

Table 2. Root mean square deviations between alkylbenzene 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								
C6H6	3.30	3.25	1.20	3.53	3.38	1.54	1.04	3.67	5.94
C7H8	4.26	4.13	1.63	5.58	6.70	5.79	3.87	1.71	.13
C8H10	3.92	3.86	.74	3.64	4.07	2.66	1.10	2.96	5.20
C9H12	5.54	5.49	3.19	4.26	4.59	3.23	2.70	4.55	6.62
C10H14	4.35	4.12	.79	3.95	4.13	2.49	1.19	4.00	6.38
	Standard entropy in J/K mol								
C6H6	.41	.43	.12	.69	1.34	1.74	1.79	1.51	.98
C7H8	.71	.71	1.06	.22	.93	1.90	2.54	2.86	2.98
C8H10	.84	.85	1.14	.76	.62	.93	1.06	.91	.56
C9H12	1.29	1.28	1.28	1.57	2.04	2.48	2.76	2.90	3.01
C10H14	2.53	2.54	2.13	2.54	3.18	3.63	3.73	3.46	2.93
	Standard enthalpy of formation in kJ/mol								
C6H6	.08	.06	.07	.16	.50	.75	.77	.52	.09
C7H8	.59	.59	.38	.73	1.32	2.00	2.47	2.73	2.84
C8H10	1.26	1.25	1.03	1.19	1.53	1.88	2.00	1.91	1.67
C9H12	2.00	1.99	1.63	1.66	1.90	2.21	2.27	2.17	2.00
C10H14	2.19	2.18	1.98	2.10	2.35	2.63	2.65	2.44	2.10
	Standard Gibbs energy of formation in kJ/mol								
C6H6	.10	.09	.12	.17	.28	.41	.61	.74	.81
C7H8	.71	.73	.80	.91	.83	.75	.48	.28	.01
C8H10	1.39	1.37	1.47	1.58	1.58	1.61	1.53	1.53	1.55
C9H12	1.79	1.78	1.80	1.87	1.89	2.01	2.06	2.24	2.47
C10H14	1.52	1.52	1.36	1.26	1.16	1.13	1.25	1.37	1.51

C°_{P300}, C°_{P400}, C°_{P500}, C°_{P600}, C°_{P800}, C°_{P1000}, and C°_{P1500}. In further steps in the calculation the heat capacity values were fit to the equation

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

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 200 to 1000 K.

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

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

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_6H_6 through C_9H_{12} and for the seven isomers of $C_{10}H_{14}$ for which they give values. 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_6H_6 and C_7H_8 this yields the magnitudes of the deviations, and for the higher homologous series it yields the root-mean-square deviations as a function of temperature. Even for the higher homologs the root-mean-square deviations in $\Delta_f G^\circ$ average less than 2 kJ mol^{-1}.

4. Tables of Standard Thermodynamic Properties of Alkylbenzene 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

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

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 $(4-n)$ in moles of gas in the formation reaction.[20]

In Tables 3 to 8, the Stull, Westrum, and Sinke tables have been used to calculate the isomer group properties for C_6H_6 to C_9H_{12}, and the Benson method has been used to calculate the isomer group properties for $C_{10}H_{14}$ to $C_{12}H_{18}$. For each property the increments in going from one carbon number to the next are provided. These increments provide a basis for a linear extrapolation of standard thermodynamic properties of alkane isomer groups to higher carbon numbers. In a general way we would expect these increments to approach constant values as the carbon number increases at constant temperature. At lower temperatures, constant values are not approached for some properties, and this indicates that extrapolations are correspondingly uncertain. The limiting increments per carbon atom are quite similar to those for the alkanes, but there are some differences.[2] The limiting increments in $\Delta_f H^\circ$(I) are about 5 kJ mol^{-1} more negative for the alkylbenzenes than for the alkanes above 500 K. The increments in C°_P(I) and S°(I) are remarkably similar for the two homologous series above 400 K.

Table 7 gives

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

the standard enthalpy for an isomer group relative to the isomer group at 298.15 K. Table 8 gives values for

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

the standard enthalpy for the isomer group relative to the

elements at 298.15 K. This quantity allows the direct calculation of heat effects when the reactants and products are at different temperatures.

5. Equilibrium Mole Fractions Within Alkylbenzene 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 $\Delta_f G_i^\circ$ 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 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.[21] For example, the two forms of 1-methylpropylbenzene are represented by 1R and 1S, and the racemic mixture is represented by 1(RS)-methylpropylbenzene. 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.

Table 9 shows that in general the more highly branched isomers have very low equilibrium mole fractions at any temperature. The isomers with more methyl groups, and more branches have more positive standard Gibbs energies of formation. 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.

It is of interest to note that if certain isomers are excluded by the catalyst, the equilibrium mole fractions of the remaining isomers may be calculated from these tables by simply excluding certain isomers and renormalizing the total mole fraction to unity. The calculation of the standard Gibbs energy of formation of the restricted isomer group is more complicated. If the standard Gibbs energy of formation of the restricted isomer group (RIG) that is in equilibrium is represented by $\Delta_f G^\circ$ (RIG) and the standard Gibbs energy of formation of the excluded isomer group (EXCLIG) is represented by $\Delta_f G^\circ$ (EXCLIG), then the standard Gibbs energy of formation of the whole isomer group and of the restricted isomer group are given by the following equations:

$$\exp[-\Delta_f G^\circ(\mathrm{I})/RT] = \exp[-\Delta_f G^\circ(\mathrm{RIG})/RT] + \exp[-\Delta_f G^\circ(\mathrm{EXCLIG})/RT], \quad (7)$$

$$\Delta_f G^\circ(\mathrm{RIG}) = -RT\ln\{\exp[-\Delta_f G^\circ(\mathrm{I})/RT] - \exp[-\Delta_f G^\circ(\mathrm{EXCLIG})/RT]\}. \quad (8)$$

6. Standard Thermodynamic Properties of Individual Alkylbenzene Species

The values of C_P°, S°, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ for all the alkylbenzene species through $C_{12}H_{18}$ are given in Tables 10 to 13 in joules for a standard state pressure of 1 bar. The values for C_6H_6 through C_9H_{12} have been converted from the tables of Stull, Westrum, and Sinke,[7] and the values for $C_{10}H_{14}$ through $C_{12}H_{18}$ have been calculated using the Benson method.[18] The values for chiral forms are for the racemates.

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

T/K	C6H6	C7H8	C8H10	C9H12	C10H14	C11H16	C12H18
298.15	81.67	103.64	129.92	160.24	210.7	261.6	268.6
300.00	82.22	104.35	130.64	161.06	211.6	262.2	269.1
400.00	111.88	140.08	170.50	207.72	253.4	293.0	308.3
500.00	137.24	171.46	206.15	249.55	289.3	327.3	353.9
600.00	157.90	197.48	236.08	284.11	322.8	362.7	397.5
700.00	174.68	218.95	260.98	312.31	353.8	396.6	437.4
800.00	188.53	236.86	281.79	335.43	381.8	427.7	473.0
900.00	200.12	252.00	299.29	354.67	406.6	455.3	504.3
1000.00	209.87	264.93	314.15	370.94	427.8	479.1	531.1

Table 3a. Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9	C11-C10	C12-C11
298.15	21.97	26.28	30.31	50.4	50.9	7.0
300.00	22.13	26.30	30.41	50.5	50.6	6.9
400.00	28.20	30.42	37.22	45.6	39.7	15.3
500.00	34.23	34.69	43.40	39.7	38.0	26.7
600.00	39.58	38.60	48.03	38.7	39.9	34.8
700.00	44.27	42.03	51.32	41.5	42.8	40.8
800.00	48.33	44.94	53.63	46.4	45.9	45.3
900.00	51.88	47.28	55.38	51.9	48.7	49.0
1000.00	55.06	49.22	56.79	56.9	51.3	52.0

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

T/K	C6H6	C7H8	C8H10	C9H12	C10H14	C11H16	C12H18
298.15	269.31	320.77	363.85	399.28	435.2	471.0	522.1
300.00	269.85	321.44	364.65	400.26	436.5	472.7	523.8
400.00	297.63	356.46	407.81	453.12	503.4	552.3	606.1
500.00	325.42	391.19	449.80	504.10	563.8	621.3	679.8
600.00	352.32	424.83	490.09	552.72	619.6	684.1	748.2
700.00	377.97	456.92	528.43	598.72	671.7	742.6	812.6
800.00	402.23	487.34	564.66	641.95	720.8	797.6	873.3
900.00	425.12	516.12	598.90	682.64	767.2	849.6	930.9
1000.00	446.71	543.40	631.22	720.86	811.2	898.8	985.5

Table 4a. Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9	C11-C10	C12-C11
298.15	51.46	43.08	35.42	36.0	35.8	51.1
300.00	51.59	43.21	35.61	36.3	36.1	51.1
400.00	58.83	51.35	45.31	50.3	48.9	53.8
500.00	65.77	58.62	54.30	59.7	57.4	58.5
600.00	72.51	65.27	62.63	66.8	64.5	64.2
700.00	78.95	71.51	70.29	73.0	70.9	70.0
800.00	85.10	77.32	77.30	78.8	76.8	75.8
900.00	91.00	82.78	83.73	84.6	82.4	81.3
1000.00	96.69	87.82	89.64	90.3	87.6	86.6

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

T/K	C6H6	C7H8	C8H10	C9H12	C10H14	C11H16	C12H18
298.15	82.93	50.00	17.76	-14.33	-43.8	-69.1	-91.1
300.00	82.80	49.87	17.59	-14.53	-43.9	-69.2	-91.3
400.00	77.66	43.26	9.91	-22.75	-51.1	-75.9	-101.0
500.00	73.39	37.87	3.51	-29.34	-57.7	-82.9	-110.1
600.00	69.91	33.56	-1.64	-34.43	-63.3	-89.2	-117.8
700.00	67.11	30.29	-5.61	-38.11	-67.8	-94.2	-123.7
800.00	64.89	27.82	-8.60	-40.74	-70.9	-97.7	-127.8
900.00	63.18	26.11	-10.70	-42.40	-72.6	-99.8	-130.1
1000.00	62.01	25.15	-11.94	-43.15	-73.1	-100.4	-130.8

Table 5a. Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9	C11-C10	C12-C11
298.15	-32.93	-32.24	-32.08	-29.4	-25.3	-22.1
300.00	-32.93	-32.28	-32.12	-29.4	-25.3	-22.1
400.00	-34.39	-33.35	-32.66	-28.4	-24.8	-25.1
500.00	-35.52	-34.36	-32.85	-28.4	-25.2	-27.2
600.00	-36.36	-35.19	-32.79	-28.9	-25.9	-28.0
700.00	-36.82	-35.90	-32.50	-29.7	-26.4	-29.5
800.00	-37.07	-36.42	-32.15	-30.1	-26.9	-30.1
900.00	-37.07	-36.81	-31.70	-30.2	-27.2	-30.4
1000.00	-36.86	-37.08	-31.21	-30.0	-27.3	-30.4

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

T/K	C6H6	C7H8	C8H10	C9H12	C10H14	C11H16	C12H18
298.15	129.73	122.10	117.71	115.71	116.3	121.0	124.4
300.00	130.02	122.56	118.29	116.49	117.3	122.2	125.7
400.00	146.57	147.83	153.09	161.51	172.2	187.0	199.6
500.00	164.29	174.64	189.65	208.36	228.8	253.5	275.8
600.00	182.80	202.37	227.34	256.35	286.6	321.4	353.7
700.00	201.86	230.81	265.87	305.18	345.3	390.3	432.8
800.00	221.26	259.59	304.83	354.35	404.6	459.8	512.6
900.00	240.90	288.70	344.16	403.87	464.1	529.5	592.7
1000.00	260.76	317.93	383.70	453.54	523.7	599.5	673.1

Table 6a. Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9	C11-C10	C12-C11
298.15	-7.62	-4.40	-2.00	.6	4.7	3.4
300.00	-7.46	-4.27	-1.81	.8	4.9	3.5
400.00	1.26	5.27	8.42	10.7	14.8	12.6
500.00	10.35	15.02	18.71	20.4	24.7	22.2
600.00	19.56	24.98	29.01	30.3	34.8	32.3
700.00	28.95	35.06	39.31	40.1	45.0	42.5
800.00	38.33	45.25	49.51	50.2	55.2	52.8
900.00	47.80	55.46	59.71	60.2	65.5	63.2
1000.00	57.18	65.77	69.84	70.2	75.8	73.6

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

T/K	C6H6	C7H8	C8H10	C9H12	C10H14	C11H16	C12H18
298.15	.00	.00	.00	.00	.0	.0	.0
300.00	.14	.21	.24	.28	.4	.5	.5
400.00	9.83	12.36	15.24	18.66	23.7	28.2	29.2
500.00	22.29	27.95	34.07	41.56	50.9	59.2	62.3
600.00	37.07	46.39	56.19	68.23	81.5	93.7	99.9
700.00	53.72	67.29	81.10	98.14	115.4	131.7	141.7
800.00	71.89	90.09	108.25	130.53	152.2	173.0	187.3
900.00	91.32	114.53	137.31	165.04	191.6	217.1	236.2
1000.00	111.90	140.44	168.08	201.43	233.4	263.9	288.0

Table 7a. Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9	C11-C10	C12-C11
298.15	.00	.00	.00	.0	.0	.0
300.00	.07	.03	.04	.1	.1	.0
400.00	2.53	2.88	3.42	5.1	4.5	1.0
500.00	5.65	6.13	7.48	9.3	8.3	3.1
600.00	9.32	9.80	12.04	13.3	12.2	6.2
700.00	13.57	13.80	17.05	17.2	16.3	10.0
800.00	18.20	18.16	22.28	21.6	20.8	14.3
900.00	23.21	22.78	27.73	26.6	25.5	19.0
1000.00	28.54	27.64	33.35	31.9	30.5	24.1

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

T/K	C6H6	C7H8	C8H10	C9H12	C10H14	C11H16	C12H18
298.15	82.93	50.00	17.76	-14.33	-43.8	-69.1	-91.1
300.00	83.07	50.21	18.00	-14.05	-43.4	-68.6	-90.6
400.00	92.76	62.36	33.00	4.34	-20.0	-40.8	-61.9
500.00	105.22	77.95	51.83	27.23	7.1	-9.9	-28.8
600.00	120.00	96.39	73.95	53.91	37.7	24.6	8.8
700.00	136.65	117.29	98.86	83.82	71.6	62.6	50.6
800.00	154.82	140.09	126.01	116.20	108.4	103.9	96.1
900.00	174.25	164.53	155.07	150.72	147.8	148.0	145.0
1000.00	194.82	190.44	185.83	187.10	189.6	194.8	196.9

Table 8a. Increments per carbon atom

T/K	C7-C6	C8-C7	C9-C8	C10-C9	C11-C10	C12-C11
298.15	-32.93	-32.24	-32.08	-29.4	-25.3	-22.1
300.00	-32.86	-32.21	-32.05	-29.3	-25.2	-22.0
400.00	-30.40	-29.36	-28.66	-24.4	-20.8	-21.1
500.00	-27.28	-26.11	-24.60	-20.1	-17.0	-18.9
600.00	-23.61	-22.44	-20.04	-16.2	-13.1	-15.8
700.00	-19.36	-18.44	-15.04	-12.2	-9.0	-12.1
800.00	-14.73	-14.08	-9.81	-7.8	-4.5	-7.7
900.00	-9.72	-9.46	-4.35	-2.9	.2	-3.0
1000.00	-4.38	-4.60	1.27	2.5	5.2	2.0

Table 9. Equilibrium mole fractions within alkylbenzene isomer groups

T/K	298.15	300	400	500	600	700	800	900	1000
C8H10									
ethylbenzene	.0053	.0054	.0180	.0371	.0599	.0845	.1095	.1330	.1556
1,3-dimethylbenzene	.5940	.5963	.5593	.5284	.5002	.4776	.4566	.4377	.4214
1,2-dimethylbenzene	.1620	.1612	.1849	.2031	.2162	.2229	.2286	.2314	.2327
1,4-dimethylbenzene	.2388	.2370	.2378	.2315	.2236	.2150	.2054	.1979	.1903
C9H12									
propylbenzene	.0002	.0002	.0015	.0053	.0118	.0204	.0304	.0408	.0513
isopropylbenzene	.0002	.0002	.0011	.0031	.0061	.0095	.0131	.0166	.0199
1-ethyl-3-methylbenzene	.0123	.0126	.0425	.0828	.1230	.1597	.1896	.2136	.2310
1-ethyl-2-methylbenzene	.0019	.0020	.0093	.0228	.0403	.0592	.0771	.0939	.1081
1-ethyl-4-methylbenzene	.0111	.0114	.0335	.0594	.0836	.1030	.1168	.1270	.1342
1,2,3-trimethylbenzene	.0264	.0264	.0415	.0506	.0541	.0543	.0526	.0502	.0476
1,2,4-trimethylbenzene	.5687	.5677	.5679	.5329	.4827	.4307	.3836	.3417	.3078
1,3,5-trimethylbenzene	.3793	.3796	.3027	.2431	.1984	.1632	.1367	.1161	.1002
C10H14									
butylbenzene	.0000	.0000	.0001	.0006	.0016	.0032	.0052	.0076	.0102
1,3-diethylbenzene	.0006	.0006	.0036	.0091	.0157	.0221	.0279	.0330	.0374
1,2-diethylbenzene	.0001	.0001	.0008	.0025	.0049	.0077	.0108	.0139	.0169
1,4-diethylbenzene	.0003	.0003	.0018	.0046	.0078	.0110	.0139	.0165	.0187
1,2,3,4-tetramethylbenzene	.0798	.0799	.0736	.0636	.0549	.0481	.0429	.0388	.0355
1,2,3,5-tetramethylbenzene	.4698	.4671	.3306	.2361	.1760	.1371	.1107	.0922	.0785
1,2,4,5-tetramethylbenzene	.2349	.2335	.1653	.1180	.0880	.0685	.0554	.0461	.0393

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

T/K	298.15	300	400	500	600	700	800	900	1000
1-ethyl-2,3-dimethylbenzene	.0056	.0058	.0155	.0250	.0327	.0386	.0430	.0464	.0489
1-ethyl-2,4-dimethylbenzene	.0332	.0339	.0694	.0929	.1050	.1100	.1112	.1103	.1083
1-ethyl-2,5-dimethylbenzene	.0332	.0339	.0694	.0929	.1050	.1100	.1112	.1103	.1083
1-ethyl-2,6-dimethylbenzene	.0028	.0029	.0077	.0125	.0164	.0193	.0215	.0232	.0245
1-ethyl-3,4-dimethylbenzene	.0332	.0339	.0694	.0929	.1050	.1100	.1112	.1103	.1083
1-ethyl-3,5-dimethylbenzene	.0977	.0991	.1559	.1725	.1683	.1567	.1436	.1311	.1199
1-propyl-2-methylbenzene	.0002	.0002	.0018	.0053	.0102	.0157	.0212	.0266	.0316
1-propyl-3-methylbenzene	.0014	.0014	.0082	.0198	.0327	.0447	.0548	.0632	.0699
1-propyl-4-methylbenzene	.0007	.0007	.0041	.0099	.0164	.0223	.0274	.0316	.0350
1-isopropyl-2-methylbenzene	.0006	.0007	.0027	.0056	.0084	.0109	.0131	.0149	.0164
1-isopropyl-3-methylbenzene	.0037	.0038	.0122	.0206	.0270	.0311	.0338	.0354	.0363
1-isopropyl-4-methylbenzene	.0019	.0019	.0061	.0103	.0135	.0156	.0169	.0177	.0182
2-methylpropylbenzene	.0001	.0001	.0009	.0028	.0053	.0082	.0110	.0137	.0162
1(RS)-methylpropylbenzene	.0001	.0001	.0006	.0024	.0052	.0089	.0129	.0171	.0212
tert-butylbenzene	.0000	.0000	.0000	.0001	.0002	.0003	.0004	.0005	.0006
C11H16									
pentamethylbenzene	.4482	.4419	.2123	.1182	.0757	.0538	.0411	.0330	.0276
1-ethyl-2,3,4-trimethylbenzene	.0317	.0321	.0446	.0465	.0452	.0432	.0413	.0395	.0380
1-ethyl-2,3,5-trimethylbenzene	.1864	.1876	.2003	.1727	.1449	.1230	.1066	.0940	.0842
1-ethyl-2,3,6-trimethylbenzene	.0317	.0321	.0446	.0465	.0452	.0432	.0413	.0395	.0380
1-ethyl-2,4,6-trimethylbenzene	.0932	.0938	.1002	.0864	.0724	.0615	.0533	.0470	.0421
1-ethyl-3,4,5-trimethylbenzene	.0932	.0938	.1002	.0864	.0724	.0615	.0533	.0470	.0421
1,2-diethyl-3-methylbenzene	.0011	.0012	.0047	.0092	.0135	.0173	.0207	.0237	.0262
1,2-diethyl-4-methylbenzene	.0066	.0068	.0210	.0340	.0432	.0494	.0535	.0562	.0581
1,3-diethyl-2-methylbenzene	.0006	.0006	.0023	.0046	.0067	.0087	.0104	.0118	.0131
1,3-diethyl-4-methylbenzene	.0066	.0068	.0210	.0340	.0432	.0494	.0535	.0562	.0581
1,3-diethyl-5-methylbenzene	.0194	.0199	.0472	.0631	.0693	.0703	.0691	.0668	.0643
1,4-diethyl-2-methylbenzene	.0066	.0068	.0210	.0340	.0432	.0494	.0535	.0562	.0581
1-propyl-2,3-dimethylbenzene	.0013	.0014	.0053	.0099	.0141	.0175	.0204	.0227	.0246
1-propyl-2,4-dimethylbenzene	.0077	.0080	.0237	.0368	.0451	.0500	.0526	.0539	.0543
1-propyl-2,5-dimethylbenzene	.0077	.0080	.0237	.0368	.0451	.0500	.0526	.0539	.0543
1-propyl-2,6-dimethylbenzene	.0007	.0007	.0026	.0050	.0070	.0088	.0102	.0113	.0123
1-isopropyl-2,3-dimethylbenzene	.0035	.0036	.0078	.0103	.0116	.0122	.0125	.0127	.0127
1-isopropyl-2,4-dimethylbenzene	.0209	.0213	.0351	.0384	.0372	.0348	.0324	.0301	.0282
1-isopropyl-2,5-dimethylbenzene	.0209	.0213	.0351	.0384	.0372	.0348	.0324	.0301	.0282
1-isopropyl-2,6-dimethylbenzene	.0018	.0018	.0039	.0052	.0058	.0061	.0063	.0063	.0064
1-butyl-2-dimethylbenzene	.0001	.0001	.0006	.0021	.0044	.0071	.0100	.0130	.0158
1-butyl-3-dimethylbenzene	.0003	.0003	.0028	.0078	.0141	.0203	.0259	.0309	.0351
1-butyl-4-dimethylbenzene	.0002	.0002	.0014	.0039	.0070	.0101	.0130	.0154	.0175
1-(1(RS)-methylpropyl)-2-methylbenzene	.0003	.0003	.0018	.0044	.0072	.0099	.0124	.0145	.0165
1-(1(RS)-methylpropyl)-3-methylbenzene	.0017	.0018	.0083	.0164	.0232	.0283	.0319	.0345	.0364
1-(1(RS)-methylpropyl)-4-methylbenzene	.0009	.0009	.0042	.0082	.0116	.0141	.0160	.0173	.0182
1-tert-butyl-2-methylbenzene	.0001	.0001	.0002	.0004	.0005	.0006	.0007	.0008	.0009
1-tert-butyl-3-methylbenzene	.0004	.0004	.0011	.0015	.0017	.0018	.0019	.0019	.0020
1-tert-butyl-4-methylbenzene	.0002	.0002	.0005	.0008	.0009	.0009	.0010	.0010	.0010
1-isobutyl-2-methylbenzene	.0006	.0006	.0027	.0052	.0074	.0091	.0105	.0117	.0126
1-isobutyl-3-methylbenzene	.0036	.0038	.0121	.0192	.0236	.0260	.0272	.0277	.0279
1-isobutyl-4-methylbenzene	.0018	.0019	.0060	.0096	.0118	.0130	.0136	.0139	.0139
pentylbenzene	.0000	.0000	.0000	.0002	.0007	.0014	.0025	.0037	.0051
isopentylbenzene	.0000	.0000	.0002	.0006	.0011	.0019	.0026	.0033	.0041
2(RS)-methylbutylbenzene	.0000	.0000	.0003	.0011	.0023	.0037	.0052	.0067	.0081
1(RS)-methylbutylbenzene	.0000	.0000	.0001	.0005	.0011	.0020	.0030	.0042	.0053
1(RS),2-dimethylpropylbenzene	.0001	.0001	.0005	.0012	.0019	.0026	.0032	.0037	.0042
tert-pentylbenzene	.0000	.0000	.0000	.0001	.0003	.0004	.0005	.0007	.0009
1-ethylpropylbenzene	.0000	.0000	.0001	.0002	.0006	.0010	.0015	.0021	.0027
neopentylbenzene	.0001	.0001	.0002	.0004	.0006	.0007	.0008	.0008	.0009
C12H18									
hexamethylbenzene	.0424	.0411	.0116	.0054	.0033	.0023	.0018	.0015	.0012
1-ethyl-2,3,4,5-tetramethylbenzene	.1058	.1048	.0656	.0473	.0375	.0316	.0277	.0249	.0228
1-ethyl-2,3,4,6-tetramethylbenzene	.1058	.1048	.0656	.0473	.0375	.0316	.0277	.0249	.0228
1-ethyl-2,3,5,6-tetramethylbenzene	.0529	.0524	.0328	.0236	.0187	.0158	.0138	.0124	.0114
1,2-diethyl-3,4-dimethylbenzene	.0037	.0038	.0069	.0093	.0112	.0127	.0139	.0149	.0157
1,2-diethyl-3,5-dimethylbenzene	.1294	.1301	.1390	.1283	.1150	.1029	.0926	.0841	.0770
1,2-diethyl-3,6-dimethylbenzene	.0019	.0019	.0034	.0047	.0056	.0063	.0069	.0074	.0079
1,2-diethyl-4,5-dimethylbenzene	.0110	.0111	.0155	.0173	.0179	.0181	.0179	.0177	.0174
1,3-diethyl-2,4-dimethylbenzene	.0037	.0038	.0069	.0093	.0112	.0127	.0139	.0149	.0157
1,3-diethyl-2,5-dimethylbenzene	.0220	.0222	.0309	.0345	.0358	.0361	.0359	.0354	.0348
1,3-diethyl-4,5-dimethylbenzene	.0220	.0222	.0309	.0345	.0358	.0361	.0359	.0354	.0348
1,3-diethyl-4,6-dimethylbenzene	.0110	.0111	.0155	.0173	.0179	.0181	.0179	.0177	.0174
1,4-diethyl-2,3-dimethylbenzene	.0019	.0019	.0034	.0047	.0056	.0063	.0069	.0074	.0079
1,4-diethyl-2,6-dimethylbenzene	.0110	.0111	.0155	.0173	.0179	.0181	.0179	.0177	.0174
1,4-diethyl-2,5-dimethylbenzene	.0220	.0222	.0309	.0345	.0358	.0361	.0359	.0354	.0348
1-propyl-2,3,4-trimethylbenzene	.0044	.0045	.0078	.0101	.0117	.0128	.0137	.0143	.0147
1-propyl-2,3,5-trimethylbenzene	.0258	.0260	.0348	.0374	.0375	.0365	.0353	.0339	.0325
1-propyl-2,3,6-trimethylbenzene	.0044	.0045	.0078	.0101	.0117	.0128	.0137	.0143	.0147
1-propyl-2,4,5-trimethylbenzene	.0258	.0260	.0348	.0374	.0375	.0365	.0353	.0339	.0325
1-propyl-2,4,6-trimethylbenzene	.0129	.0130	.0174	.0187	.0187	.0183	.0176	.0169	.0163
1-propyl-3,4,5-trimethylbenzene	.0129	.0130	.0174	.0187	.0187	.0183	.0176	.0169	.0163
1-isopropyl-2,3,4-trimethylbenzene	.0119	.0119	.0115	.0105	.0096	.0089	.0084	.0080	.0076
1-isopropyl-2,3,5-trimethylbenzene	.0698	.0695	.0517	.0390	.0309	.0255	.0217	.0190	.0169
1-isopropyl-2,3,6-trimethylbenzene	.0119	.0119	.0115	.0105	.0096	.0089	.0084	.0080	.0076
1-isopropyl-2,4,5-trimethylbenzene	.0698	.0695	.0517	.0390	.0309	.0255	.0217	.0190	.0169
1-isopropyl-2,4,6-trimethylbenzene	.0349	.0347	.0259	.0195	.0154	.0127	.0109	.0095	.0084
1-isopropyl-3,4,5-trimethylbenzene	.0349	.0347	.0259	.0195	.0154	.0127	.0109	.0095	.0084
1-butyl-2,3-dimethylbenzene	.0002	.0002	.0009	.0021	.0036	.0052	.0067	.0082	.0095
1-butyl-2,4-dimethylbenzene	.0011	.0011	.0041	.0080	.0117	.0148	.0174	.0194	.0210
1-butyl-2,5-dimethylbenzene	.0011	.0011	.0041	.0080	.0117	.0148	.0174	.0194	.0210
1-butyl-2,6-dimethylbenzene	.0001	.0001	.0005	.0011	.0018	.0026	.0034	.0041	.0047
1-butyl-3,4-dimethylbenzene	.0011	.0011	.0041	.0080	.0117	.0148	.0174	.0194	.0210
1-butyl-3,5-dimethylbenzene	.0031	.0032	.0092	.0148	.0187	.0211	.0225	.0231	.0232
1-(1(RS)-methylpropyl)-2,3-dimethylbenzene	.0010	.0010	.0027	.0045	.0060	.0073	.0083	.0091	.0099
1-(1(RS)-methylpropyl)-2,4-dimethylbenzene	.0058	.0059	.0122	.0166	.0192	.0207	.0214	.0217	.0218
1-(1(RS)-methylpropyl)-2,5-dimethylbenzene	.0058	.0059	.0122	.0166	.0192	.0207	.0214	.0217	.0218
1-(1(RS)-methylpropyl)-2,6-dimethylbenzene	.0005	.0005	.0014	.0022	.0030	.0036	.0041	.0046	.0049
1-(1(RS)-methylpropyl)-3,4-dimethylbenzene	.0058	.0059	.0122	.0166	.0192	.0207	.0214	.0217	.0218
1-(1(RS)-methylpropyl)-3,5-dimethylbenzene	.0170	.0173	.0274	.0309	.0308	.0295	.0277	.0258	.0241

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

T/K	298.15	300	400	500	600	700	800	900	1000
1-isobutyl-2,3-dimethylbenzene	.0021	.0021	.0040	.0053	.0061	.0067	.0071	.0073	.0075
1-isobutyl-2,4-dimethylbenzene	.0121	.0123	.0178	.0195	.0196	.0190	.0183	.0175	.0167
1-isobutyl-2,5-dimethylbenzene	.0121	.0123	.0178	.0195	.0196	.0190	.0183	.0175	.0167
1-isobutyl-2,6-dimethylbenzene	.0010	.0010	.0020	.0026	.0031	.0033	.0035	.0037	.0038
1-isobutyl-3,4-dimethylbenzene	.0121	.0123	.0178	.0195	.0196	.0190	.0183	.0175	.0167
1-isobutyl-3,5-dimethylbenzene	.0357	.0359	.0400	.0363	.0314	.0271	.0236	.0207	.0185
1-tert-butyl-2,3-dimethylbenzene	.0002	.0002	.0004	.0004	.0004	.0005	.0005	.0005	.0005
1-tert-butyl-2,4-dimethylbenzene	.0014	.0014	.0016	.0015	.0014	.0013	.0013	.0012	.0012
1-tert-butyl-2,5-dimethylbenzene	.0014	.0014	.0016	.0015	.0014	.0013	.0013	.0012	.0012
1-tert-butyl-2,6-dimethylbenzene	.0001	.0001	.0002	.0002	.0002	.0002	.0002	.0003	.0003
1-tert-butyl-3,4-dimethylbenzene	.0014	.0014	.0016	.0015	.0014	.0013	.0013	.0012	.0012
1-tert-butyl-3,5-dimethylbenzene	.0041	.0041	.0036	.0028	.0023	.0019	.0016	.0014	.0013
1-pentyl-2-methylbenzene	.0000	.0000	.0001	.0005	.0011	.0021	.0033	.0047	.0061
1-pentyl-3-methylbenzene	.0000	.0000	.0005	.0017	.0036	.0060	.0086	.0111	.0136
1-pentyl-4-methylbenzene	.0000	.0000	.0002	.0008	.0018	.0030	.0043	.0056	.0068
1-(1(RS)-methylbutyl)-2-methylbenzene	.0000	.0000	.0003	.0010	.0019	.0029	.0041	.0052	.0064
1-(1(RS)-methylbutyl)-3-methylbenzene	.0002	.0003	.0014	.0035	.0060	.0084	.0106	.0125	.0141
1-(1(RS)-methylbutyl)-4-methylbenzene	.0001	.0001	.0007	.0018	.0030	.0042	.0053	.0062	.0070
1-(1-ethylpropyl)-2-methylbenzene	.0000	.0000	.0002	.0005	.0009	.0015	.0020	.0026	.0032
1-(1-ethylpropyl)-3-methylbenzene	.0001	.0001	.0007	.0018	.0030	.0042	.0053	.0062	.0070
1-(1-ethylpropyl)-4-methylbenzene	.0001	.0001	.0004	.0009	.0015	.0021	.0026	.0031	.0035
1-(3-methylbutyl)-2-methylbenzene	.0001	.0001	.0005	.0011	.0019	.0027	.0035	.0042	.0049
1-(3-methylbutyl)-3-methylbenzene	.0005	.0005	.0021	.0042	.0061	.0077	.0090	.0100	.0108
1-(3-methylbutyl)-4-methylbenzene	.0003	.0003	.0011	.0021	.0031	.0039	.0045	.0050	.0054
1-(2(RS)-methylbutyl)-2-methylbenzene	.0002	.0002	.0009	.0022	.0038	.0054	.0070	.0084	.0097
1-(2(RS)-methylbutyl)-3-methylbenzene	.0010	.0010	.0042	.0083	.0122	.0155	.0180	.0200	.0216
1-(2(RS)-methylbutyl)-4-methylbenzene	.0005	.0005	.0021	.0042	.0061	.0077	.0090	.0100	.0108
1-(2,2-dimethylpropyl)-2-methylbenzene	.0000	.0000	.0001	.0003	.0004	.0006	.0007	.0009	.0010
1-(2,2-dimethylpropyl)-3-methylbenzene	.0002	.0002	.0006	.0010	.0013	.0016	.0019	.0021	.0023
1-(2,2-dimethylpropyl)-4-methylbenzene	.0001	.0001	.0003	.0005	.0007	.0008	.0009	.0010	.0011
1-(1(RS),2-dimethylpropyl)-2-methylbenzene	.0005	.0005	.0014	.0023	.0031	.0038	.0043	.0047	.0051
1-(1(RS),2-dimethylpropyl)-3-methylbenzene	.0027	.0028	.0062	.0087	.0101	.0108	.0111	.0112	.0112
1-(1(RS),2-dimethylpropyl)-4-methylbenzene	.0014	.0014	.0031	.0043	.0050	.0054	.0055	.0056	.0056
hexylbenzene	.0000	.0000	.0000	.0000	.0001	.0002	.0004	.0007	.0010
1(RS)-methylpentylbenzene	.0000	.0000	.0000	.0001	.0003	.0006	.0010	.0015	.0021
2(RS)-methylpentylbenzene	.0000	.0000	.0001	.0002	.0006	.0011	.0017	.0024	.0031
3(RS)-methylpentylbenzene	.0000	.0000	.0001	.0002	.0006	.0011	.0017	.0024	.0031
4-methylpentylbenzene	.0000	.0000	.0000	.0001	.0003	.0006	.0009	.0012	.0016
1(RS),2(RS)-dimethylbutylbenzene	.0000	.0000	.0001	.0002	.0005	.0008	.0011	.0013	.0016
1(RS),2(SR)-dimethylbutylbenzene	.0000	.0000	.0001	.0002	.0005	.0008	.0011	.0013	.0016
1(RS),3-dimethylbutylbenzene	.0000	.0000	.0001	.0002	.0005	.0008	.0011	.0013	.0016
2(RS),3-dimethylbutylbenzene	.0000	.0000	.0002	.0006	.0010	.0014	.0018	.0022	.0025
1,1-dimethylbutylbenzene	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0003
2,2-dimethylbutylbenzene	.0000	.0000	.0001	.0003	.0004	.0006	.0008	.0009	.0011
3,3-dimethylbutylbenzene	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0003	.0004
1(RS)-methyl-2,2-dimethylpropylbenzene	.0000	.0000	.0001	.0002	.0002	.0003	.0003	.0003	.0004
1-ethyl-1-methylpropylbenzene	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0003
1,1,2-trimethylpropylbenzene	.0000	.0000	.0000	.0001	.0001	.0001	.0002	.0002	.0003

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

T/K	298.15	300	400	500	600	700	800	900	1000
benzene	81.67	82.22	111.88	137.24	157.90	174.68	188.53	200.12	209.87
toluene	103.64	104.35	140.08	171.46	197.48	218.95	236.86	252.00	264.93
C8H10									
ethylbenzene	128.41	129.20	170.54	206.48	236.14	260.58	280.96	298.19	312.84
1,3-dimethylbenzene	127.57	128.28	167.49	202.63	232.25	257.02	277.86	295.52	310.58
1,2-dimethylbenzene	133.26	133.97	171.67	205.48	234.22	258.40	278.82	296.23	311.08
1,4-dimethylbenzene	126.86	127.57	166.10	201.08	230.79	255.73	276.73	294.51	309.70
C9H12									
propylbenzene	152.34	153.22	200.08	241.21	275.56	303.88	327.61	347.69	364.68
isopropylbenzene	151.71	152.59	200.83	242.25	276.98	305.01	328.86	348.53	365.26
1-ethyl-3-methylbenzene	152.21	153.09	198.74	239.32	273.63	301.67	325.52	346.02	363.17
1-ethyl-2-methylbenzene	157.90	158.74	202.92	242.25	275.31	303.34	326.77	346.44	363.59
1-ethyl-4-methylbenzene	151.54	152.38	197.48	238.07	271.96	300.41	324.68	344.76	362.33
1,2,3-trimethylbenzene	154.18	154.98	196.23	234.72	267.78	296.65	320.91	341.41	359.41
1,2,4-trimethylbenzene	154.01	154.77	196.48	235.39	268.99	297.57	321.88	342.54	360.24
1,3,5-trimethylbenzene	150.25	151.04	194.18	233.97	268.11	297.02	321.50	342.29	360.12
C10H14									
butylbenzene	180.5	181.4	227.9	270.4	308.9	340.5	374.1	400.7	423.9
1,3-diethylbenzene	182.2	183.1	229.0	271.0	309.0	343.1	373.2	399.4	421.6
1,2-diethylbenzene	187.5	188.4	234.2	276.0	313.7	347.4	377.2	402.9	424.6
1,4-diethylbenzene	182.2	183.1	229.0	271.0	309.0	343.1	373.2	399.4	421.6
1,2,3,4-tetramethylbenzene	192.7	193.6	237.3	277.4	313.7	346.3	375.2	400.4	421.9
1,2,3,5-tetramethylbenzene	187.4	188.2	232.1	272.4	309.0	341.9	371.2	396.9	418.8
1,2,4,5-tetramethylbenzene	187.4	188.2	232.1	272.4	309.0	341.9	371.2	396.9	418.8
1-ethyl-2,3-dimethylbenzene	190.1	191.0	235.8	276.7	313.7	346.9	376.2	401.6	423.2
1-ethyl-2,4-dimethylbenzene	184.8	185.6	230.6	271.7	309.0	342.5	372.2	398.1	420.2
1-ethyl-2,5-dimethylbenzene	184.8	185.6	230.6	271.7	309.0	342.5	372.2	398.1	420.2
1-ethyl-2,6-dimethylbenzene	190.1	191.0	235.8	276.7	313.7	346.9	376.2	401.6	423.2
1-ethyl-3,4-dimethylbenzene	184.8	185.6	230.6	271.7	309.0	342.5	372.2	398.1	420.2
1-ethyl-3,5-dimethylbenzene	179.4	180.3	225.4	266.7	304.3	338.1	368.2	394.6	417.2
1-propyl-2-methylbenzene	185.3	186.2	231.8	273.5	311.3	345.2	375.1	401.2	423.3
1-propyl-3-methylbenzene	180.0	180.9	226.6	268.5	306.6	340.8	371.1	397.6	420.2
1-propyl-4-methylbenzene	180.0	180.9	226.6	268.5	306.6	340.8	371.1	397.6	420.2
1-isopropyl-2-methylbenzene	184.6	185.5	231.5	273.5	311.6	345.8	375.9	402.1	424.4
1-isopropyl-3-methylbenzene	179.2	180.1	226.3	268.6	306.9	341.4	371.9	398.6	421.3
1-isopropyl-4-methylbenzene	179.2	180.1	226.3	268.6	306.9	341.4	371.9	398.6	421.3
2-methylpropylbenzene	179.8	180.7	227.5	270.4	309.2	344.0	374.8	401.6	424.4
1(RS)-methylpropylbenzene	179.8	180.7	227.6	270.4	309.3	344.1	374.9	401.6	424.4
tert-butylbenzene	182.0	182.9	231.1	275.0	314.6	350.0	381.0	407.8	430.3

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

T/K	298.15	300	400	500	600	700	800	900	1000
C11H16									
pentamethylbenzene	221.0	222.0	270.3	314.5	354.6	390.7	422.6	450.4	474.1
1-ethyl-2,3,4-trimethylbenzene	218.4	219.4	268.7	313.8	354.6	391.2	423.6	451.7	475.5
1-ethyl-2,3,5-trimethylbenzene	213.1	214.0	263.5	308.8	350.0	386.9	419.6	448.1	472.5
1-ethyl-2,3,6-trimethylbenzene	218.4	219.4	268.7	313.8	354.6	391.2	423.6	451.7	475.5
1-ethyl-2,4,6-trimethylbenzene	213.1	214.0	263.5	308.8	350.0	386.9	419.6	448.1	472.5
1-ethyl-3,4,5-trimethylbenzene	213.1	214.0	263.5	308.8	350.0	386.9	419.6	448.1	472.5
1,2-diethyl-3-methylbenzene	215.8	216.8	267.1	313.1	354.7	391.8	424.6	452.9	476.9
1,2-diethyl-4-methylbenzene	210.5	211.4	262.0	308.1	350.0	387.5	420.6	449.4	473.8
1,3-diethyl-2-methylbenzene	215.8	216.8	267.1	313.1	354.7	391.8	424.6	452.9	476.9
1,3-diethyl-4-methylbenzene	210.5	211.4	262.0	308.1	350.0	387.5	420.6	449.4	473.8
1,3-diethyl-5-methylbenzene	205.1	206.1	256.8	303.2	345.3	383.1	416.6	445.9	470.8
1,4-diethyl-2-methylbenzene	210.5	211.4	262.0	308.1	350.0	387.5	420.6	449.4	473.8
1-propyl-2,3-dimethylbenzene	213.6	214.6	264.8	310.7	352.3	389.5	422.5	451.2	475.5
1-propyl-2,4-dimethylbenzene	208.3	209.2	259.6	305.7	347.6	385.2	418.5	447.7	472.5
1-propyl-2,5-dimethylbenzene	208.3	209.2	259.6	305.7	347.6	385.2	418.5	447.7	472.5
1-propyl-2,6-dimethylbenzene	213.6	214.6	264.8	310.7	352.3	389.5	422.5	451.2	475.5
1-isopropyl-2,3-dimethylbenzene	212.9	213.8	264.5	310.7	352.6	390.1	423.3	452.2	476.6
1-isopropyl-2,4-dimethylbenzene	207.5	208.5	259.3	305.7	347.9	385.8	419.3	448.6	473.6
1-isopropyl-2,5-dimethylbenzene	207.5	208.5	259.3	305.7	347.9	385.8	419.3	448.6	473.6
1-isopropyl-2,6-dimethylbenzene	212.9	213.8	264.5	310.7	352.6	390.1	423.3	452.2	476.6
1-butyl-2-dimethylbenzene	208.8	209.8	260.8	307.5	349.9	387.9	421.5	450.7	475.6
1-butyl-3-dimethylbenzene	203.4	204.4	255.7	302.6	345.2	383.5	417.5	447.2	472.6
1-butyl-4-dimethylbenzene	203.4	204.4	255.7	302.6	345.2	383.5	417.5	447.2	472.6
1-(1(RS)-methylpropyl)-2-methylbenzene	208.1	209.1	260.5	307.6	350.2	388.4	422.3	451.7	476.7
1-(1(RS)-methylpropyl)-3-methylbenzene	202.7	203.7	255.3	302.6	345.5	384.1	418.3	448.1	473.6
1-(1(RS)-methylpropyl)-4-methylbenzene	202.7	203.7	255.3	302.6	345.5	384.1	418.3	448.1	473.6
1-tert-butyl-2-methylbenzene	210.3	211.3	264.1	312.2	355.6	394.3	428.4	457.9	482.6
1-tert-butyl-3-methylbenzene	204.9	205.9	258.9	307.2	350.9	390.0	424.5	454.3	479.6
1-tert-butyl-4-methylbenzene	204.9	205.9	258.9	307.2	350.9	390.0	424.5	454.3	479.6
1-isobutyl-2-methylbenzene	208.0	209.0	260.5	307.5	350.2	388.4	422.2	451.6	476.6
1-isobutyl-3-methylbenzene	202.7	203.7	255.3	302.6	345.5	384.0	418.3	448.1	473.6
1-isobutyl-4-methylbenzene	202.7	203.7	255.3	302.6	345.5	384.0	418.3	448.1	473.6
pentylbenzene	204.0	205.0	256.9	304.4	347.5	386.2	420.4	450.2	475.6
isopentylbenzene	203.2	204.2	256.6	304.4	347.8	386.7	421.2	451.2	476.7
2(RS)-methylbutylbenzene	203.2	204.2	256.6	304.4	347.8	386.7	421.2	451.2	476.7
1(RS)-methylbutylbenzene	203.2	204.3	256.6	304.4	347.8	386.8	421.2	451.2	476.7
1(RS),2-dimethylpropylbenzene	202.5	203.5	256.2	304.4	348.1	387.3	422.0	452.1	477.8
tert-pentylbenzene	205.5	206.5	260.1	309.0	353.2	392.7	427.4	457.4	482.6
1-ethylpropylbenzene	203.2	204.3	256.6	304.4	347.8	386.8	421.2	451.2	476.7
neopentylbenzene	206.3	207.3	260.7	309.3	353.3	392.6	427.2	457.1	482.4
C12H18									
hexamethylbenzene	254.7	255.7	308.4	356.6	400.3	439.4	474.0	504.0	529.4
1-ethyl-2,3,4,5-tetramethylbenzene	246.7	247.7	301.7	351.0	395.6	435.6	471.0	501.7	527.8
1-ethyl-2,3,4,6-tetramethylbenzene	246.7	247.7	301.7	351.0	395.6	435.6	471.0	501.7	527.8
1-ethyl-2,3,5,6-tetramethylbenzene	246.7	247.7	301.7	351.0	395.6	435.6	471.0	501.7	527.8
1,2-diethyl-3,4-dimethylbenzene	244.1	245.2	300.1	350.3	395.6	436.2	472.0	502.9	529.1
1,2-diethyl-3,5-dimethylbenzene	233.4	234.4	289.7	340.3	386.2	427.5	464.0	495.9	523.1
1,2-diethyl-3,6-dimethylbenzene	244.1	245.2	300.1	350.3	395.6	436.2	472.0	502.9	529.1
1,2-diethyl-4,5-dimethylbenzene	238.7	239.8	294.9	345.3	390.9	431.8	468.0	499.4	526.1
1,3-diethyl-2,4-dimethylbenzene	244.1	245.2	300.1	350.3	395.6	436.2	472.0	502.9	529.1
1,3-diethyl-2,5-dimethylbenzene	238.7	239.8	294.9	345.3	390.9	431.8	468.0	499.4	526.1
1,3-diethyl-4,5-dimethylbenzene	238.7	239.8	294.9	345.3	390.9	431.8	468.0	499.4	526.1
1,3-diethyl-4,6-dimethylbenzene	238.7	239.8	294.9	345.3	390.9	431.8	468.0	499.4	526.1
1,4-diethyl-2,3-dimethylbenzene	244.1	245.2	300.1	350.3	395.6	436.2	472.0	502.9	529.1
1,4-diethyl-2,6-dimethylbenzene	238.7	239.8	294.9	345.3	390.9	431.8	468.0	499.4	526.1
1,4-diethyl-2,5-dimethylbenzene	238.7	239.8	294.9	345.3	390.9	431.8	468.0	499.4	526.1
1-propyl-2,3,4-trimethylbenzene	241.9	242.9	297.7	347.8	393.2	433.9	469.9	501.2	527.8
1-propyl-2,3,5-trimethylbenzene	236.5	237.6	292.5	342.9	388.5	429.6	465.9	497.7	524.8
1-propyl-2,3,6-trimethylbenzene	241.9	242.9	297.7	347.8	393.2	433.9	469.9	501.2	527.8
1-propyl-2,4,5-trimethylbenzene	236.5	237.6	292.5	342.9	388.5	429.6	465.9	497.7	524.8
1-propyl-2,4,6-trimethylbenzene	236.5	237.6	292.5	342.9	388.5	429.6	465.9	497.7	524.8
1-propyl-3,4,5-trimethylbenzene	236.5	237.6	292.5	342.9	388.5	429.6	465.9	497.7	524.8
1-isopropyl-2,3,4-trimethylbenzene	241.2	242.2	297.4	347.9	393.6	434.5	470.7	502.2	528.9
1-isopropyl-2,3,5-trimethylbenzene	235.8	236.9	292.2	342.9	388.9	430.2	466.7	498.7	525.9
1-isopropyl-2,3,6-trimethylbenzene	241.2	242.2	297.4	347.9	393.6	434.5	470.7	502.2	528.9
1-isopropyl-2,4,5-trimethylbenzene	235.8	236.9	292.2	342.9	388.9	430.2	466.7	498.7	525.9
1-isopropyl-2,4,6-trimethylbenzene	235.8	236.9	292.2	342.9	388.9	430.2	466.7	498.7	525.9
1-isopropyl-3,4,5-trimethylbenzene	235.8	236.9	292.2	342.9	388.9	430.2	466.7	498.7	525.9
1-butyl-2,3-dimethylbenzene	237.1	238.2	293.8	344.7	390.8	432.2	468.9	500.7	527.9
1-butyl-2,4-dimethylbenzene	231.7	232.8	288.6	339.7	386.1	427.9	464.9	497.2	524.8
1-butyl-2,5-dimethylbenzene	231.7	232.8	288.6	339.7	386.1	427.9	464.9	497.2	524.8
1-butyl-2,6-dimethylbenzene	237.1	238.2	293.8	344.7	390.8	432.2	468.9	500.7	527.9
1-butyl-3,4-dimethylbenzene	231.7	232.8	288.6	339.7	386.1	427.9	464.9	497.2	524.8
1-butyl-3,5-dimethylbenzene	226.4	227.4	283.4	334.8	381.4	423.5	460.9	493.7	521.8
1-(1(RS)-methylpropyl)-2,3-dimethylbenzene	236.3	237.4	293.5	344.7	391.2	432.8	469.7	501.7	528.9
1-(1(RS)-methylpropyl)-2,4-dimethylbenzene	231.0	232.1	288.3	339.8	386.5	428.5	465.7	498.2	525.9
1-(1(RS)-methylpropyl)-2,5-dimethylbenzene	231.0	232.1	288.3	339.8	386.5	428.5	465.7	498.2	525.9
1-(1(RS)-methylpropyl)-2,6-dimethylbenzene	236.3	237.4	293.5	344.7	391.2	432.8	469.7	501.7	528.9
1-(1(RS)-methylpropyl)-3,4-dimethylbenzene	231.0	232.1	288.3	339.8	386.5	428.5	465.7	498.2	525.9
1-(1(RS)-methylpropyl)-3,5-dimethylbenzene	225.6	226.7	283.1	334.8	381.8	424.1	461.7	494.6	522.9
1-isobutyl-2,3-dimethylbenzene	236.3	237.4	293.5	344.7	391.1	432.8	469.6	501.7	528.9
1-isobutyl-2,4-dimethylbenzene	231.0	232.1	288.3	339.7	386.4	428.4	465.7	498.1	525.9
1-isobutyl-2,5-dimethylbenzene	231.0	232.1	288.3	339.7	386.4	428.4	465.7	498.1	525.9
1-isobutyl-2,6-dimethylbenzene	236.3	237.4	293.5	344.7	391.1	432.8	469.6	501.7	528.9
1-isobutyl-3,4-dimethylbenzene	231.0	232.1	288.3	339.7	386.4	428.4	465.7	498.1	525.9
1-isobutyl-3,5-dimethylbenzene	225.6	226.7	283.1	334.8	381.7	424.1	461.7	494.6	522.9
1-tert-butyl-2,3-dimethylbenzene	238.5	239.7	297.0	349.3	396.5	438.7	475.8	507.9	534.9
1-tert-butyl-2,4-dimethylbenzene	233.2	234.3	291.8	344.3	391.8	434.4	471.9	504.4	531.8
1-tert-butyl-2,5-dimethylbenzene	233.2	234.3	291.8	344.3	391.8	434.4	471.9	504.4	531.8
1-tert-butyl-2,6-dimethylbenzene	238.5	239.7	297.0	349.3	396.5	438.7	475.8	507.9	534.9
1-tert-butyl-3,4-dimethylbenzene	233.2	234.3	291.8	344.3	391.8	434.4	471.9	504.4	531.8
1-tert-butyl-3,5-dimethylbenzene	227.8	228.9	286.6	339.4	387.2	430.0	467.9	500.8	528.8
1-pentyl-2-methylbenzene	232.3	233.4	289.9	341.6	388.5	430.5	467.8	500.3	527.9
1-pentyl-3-methylbenzene	226.9	228.0	284.7	336.6	383.8	426.2	463.8	496.7	524.9
1-pentyl-4-methylbenzene	226.9	228.0	284.7	336.6	383.8	426.2	463.8	496.7	524.9
1-(1(RS)-methylbutyl)-2-methylbenzene	231.5	232.6	289.5	341.6	388.8	431.1	468.6	501.2	529.0
1-(1(RS)-methylbutyl)-3-methylbenzene	226.2	227.3	284.3	336.6	384.1	426.8	464.6	497.7	526.0

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

T/K	298.15	300	400	500	600	700	800	900	1000
1-(1(RS)-methylbutyl)-4-methylbenzene	226.2	227.3	284.3	336.6	384.1	426.8	464.6	497.7	526.0
1-(1-ethylpropyl)-2-methylbenzene	231.5	232.6	289.5	341.6	388.8	431.1	468.6	501.2	529.0
1-(1-ethylpropyl)-3-methylbenzene	226.2	227.3	284.3	336.6	384.1	426.8	464.6	497.7	526.0
1-(1-ethylpropyl)-4-methylbenzene	226.2	227.3	284.3	336.6	384.1	426.8	464.6	497.7	526.0
1-(3-methylbutyl)-2-methylbenzene	231.5	232.6	289.5	341.6	388.8	431.1	468.6	501.2	529.0
1-(3-methylbutyl)-3-methylbenzene	226.2	227.3	284.3	336.6	384.1	426.7	464.6	497.7	525.9
1-(3-methylbutyl)-4-methylbenzene	226.2	227.3	284.3	336.6	384.1	426.7	464.6	497.7	525.9
1-(2(RS)-methylbutyl)-2-methylbenzene	231.5	232.6	289.5	341.6	388.8	431.1	468.6	501.2	529.0
1-(2(RS)-methylbutyl)-3-methylbenzene	226.2	227.3	284.3	336.6	384.1	426.7	464.6	497.7	525.9
1-(2(RS)-methylbutyl)-4-methylbenzene	226.2	227.3	284.3	336.6	384.1	426.7	464.6	497.7	525.9
1-(2,2-dimethylpropyl)-2-methylbenzene	233.7	234.9	293.1	346.2	394.2	437.0	474.8	507.4	534.9
1-(2,2-dimethylpropyl)-3-methylbenzene	228.4	229.5	287.9	341.2	389.5	432.7	470.8	503.9	531.9
1-(2,2-dimethylpropyl)-4-methylbenzene	228.4	229.5	287.9	341.2	389.5	432.7	470.8	503.9	531.9
1-(1(RS),2-dimethylpropyl)-2-methylbenzene	230.8	231.9	289.2	341.6	389.1	431.7	469.4	502.2	530.0
1-(1(RS),2-dimethylpropyl)-3-methylbenzene	225.4	226.5	284.0	336.6	384.4	427.3	465.4	498.6	527.0
1-(1(RS),2-dimethylpropyl)-4-methylbenzene	225.4	226.5	284.0	336.6	384.4	427.3	465.4	498.6	527.0
hexylbenzene	227.5	228.6	285.9	338.4	386.1	428.9	466.8	499.8	528.0
1(RS)-methylpentylbenzene	226.7	227.8	285.6	338.5	386.4	429.4	467.6	500.8	529.0
2(RS)-methylpentylbenzene	226.7	227.8	285.6	338.4	386.4	429.4	467.5	500.7	529.0
3(RS)-methylpentylbenzene	226.7	227.8	285.6	338.4	386.4	429.4	467.5	500.7	529.0
4-methylpentylbenzene	226.7	227.8	285.6	338.4	386.4	429.4	467.5	500.7	529.0
1(RS),2(RS)-dimethylbutylbenzene	226.0	227.1	285.3	338.5	386.7	430.0	468.3	501.7	530.1
1(RS),2(SR)-dimethylbutylbenzene	226.0	227.1	285.3	338.5	386.7	430.0	468.3	501.7	530.1
1(RS),3-dimethylbutylbenzene	226.0	227.1	285.3	338.5	386.7	430.0	468.3	501.7	530.1
2(RS),3-dimethylbutylbenzene	226.0	227.1	285.2	338.4	386.7	430.0	468.3	501.6	530.0
1,1-dimethylbutylbenzene	228.9	230.1	289.1	343.0	391.8	435.3	473.7	506.9	535.0
2,2-dimethylbutylbenzene	229.7	230.9	289.7	343.4	391.9	435.3	473.6	506.7	534.7
3,3-dimethylbutylbenzene	229.7	230.9	289.7	343.4	391.9	435.3	473.6	506.7	534.7
1(RS)-methyl-2,2-dimethylpropylbenzene	229.0	230.1	289.3	343.4	392.2	435.9	474.4	507.7	535.8
1-ethyl-1-methylpropylbenzene	228.9	230.1	289.1	343.0	391.8	435.3	473.7	506.9	535.0
1,1,2-trimethylpropylbenzene	228.2	229.3	288.8	343.0	392.1	435.9	474.5	507.9	536.0

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

T/K	298.15	300	400	500	600	700	800	900	1000
benzene	269.31	269.85	297.63	325.42	352.32	377.97	402.23	425.12	446.71
toluene	320.77	321.44	356.46	391.19	424.83	456.92	487.34	516.12	543.40
C8H10									
ethylbenzene	360.56	361.40	404.33	446.38	486.71	524.99	561.18	595.28	627.46
1,3-dimethylbenzene	357.80	358.60	400.98	442.23	481.86	519.60	555.28	589.09	621.02
1,2-dimethylbenzene	352.86	353.70	397.51	439.56	479.60	517.59	553.44	587.33	619.34
1,4-dimethylbenzene	352.53	353.32	395.41	436.33	475.66	513.19	548.72	582.40	614.24
C9H12									
propylbenzene	400.77	401.73	452.36	501.56	548.67	593.32	635.49	675.28	712.81
isopropylbenzene	388.68	389.64	440.31	489.68	537.04	581.90	624.24	664.11	701.72
1-ethyl-3-methylbenzene	404.28	405.25	455.66	504.49	551.27	595.58	637.46	677.04	714.40
1-ethyl-2-methylbenzene	399.35	400.35	452.19	501.81	548.97	593.57	635.66	675.28	712.73
1-ethyl-4-methylbenzene	399.01	399.97	450.10	498.63	545.12	589.26	630.97	670.43	707.67
1,2,3-trimethylbenzene	384.95	385.92	436.25	484.24	530.06	573.53	614.78	653.78	690.72
1,2,4-trimethylbenzene	395.87	396.84	447.17	495.29	541.23	584.91	626.25	665.41	702.44
1,3,5-trimethylbenzene	385.41	386.38	435.79	483.53	529.26	572.82	614.11	653.23	690.22
C10H14									
butylbenzene	439.4	440.5	499.2	554.6	607.4	657.7	705.6	751.2	794.6
1,3-diethylbenzene	437.3	438.5	497.5	553.2	606.0	656.3	704.1	749.6	792.8
1,2-diethylbenzene	430.6	431.7	492.3	549.1	602.8	653.8	702.2	748.1	791.7
1,4-diethylbenzene	431.6	432.7	491.7	547.4	600.2	650.5	698.3	743.8	787.1
1,2,3,4-tetramethylbenzene	414.3	415.5	477.3	534.6	588.5	639.3	687.5	733.1	776.5
1,2,3,5-tetramethylbenzene	421.1	422.2	482.5	538.7	591.6	641.8	689.4	734.6	777.6
1,2,4,5-tetramethylbenzene	415.3	416.5	476.7	532.9	585.9	636.0	683.6	728.8	771.8
1-ethyl-2,3-dimethylbenzene	428.2	429.4	490.6	547.6	601.4	652.3	700.6	746.4	789.9
1-ethyl-2,4-dimethylbenzene	435.0	436.1	495.8	551.7	604.6	654.8	702.5	747.9	791.0
1-ethyl-2,5-dimethylbenzene	435.0	436.1	495.8	551.7	604.6	654.8	702.5	747.9	791.0
1-ethyl-2,6-dimethylbenzene	422.5	423.6	484.8	541.9	595.6	646.5	694.8	740.6	784.1
1-ethyl-3,4-dimethylbenzene	435.0	436.1	495.8	551.7	604.6	654.8	702.5	747.9	791.0
1-ethyl-3,5-dimethylbenzene	435.9	437.0	495.2	550.0	602.0	651.5	698.6	743.6	786.3
1-propyl-2-methylbenzene	436.7	437.8	497.7	554.0	607.3	657.9	706.0	751.7	795.1
1-propyl-3-methylbenzene	443.4	444.5	502.9	558.1	610.5	660.3	707.9	753.2	796.2
1-propyl-4-methylbenzene	437.7	438.8	497.2	552.3	604.7	654.6	702.1	747.4	790.5
1-isopropyl-2-methylbenzene	425.5	426.6	486.4	542.6	595.9	646.6	694.7	740.6	784.1
1-isopropyl-3-methylbenzene	432.2	433.3	491.5	546.7	599.1	649.0	696.6	742.0	785.2
1-isopropyl-4-methylbenzene	426.4	427.5	485.8	540.9	593.3	643.3	690.9	736.3	779.5
2-methylpropylbenzene	433.9	435.0	493.5	549.0	601.8	652.1	700.1	745.8	789.4
1(RS)-methylpropylbenzene	439.7	440.8	499.3	554.8	607.5	657.9	705.9	751.6	795.2
tert-butylbenzene	401.4	402.5	461.8	518.2	571.9	623.1	671.9	718.4	762.5
C11H16									
pentamethylbenzene	445.3	446.6	517.2	582.4	643.3	700.7	755.0	806.4	855.2
1-ethyl-2,3,4-trimethylbenzene	459.2	460.5	530.5	595.4	656.3	713.7	768.1	819.7	868.5
1-ethyl-2,3,5-trimethylbenzene	465.9	467.2	535.7	599.4	659.4	716.2	770.0	821.2	869.7
1-ethyl-2,3,6-trimethylbenzene	459.2	460.5	530.5	595.4	656.3	713.7	768.1	819.7	868.5
1-ethyl-2,4,6-trimethylbenzene	460.1	461.5	529.9	593.7	653.7	710.4	764.3	815.4	863.9
1-ethyl-3,4,5-trimethylbenzene	460.1	461.5	529.9	593.7	653.7	710.4	764.3	815.4	863.9
1,2-diethyl-3-methylbenzene	467.3	468.6	538.0	602.6	663.5	721.0	775.5	827.2	876.2
1,2-diethyl-4-methylbenzene	474.0	475.3	543.2	606.7	666.6	723.4	777.4	828.6	877.3
1,3-diethyl-2-methylbenzene	461.5	462.9	532.2	596.9	657.7	715.2	769.7	821.4	870.4
1,3-diethyl-4-methylbenzene	474.0	475.3	543.2	606.7	666.6	723.4	777.4	828.6	877.3
1,3-diethyl-5-methylbenzene	475.0	476.3	542.6	605.0	664.0	720.1	773.5	824.3	872.6
1,4-diethyl-2-methylbenzene	474.0	475.3	543.2	606.7	666.6	723.4	777.4	828.6	877.3
1-propyl-2,3-dimethylbenzene	467.6	469.0	537.7	601.8	662.1	719.3	773.5	825.0	873.8

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

T/K	298.15	300	400	500	600	700	800	900	1000
1-propyl-2,4-dimethylbenzene	474.4	475.7	542.8	605.8	665.3	721.8	775.4	826.4	874.9
1-propyl-2,5-dimethylbenzene	474.4	475.7	542.8	605.8	665.3	721.8	775.4	826.4	874.9
1-propyl-2,6-dimethylbenzene	461.9	463.2	531.9	596.0	656.4	713.5	767.8	819.2	868.1
1-isopropyl-2,3-dimethylbenzene	456.4	457.7	526.3	590.3	650.8	708.0	762.3	813.9	862.8
1-isopropyl-2,4-dimethylbenzene	463.1	464.4	531.5	594.4	653.9	710.5	764.2	815.3	863.9
1-isopropyl-2,5-dimethylbenzene	463.1	464.4	531.5	594.4	653.9	710.5	764.2	815.3	863.9
1-isopropyl-2,6-dimethylbenzene	450.6	452.0	520.5	584.6	645.0	702.2	756.5	808.1	857.0
1-butyl-2-dimethylbenzene	476.1	477.4	544.8	608.1	668.0	724.9	778.9	830.3	879.1
1-butyl-3-dimethylbenzene	482.8	484.1	550.0	612.2	671.2	727.3	780.8	831.7	880.2
1-butyl-4-dimethylbenzene	477.1	478.3	544.3	606.4	665.4	721.6	775.0	826.0	874.4
1-(1(RS)-methylpropyl)-2-methylbenzene	470.6	471.9	539.2	602.5	662.4	719.3	773.4	824.9	873.8
1-(1(RS)-methylpropyl)-3-methylbenzene	477.4	478.6	544.4	606.5	665.6	721.8	775.3	826.4	875.0
1-(1(RS)-methylpropyl)-4-methylbenzene	471.6	472.9	538.6	600.8	659.8	716.0	769.6	820.6	869.2
1-tert-butyl-2-methylbenzene	438.1	439.4	507.5	571.7	632.5	690.3	745.2	797.4	847.0
1-tert-butyl-3-methylbenzene	444.8	446.1	512.7	575.7	635.7	692.7	747.1	798.9	848.1
1-tert-butyl-4-methylbenzene	439.0	440.3	506.9	570.0	629.9	687.0	741.4	793.1	842.3
1-isobutyl-2-methylbenzene	464.9	466.2	533.5	596.7	656.6	713.5	767.7	819.1	868.0
1-isobutyl-3-methylbenzene	471.6	472.9	538.6	600.8	659.8	716.0	769.6	820.6	869.2
1-isobutyl-4-methylbenzene	465.8	467.1	532.9	595.0	654.0	710.2	763.8	814.8	863.4
pentylbenzene	478.8	480.1	546.3	608.8	668.1	724.7	778.5	829.8	878.6
isopentylbenzene	467.6	468.8	534.9	597.3	656.7	713.3	767.3	818.7	867.5
2(RS)-methylbutylbenzene	473.3	474.6	540.6	603.1	662.5	719.1	773.0	824.4	873.3
1(RS)-methylbutylbenzene	473.3	474.6	540.6	603.1	662.5	719.1	773.1	824.4	873.3
1(RS),2-dimethylpropylbenzene	462.1	463.4	529.2	591.7	651.1	707.8	761.8	813.3	862.3
tert-pentylbenzene	449.9	451.2	518.0	581.4	641.7	699.2	754.0	806.1	855.6
1-ethylpropylbenzene	467.6	468.8	534.9	597.3	656.8	713.4	767.3	818.7	867.6
neopentylbenzene	440.8	442.0	509.1	572.6	632.9	690.4	745.1	797.2	846.8
C12H18									
hexamethylbenzene	454.6	456.2	537.1	611.1	680.1	744.8	805.8	863.4	917.8
1-ethyl-2,3,4,5-tetramethylbenzene	490.1	491.6	570.4	643.1	711.1	775.2	835.7	893.0	947.2
1-ethyl-2,3,4,6-tetramethylbenzene	490.1	491.6	570.4	643.1	711.1	775.2	835.7	893.0	947.2
1-ethyl-2,3,5,6-tetramethylbenzene	484.4	485.9	564.7	637.3	705.4	769.4	829.9	887.2	941.5
1,2-diethyl-3,4-dimethylbenzene	498.2	499.8	577.9	650.4	718.3	782.4	843.0	900.5	954.9
1,2-diethyl-3,5-dimethylbenzene	511.7	513.2	588.3	658.5	724.6	787.3	846.9	903.4	957.1
1,2-diethyl-3,6-dimethylbenzene	492.5	494.0	572.2	644.6	712.6	776.6	837.3	894.7	949.1
1,2-diethyl-4,5-dimethylbenzene	499.2	500.7	577.3	648.7	715.7	779.1	839.2	896.2	950.2
1,3-diethyl-2,4-dimethylbenzene	498.2	499.8	577.9	650.4	718.3	782.4	843.0	900.5	954.9
1,3-diethyl-2,5-dimethylbenzene	505.0	506.5	583.1	654.4	721.5	784.9	844.9	901.9	956.0
1,3-diethyl-4,5-dimethylbenzene	505.0	506.5	583.1	654.4	721.5	784.9	844.9	901.9	956.0
1,3-diethyl-4,6-dimethylbenzene	499.2	500.7	577.3	648.7	715.7	779.1	839.2	896.2	950.2
1,4-diethyl-2,3-dimethylbenzene	492.5	494.0	572.2	644.6	712.6	776.6	837.3	894.7	949.1
1,4-diethyl-2,6-dimethylbenzene	499.2	500.7	577.3	648.7	715.7	779.1	839.2	896.2	950.2
1,4-diethyl-2,5-dimethylbenzene	505.0	506.5	583.1	654.4	721.5	784.9	844.9	901.9	956.0
1-propyl-2,3,4-trimethylbenzene	498.6	500.1	577.6	649.5	717.0	780.7	841.1	898.3	952.5
1-propyl-2,3,5-trimethylbenzene	505.3	506.8	582.8	653.5	720.2	783.2	843.0	899.7	953.6
1-propyl-2,3,6-trimethylbenzene	498.6	500.1	577.6	649.5	717.0	780.7	841.1	898.3	952.5
1-propyl-2,4,5-trimethylbenzene	505.3	506.8	582.8	653.5	720.2	783.2	843.0	899.7	953.6
1-propyl-2,4,6-trimethylbenzene	499.6	501.0	577.0	647.8	714.4	777.4	837.2	894.0	947.9
1-propyl-3,4,5-trimethylbenzene	499.6	501.0	577.0	647.8	714.4	777.4	837.2	894.0	947.9
1-isopropyl-2,3,4-trimethylbenzene	487.4	488.8	566.2	638.1	705.6	769.4	829.9	887.2	941.5
1-isopropyl-2,3,5-trimethylbenzene	494.1	495.6	571.4	642.1	708.8	771.9	831.8	888.6	942.6
1-isopropyl-2,3,6-trimethylbenzene	487.4	488.8	566.2	638.1	705.6	769.4	829.9	887.2	941.5
1-isopropyl-2,4,5-trimethylbenzene	494.1	495.6	571.4	642.1	708.8	771.9	831.8	888.6	942.6
1-isopropyl-2,4,6-trimethylbenzene	488.3	489.8	565.6	636.4	703.0	766.1	826.0	882.9	936.8
1-isopropyl-3,4,5-trimethylbenzene	488.3	489.8	565.6	636.4	703.0	766.1	826.0	882.9	936.8
1-butyl-2,3-dimethylbenzene	507.0	508.5	584.8	655.9	722.9	786.3	846.5	903.6	957.8
1-butyl-2,4-dimethylbenzene	513.8	515.2	589.9	659.9	726.0	788.8	848.4	905.0	958.9
1-butyl-2,5-dimethylbenzene	513.8	515.2	589.9	659.9	726.0	788.8	848.4	905.0	958.9
1-butyl-2,6-dimethylbenzene	501.3	502.8	579.0	650.1	717.1	780.5	840.7	897.8	952.0
1-butyl-3,4-dimethylbenzene	513.8	515.2	589.9	659.9	726.0	788.8	848.4	905.0	958.9
1-butyl-3,5-dimethylbenzene	514.8	516.2	589.4	658.2	723.4	785.5	844.5	900.7	954.2
1-(1(RS)-methylpropyl)-2,3-dimethylbenzene	501.6	503.0	579.1	650.2	717.3	780.7	841.0	898.2	952.5
1-(1(RS)-methylpropyl)-2,4-dimethylbenzene	508.3	509.8	584.3	654.3	720.4	783.2	842.9	899.7	953.6
1-(1(RS)-methylpropyl)-2,5-dimethylbenzene	508.3	509.8	584.3	654.3	720.4	783.2	842.9	899.7	953.6
1-(1(RS)-methylpropyl)-2,6-dimethylbenzene	495.8	497.3	573.4	644.5	711.5	775.0	835.2	892.5	946.8
1-(1(RS)-methylpropyl)-3,4-dimethylbenzene	508.3	509.8	584.3	654.3	720.4	783.2	842.9	899.7	953.6
1-(1(RS)-methylpropyl)-3,5-dimethylbenzene	509.3	510.7	583.7	652.6	717.8	779.9	839.0	895.4	949.0
1-isobutyl-2,3-dimethylbenzene	495.8	497.3	573.4	644.4	711.5	775.0	835.2	892.4	946.7
1-isobutyl-2,4-dimethylbenzene	502.6	504.0	578.6	648.5	714.6	777.4	837.1	893.9	947.8
1-isobutyl-2,5-dimethylbenzene	502.6	504.0	578.6	648.5	714.6	777.4	837.1	893.9	947.8
1-isobutyl-2,6-dimethylbenzene	490.1	491.5	567.6	638.7	705.7	769.2	829.4	886.7	941.0
1-isobutyl-3,4-dimethylbenzene	502.6	504.0	578.6	648.5	714.6	777.4	837.1	893.9	947.8
1-isobutyl-3,5-dimethylbenzene	503.5	504.9	578.0	646.8	712.0	774.1	833.3	889.6	943.2
1-tert-butyl-2,3-dimethylbenzene	469.0	470.5	547.4	619.4	687.3	751.7	812.8	870.7	925.7
1-tert-butyl-2,4-dimethylbenzene	475.8	477.2	552.6	623.4	690.5	754.2	814.7	872.2	926.8
1-tert-butyl-2,5-dimethylbenzene	475.8	477.2	552.6	623.4	690.5	754.2	814.7	872.2	926.8
1-tert-butyl-2,6-dimethylbenzene	463.3	464.7	541.7	613.6	681.6	745.9	807.0	864.9	919.9
1-tert-butyl-3,4-dimethylbenzene	475.8	477.2	552.6	623.4	690.5	754.2	814.7	872.2	926.8
1-tert-butyl-3,5-dimethylbenzene	476.7	478.1	552.0	621.7	687.9	750.9	810.8	867.9	922.1
1-pentyl-2-methylbenzene	515.5	517.0	591.9	662.3	728.8	791.9	851.8	908.9	963.0
1-pentyl-3-methylbenzene	522.2	523.7	597.1	666.3	731.9	794.3	853.7	910.3	964.2
1-pentyl-4-methylbenzene	516.5	517.9	591.4	660.5	726.2	788.6	848.0	904.6	958.4
1-(1(RS)-methylbutyl)-2-methylbenzene	510.0	511.5	586.3	656.6	723.1	786.3	846.4	903.5	957.8
1-(1(RS)-methylbutyl)-3-methylbenzene	516.8	518.2	591.5	660.7	726.3	788.8	848.3	905.0	958.9
1-(1(RS)-methylbutyl)-4-methylbenzene	511.0	512.4	585.7	654.9	720.5	783.0	842.5	899.2	953.1
1-(1-ethylpropyl)-2-methylbenzene	504.3	505.7	580.6	650.8	717.4	780.5	840.6	897.7	952.0
1-(1-ethylpropyl)-3-methylbenzene	511.0	512.4	585.7	654.9	720.5	783.0	842.5	899.2	953.1
1-(1-ethylpropyl)-4-methylbenzene	505.3	506.7	580.0	649.1	714.8	777.2	836.8	893.4	947.4
1-(3-methylbutyl)-2-methylbenzene	504.3	505.7	580.5	650.8	717.4	780.5	840.6	897.7	952.0
1-(3-methylbutyl)-3-methylbenzene	511.0	512.4	585.7	654.9	720.5	783.0	842.5	899.2	953.1
1-(3-methylbutyl)-4-methylbenzene	505.3	506.7	580.0	649.1	714.8	777.2	836.7	893.4	947.3
1-(2(RS)-methylbutyl)-2-methylbenzene	510.0	511.5	586.3	656.6	723.1	786.3	846.4	903.5	957.8
1-(2(RS)-methylbutyl)-3-methylbenzene	516.8	518.2	591.5	660.6	726.3	788.8	848.3	904.9	958.9
1-(2(RS)-methylbutyl)-4-methylbenzene	511.0	512.4	585.7	654.9	720.5	783.0	842.5	899.2	953.1
1-(2,2-dimethylpropyl)-2-methylbenzene	486.6	488.1	563.7	634.9	702.4	766.4	827.3	885.1	940.1
1-(2,2-dimethylpropyl)-3-methylbenzene	493.4	494.8	568.9	639.0	705.5	768.9	829.2	886.6	941.2
1-(2,2-dimethylpropyl)-4-methylbenzene	487.6	489.0	563.1	633.2	699.8	763.1	823.4	880.8	935.4
1-(1(RS),2-dimethylpropyl)-2-methylbenzene	498.8	500.3	574.9	645.2	711.7	775.0	835.1	892.4	946.7

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

T/K	298.15	300	400	500	600	700	800	900	1000
1-(1(RS),2-dimethylpropyl)-3-methylbenzene	505.6	507.0	580.1	649.2	714.9	777.4	837.0	893.8	947.9
1-(1(RS),2-dimethylpropyl)-4-methylbenzene	499.8	501.2	574.3	643.5	709.1	771.7	831.3	888.1	942.1
hexylbenzene	512.4	513.9	587.6	657.1	723.1	785.9	845.7	902.6	956.8
1(RS)-methylpentylbenzene	512.7	514.2	587.7	657.2	723.3	786.1	846.0	903.0	957.3
2(RS)-methylpentylbenzene	512.7	514.2	587.7	657.2	723.2	786.1	846.0	903.0	957.3
3(RS)-methylpentylbenzene	512.7	514.2	587.7	657.2	723.2	786.1	846.0	903.0	957.3
4-methylpentylbenzene	507.0	508.4	582.0	651.5	717.5	780.3	840.2	897.2	951.5
1(RS),2(RS)-dimethylbutylbenzene	501.5	502.9	576.3	645.8	711.8	774.8	834.8	891.9	946.3
1(RS),2(SR)-dimethylbutylbenzene	501.5	502.9	576.3	645.8	711.8	774.8	834.8	891.9	946.3
1(RS),3-dimethylbutylbenzene	501.5	502.9	576.3	645.8	711.8	774.8	834.8	891.9	946.3
2(RS),3-dimethylbutylbenzene	501.5	502.9	576.3	645.8	711.8	774.8	834.7	891.9	946.2
1,1-dimethylbutylbenzene	489.3	490.7	565.1	635.5	702.5	766.2	826.9	884.7	939.6
2,2-dimethylbutylbenzene	489.3	490.7	565.3	635.8	702.8	766.5	827.2	885.0	939.8
3,3-dimethylbutylbenzene	480.2	481.6	556.2	626.7	693.7	757.4	818.1	875.8	930.7
1(RS)-methyl-2,2-dimethylpropylbenzene	474.7	476.1	550.6	621.0	688.0	751.9	812.6	870.5	925.5
1-ethyl-1-methylpropylbenzene	489.3	490.7	565.1	635.5	702.5	766.2	826.9	884.7	939.6
1,1,2-trimethylpropylbenzene	478.1	479.5	553.7	624.1	691.1	754.9	815.6	873.5	928.5

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

T/K	298.15	300	400	500	600	700	800	900	1000
benzene	82.93	82.80	77.66	73.39	69.91	67.11	64.89	63.18	62.01
toluene	50.00	49.87	43.26	37.87	33.56	30.29	27.82	26.11	25.15
C8H10									
ethylbenzene	29.79	29.62	21.88	15.52	10.38	6.40	3.35	1.13	-.21
1,3-dimethylbenzene	17.24	17.07	9.12	2.38	-3.14	-7.49	-10.88	-13.35	-14.98
1,2-dimethylbenzene	19.00	18.83	11.38	4.98	-.29	-4.48	-7.74	-10.17	-11.67
1,4-dimethylbenzene	17.95	17.78	9.71	2.85	-2.80	-7.32	-10.84	-13.43	-15.10
C9H12									
propylbenzene	7.82	7.61	-1.38	-8.79	-14.69	-19.25	-22.68	-25.10	-26.48
isopropylbenzene	3.93	3.72	-5.27	-12.55	-18.37	-22.76	-26.11	-28.41	-29.71
1-ethyl-3-methylbenzene	-1.92	-2.13	-11.21	-18.79	-24.89	-29.62	-33.30	-35.90	-37.45
1-ethyl-2-methylbenzene	1.21	1.05	-7.57	-14.77	-20.67	-25.23	-28.74	-31.30	-32.80
1-ethyl-4-methylbenzene	-3.26	-3.47	-12.64	-20.33	-26.61	-31.51	-35.27	-37.95	-39.62
1,2,3-trimethylbenzene	-9.58	-9.79	-18.91	-26.86	-33.47	-38.79	-42.93	-45.98	-47.95
1,2,4-trimethylbenzene	-13.93	-14.14	-23.26	-31.13	-37.70	-42.89	-46.90	-49.87	-51.76
1,3,5-trimethylbenzene	-16.07	-16.28	-25.69	-33.76	-40.42	-45.69	-49.79	-52.76	-54.64
C10H14									
butylbenzene	-12.2	-12.4	-22.4	-31.2	-38.5	-44.1	-48.1	-50.5	-51.5
1,3-diethylbenzene	-24.7	-24.9	-34.8	-43.5	-50.7	-56.4	-60.4	-63.0	-64.1
1,2-diethylbenzene	-22.3	-22.5	-31.9	-40.1	-46.8	-52.0	-55.7	-57.8	-58.7
1,4-diethylbenzene	-24.7	-24.9	-34.8	-43.5	-50.7	-56.4	-60.4	-63.0	-64.1
1,2,3,4-tetramethylbenzene	-43.7	-43.9	-52.9	-60.8	-67.5	-72.8	-76.6	-79.0	-80.1
1,2,3,5-tetramethylbenzene	-46.1	-46.3	-55.8	-64.3	-71.5	-77.2	-81.4	-84.1	-85.6
1,2,4,5-tetramethylbenzene	-46.1	-46.3	-55.8	-64.3	-71.5	-77.2	-81.4	-84.1	-85.6
1-ethyl-2,3-dimethylbenzene	-33.0	-33.2	-42.4	-50.5	-57.2	-62.4	-66.1	-68.4	-69.4
1-ethyl-2,4-dimethylbenzene	-35.4	-35.6	-45.3	-53.9	-61.1	-66.8	-70.9	-73.6	-74.9
1-ethyl-2,5-dimethylbenzene	-35.4	-35.6	-45.3	-53.9	-61.1	-66.8	-70.9	-73.6	-74.9
1-ethyl-2,6-dimethylbenzene	-33.0	-33.2	-42.4	-50.5	-57.2	-62.4	-66.1	-68.4	-69.4
1-ethyl-3,4-dimethylbenzene	-35.4	-35.6	-45.3	-53.9	-61.1	-66.8	-70.9	-73.6	-74.9
1-ethyl-3,5-dimethylbenzene	-37.8	-38.0	-48.2	-57.3	-65.0	-71.2	-75.7	-78.7	-80.3
1-propyl-2-methylbenzene	-22.6	-22.8	-32.4	-40.8	-47.8	-53.3	-57.1	-59.5	-60.5
1-propyl-3-methylbenzene	-25.0	-25.2	-35.3	-44.3	-51.8	-57.6	-61.9	-64.6	-65.9
1-propyl-4-methylbenzene	-25.0	-25.2	-35.3	-44.3	-51.8	-57.6	-61.9	-64.6	-65.9
1-isopropyl-2-methylbenzene	-28.4	-28.6	-38.3	-46.7	-53.7	-59.1	-62.9	-65.1	-66.0
1-isopropyl-3-methylbenzene	-30.8	-31.0	-41.2	-50.2	-57.6	-63.5	-67.6	-70.3	-71.5
1-isopropyl-4-methylbenzene	-30.8	-31.0	-41.2	-50.2	-57.6	-63.5	-67.6	-70.3	-71.5
2-methylpropylbenzene	21.5	21.8	31.9	40.7	47.9	53.5	57.4	59.8	60.7
1(RS)-methylpropylbenzene	-18.0	-18.2	-28.3	-37.1	-44.4	-50.0	-53.9	-56.2	-57.1
tert-butylbenzene	-24.2	-24.4	-34.2	-42.6	-49.3	-54.4	-57.7	-59.4	-59.7
C11H16									
pentamethylbenzene	-74.8	-75.0	-84.8	-93.5	-100.8	-106.5	-110.6	-113.1	-114.2
1-ethyl-2,3,4-trimethylbenzene	-64.1	-64.3	-74.3	-83.1	-90.4	-96.1	-100.1	-102.5	-103.5
1-ethyl-2,3,5-trimethylbenzene	-66.4	-66.7	-77.2	-86.5	-94.4	-100.5	-104.9	-107.7	-109.0
1-ethyl-2,3,6-trimethylbenzene	-64.1	-64.3	-74.3	-83.1	-90.4	-96.1	-100.1	-102.5	-103.5
1-ethyl-2,4,6-trimethylbenzene	-66.4	-66.7	-77.2	-86.5	-94.4	-100.5	-104.9	-107.7	-109.0
1-ethyl-3,4,5-trimethylbenzene	-66.4	-66.7	-77.2	-86.5	-94.4	-100.5	-104.9	-107.7	-109.0
1,2-diethyl-3-methylbenzene	-53.3	-53.6	-63.8	-72.7	-80.1	-85.7	-89.6	-91.9	-92.8
1,2-diethyl-4-methylbenzene	-55.7	-56.0	-66.7	-76.2	-84.0	-90.1	-94.4	-97.1	-98.3
1,3-diethyl-2-methylbenzene	-53.3	-53.6	-63.8	-72.7	-80.1	-85.7	-89.6	-91.9	-92.8
1,3-diethyl-4-methylbenzene	-55.7	-56.0	-66.7	-76.2	-84.0	-90.1	-94.4	-97.1	-98.3
1,3-diethyl-5-methylbenzene	-58.1	-58.4	-69.6	-79.6	-87.9	-94.5	-99.2	-102.3	-103.8
1,4-diethyl-2-methylbenzene	-55.7	-56.0	-66.7	-76.2	-84.0	-90.1	-94.4	-97.1	-98.3
1-propyl-2,3-dimethylbenzene	-53.6	-53.9	-64.3	-73.5	-81.1	-87.0	-91.1	-93.6	-94.6
1-propyl-2,4-dimethylbenzene	-56.0	-56.3	-67.2	-76.9	-85.0	-91.3	-95.9	-98.7	-100.1
1-propyl-2,5-dimethylbenzene	-56.0	-56.3	-67.2	-76.9	-85.0	-91.3	-95.9	-98.7	-100.1
1-propyl-2,6-dimethylbenzene	-53.6	-53.9	-64.3	-73.5	-81.1	-87.0	-91.1	-93.6	-94.6
1-isopropyl-2,3-dimethylbenzene	-59.5	-59.7	-70.2	-79.4	-87.0	-92.8	-96.8	-99.2	-100.1
1-isopropyl-2,4-dimethylbenzene	-61.8	-62.1	-73.1	-82.8	-90.9	-97.2	-101.6	-104.4	-105.6
1-isopropyl-2,5-dimethylbenzene	-61.8	-62.1	-73.1	-82.8	-90.9	-97.2	-101.6	-104.4	-105.6
1-isopropyl-2,6-dimethylbenzene	-59.5	-59.7	-70.2	-79.4	-87.0	-92.8	-96.8	-99.2	-100.1
1-butyl-2-dimethylbenzene	-43.2	-43.5	-54.3	-63.9	-71.7	-77.8	-82.1	-84.7	-85.7
1-butyl-3-dimethylbenzene	-45.6	-45.8	-57.3	-67.3	-75.7	-82.2	-86.9	-89.8	-91.2
1-butyl-4-dimethylbenzene	-45.6	-45.8	-57.3	-67.3	-75.7	-82.2	-86.9	-89.8	-91.2
1-(1(RS)-methylpropyl)-2-methylbenzene	-49.0	-49.3	-60.2	-69.8	-77.6	-83.7	-87.8	-90.3	-91.2
1-(1(RS)-methylpropyl)-3-methylbenzene	-51.4	-51.7	-63.1	-73.2	-81.5	-88.0	-92.6	-95.5	-96.7
1-(1(RS)-methylpropyl)-4-methylbenzene	-51.4	-51.7	-63.1	-73.2	-81.5	-88.0	-92.6	-95.5	-96.7
1-tert-butyl-2-methylbenzene	-55.2	-55.5	-66.1	-75.2	-82.6	-88.1	-91.7	-93.5	-93.8
1-tert-butyl-3-methylbenzene	-57.6	-57.9	-69.0	-78.7	-86.5	-92.5	-96.4	-98.7	-99.3
1-tert-butyl-4-methylbenzene	-57.6	-57.9	-69.0	-78.7	-86.5	-92.5	-96.4	-98.7	-99.3

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

T/K	298.15	300	400	500	600	700	800	900	1000
1-isobutyl-2-methylbenzene	-52.6	-52.8	-63.8	-73.3	-81.2	-87.2	-91.4	-93.9	-94.8
1-isobutyl-3-methylbenzene	-55.0	-55.2	-66.7	-76.8	-85.1	-91.6	-96.2	-99.1	-100.3
1-isobutyl-4-methylbenzene	-55.0	-55.2	-66.7	-76.8	-85.1	-91.6	-96.2	-99.1	-100.3
pentylbenzene	-32.8	-33.0	-44.4	-54.3	-62.4	-68.7	-73.1	-75.7	-76.8
isopentylbenzene	-42.2	-42.4	-53.8	-63.7	-71.8	-78.1	-82.4	-85.0	-85.9
2(RS)-methylbutylbenzene	-42.2	-42.4	-53.8	-63.7	-71.8	-78.1	-82.4	-85.0	-85.9
1(RS)-methylbutylbenzene	-38.6	-38.9	-50.2	-60.1	-68.3	-74.5	-78.8	-81.4	-82.3
1(RS),2-dimethylpropylbenzene	-48.0	-48.2	-59.7	-69.6	-77.7	-83.9	-88.2	-90.6	-91.5
tert-pentylbenzene	-44.8	-45.0	-56.1	-65.6	-73.3	-78.9	-82.7	-84.6	-84.9
1-ethylpropylbenzene	-38.6	-38.9	-50.2	-60.1	-68.3	-74.5	-78.8	-81.4	-82.3
neopentylbenzene	-54.2	-54.4	-65.4	-74.9	-82.5	-88.2	-91.9	-93.9	-94.2
C12H18									
hexamethylbenzene	-103.4	-103.6	-113.8	-122.7	-130.1	-135.8	-139.8	-142.1	-142.8
1-ethyl-2,3,4,5-tetramethylbenzene	-95.1	-95.3	-106.2	-115.8	-123.7	-129.8	-134.1	-136.6	-137.6
1-ethyl-2,3,4,6-tetramethylbenzene	-95.1	-95.3	-106.2	-115.8	-123.7	-129.8	-134.1	-136.6	-137.6
1-ethyl-2,3,5,6-tetramethylbenzene	-95.1	-95.3	-106.2	-115.8	-123.7	-129.8	-134.1	-136.6	-137.6
1,2-diethyl-3,4-dimethylbenzene	-84.4	-84.6	-95.7	-105.4	-113.3	-119.4	-123.6	-126.1	-126.9
1,2-diethyl-3,5-dimethylbenzene	-89.2	-89.4	-101.6	-112.3	-121.2	-128.2	-133.2	-136.4	-137.9
1,2-diethyl-3,6-dimethylbenzene	-84.4	-84.6	-95.7	-105.4	-113.3	-119.4	-123.6	-126.1	-126.9
1,2-diethyl-4,5-dimethylbenzene	-86.8	-87.0	-98.6	-108.8	-117.3	-123.8	-128.4	-131.2	-132.4
1,3-diethyl-2,4-dimethylbenzene	-84.4	-84.6	-95.7	-105.4	-113.3	-119.4	-123.6	-126.1	-126.9
1,3-diethyl-2,5-dimethylbenzene	-86.8	-87.0	-98.6	-108.8	-117.3	-123.8	-128.4	-131.2	-132.4
1,3-diethyl-4,5-dimethylbenzene	-86.8	-87.0	-98.6	-108.8	-117.3	-123.8	-128.4	-131.2	-132.4
1,3-diethyl-4,6-dimethylbenzene	-86.8	-87.0	-98.6	-108.8	-117.3	-123.8	-128.4	-131.2	-132.4
1,4-diethyl-2,3-dimethylbenzene	-84.4	-84.6	-95.7	-105.4	-113.3	-119.4	-123.6	-126.1	-126.9
1,4-diethyl-2,6-dimethylbenzene	-86.8	-87.0	-98.6	-108.8	-117.3	-123.8	-128.4	-131.2	-132.4
1,4-diethyl-2,5-dimethylbenzene	-86.8	-87.0	-98.6	-108.8	-117.3	-123.8	-128.4	-131.2	-132.4
1-propyl-2,3,4-trimethylbenzene	-84.7	-84.9	-96.2	-106.2	-114.4	-120.7	-125.1	-127.7	-128.7
1-propyl-2,3,5-trimethylbenzene	-87.1	-87.3	-99.2	-109.6	-118.3	-125.0	-129.9	-132.9	-134.2
1-propyl-2,3,6-trimethylbenzene	-84.7	-84.9	-96.2	-106.2	-114.4	-120.7	-125.1	-127.7	-128.7
1-propyl-2,4,5-trimethylbenzene	-87.1	-87.3	-99.2	-109.6	-118.3	-125.0	-129.9	-132.9	-134.2
1-propyl-2,4,6-trimethylbenzene	-87.1	-87.3	-99.2	-109.6	-118.3	-125.0	-129.9	-132.9	-134.2
1-propyl-3,4,5-trimethylbenzene	-87.1	-87.3	-99.2	-109.6	-118.3	-125.0	-129.9	-132.9	-134.2
1-isopropyl-2,3,4-trimethylbenzene	-90.5	-90.7	-102.1	-112.0	-120.2	-126.5	-130.8	-133.4	-134.3
1-isopropyl-2,3,5-trimethylbenzene	-92.9	-93.1	-105.0	-115.5	-124.1	-130.9	-135.6	-138.5	-139.8
1-isopropyl-2,3,6-trimethylbenzene	-90.5	-90.7	-102.1	-112.0	-120.2	-126.5	-130.8	-133.4	-134.3
1-isopropyl-2,4,5-trimethylbenzene	-92.9	-93.1	-105.0	-115.5	-124.1	-130.9	-135.6	-138.5	-139.8
1-isopropyl-2,4,6-trimethylbenzene	-92.9	-93.1	-105.0	-115.5	-124.1	-130.9	-135.6	-138.5	-139.8
1-isopropyl-3,4,5-trimethylbenzene	-92.9	-93.1	-105.0	-115.5	-124.1	-130.9	-135.6	-138.5	-139.8
1-butyl-2,3-dimethylbenzene	-74.3	-74.5	-86.3	-96.5	-105.0	-111.5	-116.1	-118.8	-119.8
1-butyl-2,4-dimethylbenzene	-76.7	-76.9	-89.2	-100.0	-108.9	-115.9	-120.9	-123.9	-125.3
1-butyl-2,5-dimethylbenzene	-76.7	-76.9	-89.2	-100.0	-108.9	-115.9	-120.9	-123.9	-125.3
1-butyl-2,6-dimethylbenzene	-74.3	-74.5	-86.3	-96.5	-105.0	-111.5	-116.1	-118.8	-119.8
1-butyl-3,4-dimethylbenzene	-76.7	-76.9	-89.2	-100.0	-108.9	-115.9	-120.9	-123.9	-125.3
1-butyl-3,5-dimethylbenzene	-79.0	-79.3	-92.1	-103.4	-112.8	-120.3	-125.6	-129.1	-130.8
1-(1(RS)-methylpropyl)-2,3-dimethylbenzene	-80.1	-80.3	-92.1	-102.4	-110.9	-117.4	-121.8	-124.4	-125.4
1-(1(RS)-methylpropyl)-2,4-dimethylbenzene	-82.5	-82.7	-95.1	-105.9	-114.8	-121.7	-126.6	-129.6	-130.8
1-(1(RS)-methylpropyl)-2,5-dimethylbenzene	-82.5	-82.7	-95.1	-105.9	-114.8	-121.7	-126.6	-129.6	-130.8
1-(1(RS)-methylpropyl)-2,6-dimethylbenzene	-80.1	-80.3	-92.1	-102.4	-110.9	-117.4	-121.8	-124.4	-125.4
1-(1(RS)-methylpropyl)-3,4-dimethylbenzene	-82.5	-82.7	-95.1	-105.9	-114.8	-121.7	-126.6	-129.6	-130.8
1-(1(RS)-methylpropyl)-3,5-dimethylbenzene	-84.9	-85.1	-98.0	-109.3	-118.7	-126.1	-131.4	-134.8	-136.3
1-isobutyl-2,3-dimethylbenzene	-83.6	-83.9	-95.7	-106.0	-114.4	-120.9	-125.4	-128.0	-128.9
1-isobutyl-2,4-dimethylbenzene	-86.0	-86.3	-98.6	-109.4	-118.4	-125.3	-130.2	-133.2	-134.4
1-isobutyl-2,5-dimethylbenzene	-86.0	-86.3	-98.6	-109.4	-118.4	-125.3	-130.2	-133.2	-134.4
1-isobutyl-2,6-dimethylbenzene	-83.6	-83.9	-95.7	-106.0	-114.4	-120.9	-125.4	-128.0	-128.9
1-isobutyl-3,4-dimethylbenzene	-86.0	-86.3	-98.6	-109.4	-118.4	-125.3	-130.2	-133.2	-134.4
1-isobutyl-3,5-dimethylbenzene	-88.4	-88.7	-101.5	-112.8	-122.3	-129.7	-135.0	-138.3	-139.9
1-tert-butyl-2,3-dimethylbenzene	-86.3	-86.5	-98.0	-107.9	-115.9	-121.8	-125.6	-127.6	-128.0
1-tert-butyl-2,4-dimethylbenzene	-88.7	-88.9	-101.0	-111.3	-119.8	-126.1	-130.4	-132.8	-133.4
1-tert-butyl-2,5-dimethylbenzene	-88.7	-88.9	-101.0	-111.3	-119.8	-126.1	-130.4	-132.8	-133.4
1-tert-butyl-2,6-dimethylbenzene	-86.3	-86.5	-98.0	-107.9	-115.9	-121.8	-125.6	-127.6	-128.0
1-tert-butyl-3,4-dimethylbenzene	-88.7	-88.9	-101.0	-111.3	-119.8	-126.1	-130.4	-132.8	-133.4
1-tert-butyl-3,5-dimethylbenzene	-91.0	-91.3	-103.9	-114.8	-123.7	-130.5	-135.2	-138.0	-138.9
1-pentyl-2-methylbenzene	-63.8	-64.1	-76.3	-86.9	-95.7	-102.4	-107.1	-109.8	-110.9
1-pentyl-3-methylbenzene	-66.2	-66.5	-79.2	-90.3	-99.6	-106.8	-111.9	-115.0	-116.4
1-pentyl-4-methylbenzene	-66.2	-66.5	-79.2	-90.3	-99.6	-106.8	-111.9	-115.0	-116.4
1-(1(RS)-methylbutyl)-2-methylbenzene	-69.7	-69.9	-82.2	-92.8	-101.5	-108.2	-112.8	-115.5	-116.4
1-(1(RS)-methylbutyl)-3-methylbenzene	-72.0	-72.3	-85.1	-96.2	-105.4	-112.6	-117.6	-120.7	-121.9
1-(1(RS)-methylbutyl)-4-methylbenzene	-72.0	-72.3	-85.1	-96.2	-105.4	-112.6	-117.6	-120.7	-121.9
1-(1-ethylpropyl)-2-methylbenzene	-69.7	-69.9	-82.2	-92.8	-101.5	-108.2	-112.8	-115.5	-116.4
1-(1-ethylpropyl)-3-methylbenzene	-72.0	-72.3	-85.1	-96.2	-105.4	-112.6	-117.6	-120.7	-121.9
1-(1-ethylpropyl)-4-methylbenzene	-72.0	-72.3	-85.1	-96.2	-105.4	-112.6	-117.6	-120.7	-121.9
1-(3-methylbutyl)-2-methylbenzene	-73.2	-73.5	-85.7	-96.4	-105.1	-111.8	-116.4	-119.1	-120.0
1-(3-methylbutyl)-3-methylbenzene	-75.6	-75.9	-88.6	-99.8	-109.0	-116.1	-121.2	-124.2	-125.5
1-(3-methylbutyl)-4-methylbenzene	-75.6	-75.9	-88.6	-99.8	-109.0	-116.1	-121.2	-124.2	-125.5
1-(2(RS)-methylbutyl)-2-methylbenzene	-73.2	-73.5	-85.7	-96.4	-105.1	-111.8	-116.4	-119.1	-120.0
1-(2(RS)-methylbutyl)-3-methylbenzene	-75.6	-75.9	-88.6	-99.8	-109.0	-116.1	-121.2	-124.2	-125.5
1-(2(RS)-methylbutyl)-4-methylbenzene	-75.6	-75.9	-88.6	-99.8	-109.0	-116.1	-121.2	-124.2	-125.5
1-(2,2-dimethylpropyl)-2-methylbenzene	-75.9	-76.1	-88.1	-98.3	-106.5	-112.6	-116.6	-118.7	-119.0
1-(2,2-dimethylpropyl)-3-methylbenzene	-78.2	-78.5	-91.0	-101.7	-110.4	-117.0	-121.4	-123.9	-124.5
1-(2,2-dimethylpropyl)-4-methylbenzene	-78.2	-78.5	-91.0	-101.7	-110.4	-117.0	-121.4	-123.9	-124.5
1-(1(RS),2-dimethylpropyl)-2-methylbenzene	-79.0	-79.3	-91.6	-102.2	-111.0	-117.6	-122.1	-124.7	-125.6
1-(1(RS),2-dimethylpropyl)-3-methylbenzene	-81.4	-81.7	-94.5	-105.7	-114.9	-122.0	-126.9	-129.9	-131.1
1-(1(RS),2-dimethylpropyl)-4-methylbenzene	-81.4	-81.7	-94.5	-105.7	-114.9	-122.0	-126.9	-129.9	-431.1
hexylbenzene	-53.4	-53.7	-66.3	-77.3	-86.3	-93.3	-98.1	-100.9	-102.0
1(RS)-methylpentylbenzene	-59.2	-59.5	-72.2	-83.2	-92.2	-99.1	-103.8	-106.6	-107.5
2(RS)-methylpentylbenzene	-62.8	-63.1	-75.7	-86.7	-95.7	-102.6	-107.4	-110.2	-111.1
3(RS)-methylpentylbenzene	-62.8	-63.1	-75.7	-86.7	-95.7	-102.6	-107.4	-110.2	-111.1
4-methylpentylbenzene	-62.8	-63.1	-75.7	-86.7	-95.7	-102.6	-107.4	-110.2	-111.1
1(RS),2(RS)-dimethylbutylbenzene	-68.6	-68.9	-81.6	-92.6	-101.6	-108.5	-113.1	-115.8	-116.7
1(RS),2(SR)-dimethylbutylbenzene	-68.6	-68.9	-81.6	-92.6	-101.6	-108.5	-113.1	-115.8	-116.7
1(RS),3-dimethylbutylbenzene	-68.6	-68.9	-81.6	-92.6	-101.6	-108.5	-113.1	-115.8	-116.7
2(RS),3-dimethylbutylbenzene	-72.2	-72.4	-85.2	-96.2	-105.2	-112.0	-116.7	-119.4	-120.3
1,1-dimethylbutylbenzene	-65.4	-65.7	-78.1	-88.7	-97.2	-103.5	-107.6	-109.8	-110.1
2,2-dimethylbutylbenzene	-74.8	-75.1	-87.4	-97.9	-106.4	-112.7	-116.9	-119.0	-119.4
3,3-dimethylbutylbenzene	-74.8	-75.1	-87.4	-97.9	-106.4	-112.7	-116.9	-119.0	-119.4
1(RS)-methyl-2,2-dimethylpropylbenzene	-80.6	-80.9	-93.3	-103.8	-112.3	-118.6	-122.6	-124.7	-125.0
1-ethyl-1-methylpropylbenzene	-65.4	-65.7	-78.1	-88.7	-97.2	-103.5	-107.6	-109.8	-110.1
1,1,2-trimethylpropylbenzene	-74.8	-75.1	-87.5	-98.1	-106.6	-112.9	-117.0	-119.0	-119.3

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

T/K	298.15	300	400	500	600	700	800	900	1000
benzene	129.73	130.02	146.57	164.29	182.80	201.86	221.26	240.90	260.76
toluene	122.10	122.56	147.83	174.64	202.37	230.81	259.59	288.70	317.93
C8H10									
ethylbenzene	130.71	131.30	166.45	203.35	241.39	280.26	319.55	359.25	399.17
1,3-dimethylbenzene	119.00	119.58	155.02	192.31	230.80	270.17	310.05	350.34	390.89
1,2-dimethylbenzene	122.22	122.85	158.71	196.28	234.98	274.61	314.65	355.11	395.82
1,4-dimethylbenzene	121.26	121.89	157.87	195.74	234.82	274.82	315.36	356.28	397.50
C9H12									
propylbenzene	137.40	138.19	183.18	230.18	278.52	327.82	377.58	427.80	478.23
isopropylbenzene	137.15	137.94	184.10	232.32	281.83	332.30	383.19	434.54	486.10
1-ethyl-3-methylbenzene	126.60	127.40	172.01	218.72	266.81	315.86	365.41	415.42	465.72
1-ethyl-2-methylbenzene	131.25	132.00	177.08	224.07	272.37	321.63	371.39	421.57	472.04
1-ethyl-4-methylbenzene	126.85	127.65	172.81	220.10	268.73	318.41	368.63	419.31	470.24
1,2,3-trimethylbenzene	124.72	125.56	172.10	220.77	270.91	322.13	373.94	426.25	478.86
1,2,4-trimethylbenzene	117.11	117.90	163.39	210.98	259.99	310.08	360.72	411.90	463.34
1,3,5-trimethylbenzene	118.11	118.91	165.49	214.24	264.42	315.73	367.58	419.98	472.67
C10H14									
butylbenzene	146.7	147.6	202.6	259.8	318.8	378.8	439.5	500.6	561.9
1,3-diethylbenzene	134.8	135.8	190.9	248.3	307.4	367.5	428.4	489.6	551.1
1,2-diethylbenzene	139.2	140.2	195.9	253.7	313.2	373.6	434.7	496.1	557.7
1,4-diethylbenzene	136.5	137.5	193.2	251.2	310.8	371.6	433.0	494.8	556.8
1,2,3,4-tetramethylbenzene	122.6	123.6	180.9	240.2	301.1	363.0	425.5	488.4	551.5
1,2,3,5-tetramethylbenzene	118.2	119.2	175.9	234.8	295.3	356.9	419.2	481.9	544.9
1,2,4,5-tetramethylbenzene	119.9	120.9	178.2	237.7	298.8	360.9	423.8	487.1	550.7
1-ethyl-2,3-dimethylbenzene	129.2	130.2	186.1	244.1	303.7	364.3	425.5	487.1	548.8
1-ethyl-2,4-dimethylbenzene	124.8	125.8	181.1	238.7	297.9	358.2	419.2	480.6	542.2
1-ethyl-2,5-dimethylbenzene	124.8	125.8	181.1	238.7	297.9	358.2	419.2	480.6	542.2
1-ethyl-2,6-dimethylbenzene	130.9	131.9	188.4	247.0	307.2	368.3	430.1	492.2	554.6
1-ethyl-3,4-dimethylbenzene	124.8	125.8	181.1	238.7	297.9	358.2	419.2	480.6	542.2
1-ethyl-3,5-dimethylbenzene	122.1	123.1	178.4	236.1	295.5	356.1	417.5	479.3	541.4
1-propyl-2-methylbenzene	127.1	128.0	183.2	240.5	300.5	360.5	420.2	481.2	542.5
1-propyl-3-methylbenzene	132.7	133.6	188.2	245.1	303.7	363.4	423.9	484.7	545.9
1-propyl-4-methylbenzene	134.4	135.4	190.5	248.0	307.2	367.4	428.5	489.9	551.6
1-isopropyl-2-methylbenzene	134.6	135.6	191.9	250.4	310.5	371.6	433.4	495.6	557.9
1-isopropyl-3-methylbenzene	130.2	131.2	186.9	244.9	304.7	365.5	427.1	489.1	551.3
1-isopropyl-4-methylbenzene	131.9	132.9	189.2	247.8	308.1	369.5	431.7	494.3	557.1
2-methylpropylbenzene	138.9	139.9	195.4	253.2	312.7	373.3	434.6	496.2	558.0
1(RS)-methylpropylbenzene	140.8	141.7	196.6	253.9	312.8	372.8	433.5	494.5	555.8
tert-butylbenzene	146.0	147.0	205.7	266.7	329.3	392.8	456.9	521.3	585.8
C11H16									
pentamethylbenzene	123.0	124.2	192.2	262.4	334.3	407.3	481.0	555.1	629.4
1-ethyl-2,3,4-trimethylbenzene	129.6	130.8	197.3	266.3	336.9	408.6	481.0	553.7	626.7
1-ethyl-2,3,5-trimethylbenzene	125.2	126.4	192.4	260.8	331.1	402.5	474.7	547.2	620.1
1-ethyl-2,3,6-trimethylbenzene	129.6	130.8	197.3	266.3	336.9	408.6	481.0	553.7	626.7
1-ethyl-2,4,6-trimethylbenzene	126.9	128.1	194.7	263.7	334.5	406.5	479.3	552.4	625.8
1-ethyl-3,4,5-trimethylbenzene	126.9	128.1	194.7	263.7	334.5	406.5	479.3	552.4	625.8
1,2-diethyl-3-methylbenzene	137.9	139.0	204.8	273.0	342.9	413.9	485.6	557.6	629.8
1,2-diethyl-4-methylbenzene	133.5	134.6	199.8	267.6	337.1	407.8	479.3	551.1	623.2
1,3-diethyl-2-methylbenzene	139.6	140.8	207.1	275.9	346.4	417.9	490.2	562.7	635.5
1,3-diethyl-4-methylbenzene	133.5	134.6	199.8	267.6	337.1	407.8	479.3	551.1	623.2
1,3-diethyl-5-methylbenzene	130.8	131.9	197.2	265.0	334.8	405.7	477.6	549.8	622.3
1,4-diethyl-2-methylbenzene	133.5	134.6	199.8	267.6	337.1	407.8	479.3	551.1	623.2
1-propyl-2,3-dimethylbenzene	137.5	138.6	204.5	272.7	342.7	413.8	485.7	557.9	630.3
1-propyl-2,4-dimethylbenzene	133.1	134.2	199.5	267.3	336.9	407.7	479.4	551.4	623.7
1-propyl-2,5-dimethylbenzene	133.1	134.2	199.5	267.3	336.9	407.7	479.4	551.4	623.7
1-propyl-2,6-dimethylbenzene	139.2	140.4	206.8	275.6	346.2	417.8	490.3	563.1	636.1
1-isopropyl-2,3-dimethylbenzene	135.0	136.2	203.1	272.5	343.7	415.9	488.9	562.2	635.8
1-isopropyl-2,4-dimethylbenzene	130.6	131.8	198.1	267.1	337.9	409.8	482.6	555.8	629.2
1-isopropyl-2,5-dimethylbenzene	130.6	131.8	198.1	267.1	337.9	409.8	482.6	555.8	629.2
1-isopropyl-2,6-dimethylbenzene	136.7	137.9	205.4	275.4	347.1	420.0	493.5	567.4	641.5
1-butyl-2-dimethylbenzene	145.4	146.5	211.6	279.1	348.5	419.1	490.4	562.1	634.0
1-butyl-3-dimethylbenzene	141.0	142.1	206.6	273.7	342.7	413.0	484.1	555.6	627.4
1-butyl-4-dimethylbenzene	142.7	143.8	208.9	276.6	346.2	417.0	488.7	560.8	633.1
1-(1(RS)-methylpropyl)-2-methylbenzene	141.2	142.3	207.9	276.1	346.0	417.1	489.0	561.2	633.6
1-(1(RS)-methylpropyl)-3-methylbenzene	136.8	137.9	202.9	270.6	340.2	411.0	482.7	554.7	627.0
1-(1(RS)-methylpropyl)-4-methylbenzene	138.5	139.7	205.2	273.5	343.7	415.1	487.3	559.9	632.8
1-tert-butyl-2-methylbenzene	144.7	145.9	214.7	286.0	359.0	433.0	507.8	582.8	657.9
1-tert-butyl-3-methylbenzene	140.3	141.5	209.7	280.5	353.2	426.9	501.5	576.3	651.3
1-tert-butyl-4-methylbenzene	142.0	143.2	212.0	283.4	356.6	431.0	506.1	581.5	657.1
1-isobutyl-2-methylbenzene	139.3	140.5	206.7	275.4	345.9	417.6	490.1	562.9	635.9
1-isobutyl-3-methylbenzene	134.9	136.1	201.7	270.0	340.1	411.5	483.8	556.4	629.3
1-isobutyl-4-methylbenzene	136.7	137.8	204.0	272.8	343.6	415.6	488.4	561.6	635.0
pentylbenzene	155.0	156.1	221.0	288.4	357.8	428.3	499.7	571.4	643.4
isopentylbenzene	148.9	150.1	216.1	284.7	355.2	426.9	499.4	572.2	645.3
2(RS)-methylbutylbenzene	147.2	148.4	213.8	281.8	351.8	422.9	494.8	567.0	639.5
1(RS)-methylbutylbenzene	150.8	151.9	217.3	285.4	355.3	426.4	498.3	570.6	643.1
1(RS),2-dimethylpropylbenzene	144.8	145.9	212.5	281.7	352.7	425.0	498.0	571.4	645.0
tert-pentylbenzene	151.6	152.8	220.5	290.7	362.8	435.9	509.8	583.9	658.2
1-ethylpropylbenzene	152.5	153.7	219.6	288.3	358.8	430.4	502.9	575.8	648.8
neopentylbenzene	144.9	146.2	214.8	285.9	358.8	432.8	507.6	582.6	657.8
C12H18									
hexamethylbenzene	132.2	133.7	214.4	297.5	382.3	468.1	554.7	641.6	728.7
1-ethyl-2,3,4,5-tetramethylbenzene	130.0	131.4	208.6	288.5	370.1	452.9	536.5	620.4	704.5
1-ethyl-2,3,4,6-tetramethylbenzene	130.0	131.4	208.6	288.5	370.1	452.9	536.5	620.4	704.5
1-ethyl-2,3,5,6-tetramethylbenzene	131.7	133.1	210.9	291.3	373.6	456.9	541.1	625.6	710.3
1,2-diethyl-3,4-dimethylbenzene	138.3	139.6	216.1	295.2	376.1	458.2	541.0	624.2	707.6
1,2-diethyl-3,5-dimethylbenzene	129.5	130.8	206.1	284.3	364.5	446.0	528.4	611.3	694.4
1,2-diethyl-3,6-dimethylbenzene	140.0	141.4	218.4	298.1	379.6	462.2	545.7	629.4	713.4
1,2-diethyl-4,5-dimethylbenzene	135.6	136.9	213.4	292.6	373.8	456.1	539.3	622.9	706.8
1,3-diethyl-2,4-dimethylbenzene	138.3	139.6	216.1	295.2	376.1	458.2	541.0	624.2	707.6
1,3-diethyl-2,5-dimethylbenzene	133.9	135.2	211.1	289.8	370.3	452.1	534.7	617.7	701.0
1,3-diethyl-4,5-dimethylbenzene	133.9	135.2	211.1	289.8	370.3	452.1	534.7	617.7	701.0

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

T/K	298.15	300	400	500	600	700	800	900	1000
1,3-diethyl-4,6-dimethylbenzene	135.6	136.9	213.4	292.6	373.8	456.1	539.3	622.9	706.8
1,4-diethyl-2,3-dimethylbenzene	140.0	141.4	218.4	298.1	379.6	462.2	545.7	629.4	713.4
1,4-diethyl-2,6-dimethylbenzene	135.6	136.9	213.4	292.6	373.8	456.1	539.3	622.9	706.8
1,4-diethyl-2,5-dimethylbenzene	133.9	135.2	211.1	289.8	370.3	452.1	534.7	617.7	701.0
1-propyl-2,3,4-trimethylbenzene	137.9	139.2	215.7	294.9	375.9	458.1	541.2	624.5	708.2
1-propyl-2,3,5-trimethylbenzene	133.5	134.8	210.7	289.4	370.1	452.0	534.9	618.1	701.6
1-propyl-2,3,6-trimethylbenzene	137.9	139.2	215.7	294.9	375.9	458.1	541.2	624.5	708.2
1-propyl-2,4,5-trimethylbenzene	133.5	134.8	210.7	289.4	370.1	452.0	534.9	618.1	701.6
1-propyl-2,4,6-trimethylbenzene	135.2	136.6	213.0	292.3	373.6	456.1	539.5	623.3	707.3
1-propyl-3,4,5-trimethylbenzene	135.2	136.6	213.0	292.3	373.6	456.1	539.5	623.3	707.3
1-isopropyl-2,3,4-trimethylbenzene	135.4	136.8	214.4	294.7	376.9	460.2	544.4	628.9	713.6
1-isopropyl-2,3,5-trimethylbenzene	131.0	132.4	209.4	289.2	371.1	454.1	538.1	622.4	707.0
1-isopropyl-2,3,6-trimethylbenzene	135.4	136.8	214.4	294.7	376.9	460.2	544.4	628.9	713.6
1-isopropyl-2,4,5-trimethylbenzene	131.0	132.4	209.4	289.2	371.1	454.1	538.1	622.4	707.0
1-isopropyl-2,4,6-trimethylbenzene	132.7	134.1	211.7	292.1	374.5	458.2	542.7	627.6	712.8
1-isopropyl-3,4,5-trimethylbenzene	132.7	134.1	211.7	292.1	374.5	458.2	542.7	627.6	712.8
1-butyl-2,3-dimethylbenzene	145.8	147.1	222.8	301.3	381.7	463.4	545.9	628.7	711.8
1-butyl-2,4-dimethylbenzene	141.4	142.7	217.8	295.9	375.9	457.3	539.6	622.2	705.2
1-butyl-2,5-dimethylbenzene	141.4	142.7	217.8	295.9	375.9	457.3	539.6	622.2	705.2
1-butyl-2,6-dimethylbenzene	147.5	148.8	225.1	304.2	385.2	467.4	550.5	633.9	717.6
1-butyl-3,4-dimethylbenzene	141.4	142.7	217.8	295.9	375.9	457.3	539.6	622.2	705.2
1-butyl-3,5-dimethylbenzene	138.7	140.0	215.2	293.3	373.6	455.2	537.9	620.9	704.4
1-(1(RS)-methylpropyl)-2,3-dimethylbenzene	141.6	142.9	219.2	298.3	379.2	461.4	544.5	627.9	711.5
1-(1(RS)-methylpropyl)-2,4-dimethylbenzene	137.2	138.5	214.2	292.8	373.4	455.3	538.2	621.4	704.9
1-(1(RS)-methylpropyl)-2,5-dimethylbenzene	137.2	138.5	214.2	292.8	373.4	455.3	538.2	621.4	704.9
1-(1(RS)-methylpropyl)-2,6-dimethylbenzene	143.3	144.7	221.5	301.1	382.7	465.5	549.1	633.1	717.3
1-(1(RS)-methylpropyl)-3,4-dimethylbenzene	137.2	138.5	214.2	292.8	373.4	455.3	538.2	621.4	704.9
1-(1(RS)-methylpropyl)-3,5-dimethylbenzene	134.5	135.9	211.5	290.2	371.1	453.3	536.5	620.1	704.1
1-isobutyl-2,3-dimethylbenzene	139.7	141.1	218.0	297.6	379.1	461.9	545.5	629.5	713.7
1-isobutyl-2,4-dimethylbenzene	135.3	136.7	213.0	292.1	373.3	455.8	539.2	623.0	707.1
1-isobutyl-2,5-dimethylbenzene	135.3	136.7	213.0	292.1	373.3	455.8	539.2	623.0	707.1
1-isobutyl-2,6-dimethylbenzene	141.4	142.8	220.3	300.5	382.6	466.0	550.2	634.7	719.5
1-isobutyl-3,4-dimethylbenzene	135.3	136.7	213.0	292.1	373.3	455.8	539.2	623.0	707.1
1-isobutyl-3,5-dimethylbenzene	132.7	134.0	210.3	289.5	371.0	453.8	537.5	621.7	706.3
1-tert-butyl-2,3-dimethylbenzene	145.1	146.5	226.0	308.2	392.2	477.3	563.2	649.4	735.8
1-tert-butyl-2,4-dimethylbenzene	140.7	142.1	221.0	302.7	386.4	471.2	556.9	642.9	729.2
1-tert-butyl-2,5-dimethylbenzene	140.7	142.1	221.0	302.7	386.4	471.2	556.9	642.9	729.2
1-tert-butyl-2,6-dimethylbenzene	146.8	148.2	228.3	311.1	395.7	481.4	567.9	654.6	741.5
1-tert-butyl-3,4-dimethylbenzene	140.7	142.1	221.0	302.7	386.4	471.2	556.9	642.9	729.2
1-tert-butyl-3,5-dimethylbenzene	138.0	139.4	218.3	300.1	384.0	469.2	555.2	641.7	728.3
1-pentyl-2-methylbenzene	153.6	155.0	229.9	307.7	387.5	468.6	550.6	632.9	715.5
1-pentyl-3-methylbenzene	149.3	150.6	224.9	302.3	381.7	462.5	544.3	626.4	708.9
1-pentyl-4-methylbenzene	151.0	152.3	227.2	305.2	385.2	466.6	548.9	631.6	714.6
1-(1(RS)-methylbutyl)-2-methylbenzene	149.5	150.8	226.3	304.7	385.1	466.7	549.2	632.0	715.1
1-(1(RS)-methylbutyl)-3-methylbenzene	145.1	146.4	221.3	299.2	379.2	460.6	542.9	625.6	708.5
1-(1(RS)-methylbutyl)-4-methylbenzene	146.8	148.1	223.6	302.1	382.7	464.6	547.5	630.7	714.3
1-(1-ethylpropyl)-2-methylbenzene	151.2	152.5	228.6	307.6	388.5	470.7	553.8	637.2	720.9
1-(1-ethylpropyl)-3-methylbenzene	146.8	148.1	223.6	302.1	382.7	464.6	547.5	630.7	714.3
1-(1-ethylpropyl)-4-methylbenzene	148.5	149.9	225.9	305.0	386.2	468.7	552.1	635.9	720.1
1-(3-methylbutyl)-2-methylbenzene	147.6	149.0	225.1	304.0	385.0	467.2	550.2	633.7	717.4
1-(3-methylbutyl)-3-methylbenzene	143.2	144.6	220.1	298.6	379.1	461.1	543.9	627.2	710.8
1-(3-methylbutyl)-4-methylbenzene	144.9	146.3	222.4	301.4	382.6	465.1	548.5	632.4	716.5
1-(2(RS)-methylbutyl)-2-methylbenzene	145.9	147.3	222.8	301.1	381.5	463.1	545.6	628.5	711.6
1-(2(RS)-methylbutyl)-3-methylbenzene	141.5	142.8	217.8	295.7	375.7	457.0	539.3	622.0	705.0
1-(2(RS)-methylbutyl)-4-methylbenzene	143.2	144.6	220.1	298.6	379.1	461.1	543.9	627.2	710.8
1-(2,2-dimethylpropyl)-2-methylbenzene	150.3	151.6	229.5	310.0	392.5	476.2	560.6	645.4	730.3
1-(2,2-dimethylpropyl)-3-methylbenzene	145.9	147.2	224.5	304.6	386.7	470.1	554.3	638.9	723.7
1-(2,2-dimethylpropyl)-4-methylbenzene	147.6	149.0	226.8	307.5	390.2	474.1	558.9	644.1	729.4
1-(1(RS),2-dimethylpropyl)-2-methylbenzene	143.4	144.8	221.4	300.9	382.5	465.2	548.9	632.8	717.1
1-(1(RS),2-dimethylpropyl)-3-methylbenzene	139.0	140.4	216.5	295.5	376.7	459.1	542.5	626.4	710.4
1-(1(RS),2-dimethylpropyl)-4-methylbenzene	140.8	142.1	218.8	298.4	380.1	463.2	547.2	631.5	716.2
hexylbenzene	165.0	166.3	241.7	319.9	400.3	481.9	564.5	647.4	730.6
1(RS)-methylpentylbenzene	159.1	160.4	235.7	314.0	394.3	476.0	558.5	641.4	724.5
2(RS)-methylpentylbenzene	155.5	156.9	232.2	310.4	390.8	472.4	554.9	637.8	721.0
3(RS)-methylpentylbenzene	155.5	156.9	232.2	310.4	390.8	472.4	554.9	637.8	721.0
4-methylpentylbenzene	157.2	158.6	234.5	313.3	394.2	476.4	559.6	643.0	726.8
1(RS),2(RS)-dimethylbutylbenzene	153.0	154.4	230.9	310.3	391.7	474.5	558.2	642.2	726.5
1(RS),2(SR)-dimethylbutylbenzene	153.0	154.4	230.9	310.3	391.7	474.5	558.2	642.2	726.5
1(RS),3-dimethylbutylbenzene	153.0	154.4	230.9	310.3	391.7	474.5	558.2	642.2	726.5
2(RS),3-dimethylbutylbenzene	149.5	150.9	227.3	306.7	388.2	471.0	554.6	638.6	722.9
1,1-dimethylbutylbenzene	159.9	161.3	238.9	319.3	401.8	485.5	570.0	654.7	739.7
2,2-dimethylbutylbenzene	150.5	151.9	229.5	309.9	392.4	476.0	560.4	645.2	730.1
3,3-dimethylbutylbenzene	153.2	154.6	233.1	314.5	397.8	482.4	567.8	653.4	739.3
1(RS)-methyl-2,2-dimethylpropylbenzene	149.0	150.4	229.5	311.4	395.4	480.5	566.4	652.6	738.9
1-ethyl-1-methylpropylbenzene	159.9	161.3	238.9	319.3	401.8	485.5	570.0	654.7	739.7
1,1,2-trimethylpropylbenzene	153.8	155.3	234.0	315.6	399.2	484.0	569.6	655.5	741.6

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. They also provide a basis for extrapolation to estimate the standard thermodynamics properties of higher isomer groups. As the carbon number increases, the equilibrium mole fractions of individual molecular species become of less interest because there are so many of them and because gas chromatographic analytical methods yield mole fractions of isomer groups, rather than individual isomers, at higher carbon numbers.

The distribution of species within an isomer group is independent of pressure for ideal gases and is only a function of temperature, and so it is of interest to note that if any alkylbenzene species (or isomer group) is exposed to a catalyst of disproportionation and isomerization reactions, the equilibrium distribution is similarly independent of pressure for ideal gases and is only a function of temperature. Actually this statement applies to any initial mixture of alkylbenzenes. The reason is that the disproportionation reactions,

$$C_n H_{2n-6} = \tfrac{1}{2} C_{n-1} H_{2n-8} + \tfrac{1}{2} C_{n+1} H_{2n-4}, \qquad (9)$$

do not involve a change in the number of moles of gas. Calculations of equilibrium mole fractions of alkylbenzene mixtures at various H/C ratios for the mixture provide an illustration of the usefulness of data on isomer groups.[22]

8. Nomenclature

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

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

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

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

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

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

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

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

n = number of carbon atoms in a molecule

N_I = number of isomers in an isomer group

OPT = number of optical isomers

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

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

S°(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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