Standard Chemical Thermodynamic Properties of Alkanol Isomer Groups

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The chemical thermodynamic properties of alkanol(ROH) isomer groups from CH_4O to $C_4H_{10}O$ 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 $C_5H_{12}O$ to $C_8H_{18}O$ have been estimated using Benson group values. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 298.15 to 1000 K. For isomer group properties increments per carbon atom have been calculated to show the extent to which thermodynamic properties of higher isomer groups may be obtained by linear extrapolation. Values of C°_p, S°, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ are given for all species of alkanols from CH_4O to $C_8H_{18}O$ in SI units for a standard state pressure of 1 bar.

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

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1. Introduction

Earlier papers in this series have presented isomer group thermodynamic properties[1] for the alkanes,[2] alkylbenzenes,[3] alkenes,[4] alkylnaphthalenes,[5] alkylcyclopentanes and alkylcyclohexanes,[6] alkynes,[7] and alkanethiols.[8] This paper presents data on the alkanols. Chemical thermodynamic properties are given in Stull, Westrum, and Sinke[9] for all isomers of the alkanols through $C_4H_{10}O$, except that values are not given for 2-methyl-1-propanol (isobutylalcohol). A wide range of physical and thermodynamic properties of certain alkanols has been published by Wilhoit and

Zwolinski.[10] It has therefore been of interest to extend these data to all isomers through $C_8H_{18}O$ by use of the Benson group method[11] in order to see whether the increments in the various chemical thermodynamic properties become independent of carbon number beyond the lower members in this homologous series.

2. Standard Thermodynamic Properties of Alkanol Isomer Groups

When isomers are in chemical equilibrium it has been known for some time[12,13] that they can be aggregated in calculations of equilibrium mole fractions by use of the standard Gibbs energy of formation $\Delta_f G^\circ(\mathrm{I})$ of the isomer group defined by

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

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

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

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

$$\Delta_f G^\circ(\mathrm{I}) = \Delta_f H^\circ(\mathrm{I}) - T[S^\circ(\mathrm{I}) - nS^\circ_{\text{graphite}} - (n+1)S^\circ_{H_2(g)} - \tfrac{1}{2}S^\circ_{O_2(g)}], \quad (3)$$

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. Table 1 is an expanded form of the table of Blair and Henze[14] that gives the numbers of isomers of the alkanols classified according to whether oxygen is bonded to a primary, secondary, or tertiary carbon, and according to the numbers of chiral centers.

Rather than having a line in a thermodynamic table for each stereoisomer, this article follows the standard practice of giving properties of racemates. When there is one chiral center R ln 2 is added to the calculated standard entropy and $-RT$ ln 2 to the standard Gibbs energy of formation of one of the forms. For the alkanols with more chiral centers the adjustment of the entropy is R ln 4 for two centers and R ln 8 for three, since none of the species are internally compensated.

All of the references used by Stull, Westrum, and Sinke,[9] while compiling the data for their tables on the alkanols, are too numerous to mention here. The thermodynamic properties of 2-methyl-2-propanol (tertiary butyl alcohol) are from an Erratum (1 December 1972).

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

	Chiral Centers	Primary	Secondary	Tertiary	Total
CH4O	None	1			1
C2H6O	None	1			1
C3H8O	None	1	1		2
C4H10O	None	2		1	3
	One		1		1
	Total	2	1	1	4
C5H12O	None	3	1	1	5
	One	2	4		6
	Total	5	5	1	11
C6H14O	None	5		3	8
	One	6	10		16
	Two		4		4
	Total	11	14	3	28
C7H16O	None	8	2	4	14
	One	16	18	6	40
	Two	4	16		20
	Total	28	36	10	74
C8H18O	None	14		9	23
	One	40	38	14	92
	Two	20	52	4	76
	Three		8		8
	Total	74	98	27	199

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

Since data are available for all of the isomers of the alkanols only through $C_4H_{10}O$, except for 2-methyl-1-propanol, this does not provide an adequate basis for extrapolating isomer group properties to higher carbon numbers. Therefore, the Benson group method has been used to calculate the properties for all isomers through $C_8H_{18}O$ in the ideal gas state.

In order to make these calculations, the structure of each alkanol species was divided into the following Benson groups: $C(H)_3(C)$, $C(H)_2(C)_2$, $C(H)(C)_3$, $C(C)_4$, $C(H)_3(O)$, $C(C)(H)_2(O)$, $C(C)_2(H)(O)$, $C(C)_3(O)$, $O(C)(H)$, and gauche. In addition the total symmetry number (TSN) and number of optical isomers (OPT), were identified and were tabulated. In view of some of the uncertainties in some of these group values indicated by Benson, the 1,5-H repulsions, which affect only several of the most highly branched species, were omitted. In calculating symmetry numbers a report by Davies, Syverud, and Steiner[15] was very helpful. The numbers of isomers of the alkanols are exactly the same as for the alkanethiols,[8] and the numbers of Benson groups in each molecular species are the same except for the substitution of oxygen for sulfur.

The assignment of Benson groups was checked by multiplying the matrix of numbers of groups by a matrix which had in its first column the number of carbon atoms in the group, in the second column the number of hydrogen atoms in each group, and in the third column the number of oxygen atoms in each group. Matrix multiplication yields a matrix with as many rows as lines in the table for that isomer group and three columns giving the numbers of carbon atoms, hydrogen atoms, and oxygen atoms. This check prevents some possible errors in the group assignments. The computer programs used in making the Benson calculations are described in the first paper in this series.[2] In making these calculations thermodynamic properties for graphite, molecular hydro-

Table 2. Root mean square deviations between alkanol 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								
CH4O	.59	.56	.38	.06	.29	.40	.34	.15	.12
C2H6O	.93	.93	.94	1.42	1.30	.90	.45	.30	.69
C3H8O	.79	.81	.65	1.44	.83	.84	.92	.83	1.13
C4H10O	.51	.51	.61	1.59	.58	1.15	1.67	1.45	.49
	Standard entropy in J/K mol								
CH4O	.03	.00	.02	.04	.04	.01	.07	.12	.10
C2H6O	1.85	1.87	2.15	2.40	2.67	2.83	2.93	2.96	3.02
C3H8O	3.56	3.55	3.47	3.31	3.17	3.05	2.94	2.84	2.76
C4H10O	2.40	2.41	2.31	2.26	2.22	2.08	1.92	1.75	1.68
	Standard enthalpy of formation in kJ/mol								
CH4O	.42	.43	.44	.45	.44	.42	.36	.34	.33
C2H6O	.33	.36	.40	.51	.66	.76	.81	.87	.91
C3H8O	1.62	1.61	1.62	1.72	1.84	1.90	2.00	2.07	2.16
C4H10O	2.01	2.00	1.93	1.92	1.90	1.85	1.69	1.55	1.50
	Standard Gibbs energy of formation in kJ/mol								
CH4O	.42	.41	.39	.42	.39	.37	.42	.41	.39
C2H6O	.22	.25	.43	.64	.93	1.19	1.50	1.73	2.00
C3H8O	2.65	2.66	3.00	3.32	3.65	3.97	4.25	4.53	4.80
C4H10O	1.44	1.43	1.31	1.19	1.11	1.09	1.08	1.15	1.22

gen, and molecular oxygen were taken from Stull and Prophet.[16]

Table 2 shows how well the chemical thermodynamic properties calculated using the Benson method agree with the values from Stull, Westrum, and Sinke[9] for CH_4O through $C_4H_{10}O$. 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 CH_4O and C_2H_6O this yields the magnitudes of the deviations, and for C_3H_8O and $C_4H_{10}O$ it yields the root-mean-square deviations at various temperatures. The species 2-methyl-1-propanol has been omitted from these comparisons since the properties calculated for it have been calculated using the Benson method for the tables in this article.

4. Tables of Standard Thermodynamic Properties of Alkanol Isomer Groups

The conversion of thermodynamic properties from 1 atm to 1 bar is discussed in earlier papers in this series and in the NBS Tables.[17]

The remaining tables in this paper have all been calculated using values from Stull, Westrum, and Sinke for CH_4O to $C_4H_{10}O$ and values calculated using the Benson method for $C_5H_{12}O$, $C_6H_{14}O$, $C_7H_{16}O$, and $C_8H_{18}O$ species using group values from Ref. 11. Tables 3–8 give isomer group properties and the increments per carbon atom. Table 7 gives $H^\circ(I,T) - H^\circ(I,298.15\ K)$, the standard enthalpy for an isomer group relative to the isomer group at 298.15 K.

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

T/K	CH4O	C2H6O	C3H8O	C4H10O	C5H12O	C6H14O	C7H16O	C8H18O
298.15	43.89	65.44	92.83	121.28	152.57	184.9	204.5	225.4
300.00	44.02	65.73	93.37	122.20	153.49	185.8	205.5	226.6
400.00	51.42	81.00	121.09	172.93	196.84	230.3	255.6	283.0
500.00	59.50	95.27	143.96	210.78	226.19	262.8	294.9	328.5
600.00	67.03	107.49	159.05	226.11	247.78	288.3	326.6	365.5
700.00	73.72	117.95	171.45	233.27	265.93	310.2	353.4	396.8
800.00	79.66	126.90	181.61	240.10	281.62	329.2	376.1	423.1
900.00	84.89	134.68	190.52	247.83	294.76	344.9	394.8	444.6
1000.00	89.45	141.54	198.48	255.63	305.08	357.2	409.2	461.1

Table 3a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	21.55	27.39	28.45	31.3	32.3	19.6	20.9
300.00	21.71	27.64	28.83	31.3	32.3	19.7	21.0
400.00	29.58	40.09	51.85	23.9	33.5	25.3	27.4
500.00	35.77	48.69	66.82	15.4	36.6	32.1	33.6
600.00	40.46	51.56	67.06	21.7	40.5	38.3	39.0
700.00	44.22	53.50	61.83	32.7	44.3	43.2	43.4
800.00	47.24	54.71	58.50	41.5	47.5	47.0	46.9
900.00	49.79	55.83	57.31	46.9	50.2	49.9	49.8
1000.00	52.09	56.94	57.15	49.5	52.1	52.0	51.8

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

T/K	CH4O	C2H6O	C3H8O	C4H10O	C5H12O	C6H14O	C7H16O	C8H18O
298.15	239.81	282.70	310.82	327.46	379.01	419.0	464.8	509.6
300.00	240.10	283.12	311.43	328.23	379.95	420.1	466.0	511.0
400.00	253.74	304.16	342.12	370.27	430.39	480.0	532.3	584.2
500.00	266.13	323.78	371.76	413.39	477.68	535.0	593.7	652.4
600.00	277.63	342.28	399.44	453.47	520.90	585.3	650.4	715.7
700.00	288.47	359.64	424.93	488.94	560.49	631.4	702.8	774.4
800.00	298.72	376.00	448.47	520.52	597.05	674.1	751.5	829.2
900.00	308.43	391.40	470.40	549.23	631.01	713.8	796.9	880.3
1000.00	317.59	405.96	490.90	575.76	662.63	750.8	839.3	928.1

Table 4a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	42.89	28.12	16.65	51.5	40.0	45.8	44.9
300.00	43.01	28.32	16.80	51.7	40.2	45.9	45.0
400.00	50.42	37.95	28.16	60.1	49.6	52.3	51.9
500.00	57.66	47.98	41.63	64.3	57.4	58.7	58.7
600.00	64.64	57.16	54.03	67.4	64.4	65.1	65.3
700.00	71.17	65.29	64.01	71.5	70.9	71.4	71.7
800.00	77.28	72.47	72.05	76.5	77.0	77.4	77.7
900.00	82.97	79.00	78.84	81.8	82.8	83.1	83.4
1000.00	88.37	84.95	84.86	86.9	88.2	88.5	88.8

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

T/K	CH4O	C2H6O	C3H8O	C4H10O	C5H12O	C6H14O	C7H16O	C8H18O
298.15	-201.17	-234.81	-272.38	-312.34	-330.52	-354.9	-377.1	-399.0
300.00	-201.25	-234.89	-272.50	-312.49	-330.68	-355.1	-377.3	-399.2
400.00	-204.81	-239.83	-277.98	-317.92	-337.05	-362.1	-386.0	-409.5
500.00	-207.94	-243.97	-281.87	-319.98	-341.51	-367.3	-392.6	-417.3
600.00	-210.62	-247.32	-284.71	-320.54	-344.80	-371.3	-397.5	-423.1
700.00	-212.88	-250.04	-286.84	-320.91	-347.23	-374.2	-401.0	-427.2
800.00	-214.68	-252.17	-288.46	-321.38	-348.82	-376.0	-403.3	-429.7
900.00	-216.15	-253.76	-289.54	-321.69	-349.72	-377.0	-404.4	-431.1
1000.00	-217.28	-254.93	-290.15	-321.74	-350.07	-377.4	-404.8	-431.5

Table 5a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-33.64	-37.58	-39.96	-18.2	-24.4	-22.2	-21.9
300.00	-33.64	-37.61	-39.99	-18.2	-24.4	-22.2	-22.0
400.00	-35.02	-38.15	-39.94	-19.1	-25.0	-23.9	-23.5
500.00	-36.02	-37.90	-38.11	-21.5	-25.8	-25.3	-24.7
600.00	-36.69	-37.39	-35.83	-24.3	-26.5	-26.2	-25.5
700.00	-37.15	-36.81	-34.07	-26.3	-26.9	-26.9	-26.1
800.00	-37.49	-36.29	-32.93	-27.4	-27.2	-27.2	-26.5
900.00	-37.61	-35.78	-32.15	-28.0	-27.3	-27.4	-26.7
1000.00	-37.66	-35.22	-31.59	-28.3	-27.3	-27.4	-26.7

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

T/K	CH4O	C2H6O	C3H8O	C4H10O	C5H12O	C6H14O	C7H16O	C8H18O
298.15	-162.46	-168.20	-173.51	-177.79	-170.61	-166.2	-161.4	-156.0
300.00	-162.21	-167.82	-173.89	-176.96	-169.62	-165.1	-160.0	-154.5
400.00	-148.63	-144.66	-138.84	-130.84	-114.89	-100.6	-86.2	-71.3
500.00	-134.27	-120.36	-103.58	-83.80	-58.82	-34.6	-10.5	14.2
600.00	-119.23	-95.36	-67.65	-36.50	-1.93	32.4	66.4	101.0
700.00	-103.82	-69.81	-31.27	10.87	55.40	99.8	144.0	188.7
800.00	-88.15	-43.92	5.33	58.27	113.05	167.7	222.1	276.9
900.00	-72.24	-17.75	42.13	105.79	170.81	235.7	300.3	365.3
1000.00	-56.15	8.56	79.06	153.31	228.66	303.8	378.6	453.8

Table 6a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-5.74	-5.32	-4.28	7.2	4.4	4.9	5.4
300.00	-5.62	-5.07	-4.07	7.3	4.6	5.0	5.5
400.00	3.98	5.82	8.00	16.0	14.3	14.4	14.9
500.00	13.90	16.79	19.77	25.0	24.2	24.1	24.7
600.00	23.87	27.71	31.15	34.6	34.3	34.1	34.6
700.00	34.01	38.54	42.14	44.5	44.4	44.2	44.7
800.00	44.23	49.25	52.94	54.8	54.7	54.4	54.9
900.00	54.49	59.88	63.65	65.0	64.9	64.6	65.0
1000.00	64.71	70.50	74.25	75.3	75.1	74.8	75.2

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

T/K	CH4O	C2H6O	C3H8O	C4H10O	C5H12O	C6H14O	C7H16O	C8H18O
298.15	.00	.00	.00	.00	.00	.0	.0	.0
300.00	.07	.14	.18	.22	.28	.3	.4	.4
400.00	4.83	7.44	10.86	14.88	17.92	21.3	23.5	26.0
500.00	10.39	16.26	24.18	34.27	39.17	46.0	51.1	56.6
600.00	16.72	26.42	39.36	56.24	62.91	73.6	82.3	91.4
700.00	23.75	37.70	55.93	79.28	88.61	103.5	116.3	129.6
800.00	31.05	49.54	73.17	102.53	115.61	135.1	152.4	170.2
900.00	39.67	63.04	92.19	127.35	144.85	169.3	191.4	214.0
1000.00	48.40	76.86	111.70	152.55	174.87	204.4	231.6	259.3

Table 7a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	.00	.00	.00	.0	.0	.0	.0
300.00	.07	.04	.04	.1	.1	.0	.0
400.00	2.62	3.42	4.02	3.0	3.3	2.3	2.5
500.00	5.86	7.93	10.09	4.9	6.8	5.1	5.5
600.00	9.70	12.94	16.88	6.7	10.7	8.7	9.1
700.00	13.95	18.24	23.35	9.3	14.9	12.8	13.3
800.00	18.49	23.63	29.37	13.1	19.5	17.3	17.8
900.00	23.38	29.15	35.16	17.5	24.4	22.1	22.6
1000.00	28.46	34.84	40.85	22.3	29.5	27.2	27.7

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

T/K	CH4O	C2H6O	C3H8O	C4H10O	C5H12O	C6H14O	C7H16O	C8H18O
298.15	-201.17	-234.81	-272.38	-312.34	-330.52	-354.9	-377.1	-398.9
300.00	-201.10	-234.67	-272.21	-312.13	-330.24	-354.6	-376.7	-398.5
400.00	-196.34	-227.36	-261.52	-297.46	-312.60	-333.6	-353.5	-372.9
500.00	-190.77	-218.55	-248.20	-278.07	-291.35	-308.9	-325.9	-342.2
600.00	-184.45	-208.39	-233.03	-256.11	-267.62	-281.3	-294.8	-307.5
700.00	-177.42	-197.11	-216.45	-233.06	-241.91	-251.4	-260.8	-269.4
800.00	-170.12	-185.27	-199.22	-209.81	-214.91	-219.8	-224.7	-228.8
900.00	-161.50	-171.76	-180.19	-184.99	-185.67	-185.6	-185.7	-185.0
1000.00	-152.77	-157.94	-160.69	-159.80	-155.65	-150.5	-145.4	-139.7

Table 8a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-33.64	-37.58	-39.96	-18.2	-24.4	-22.2	-21.8
300.00	-33.57	-37.54	-39.92	-18.1	-24.3	-22.1	-21.8
400.00	-31.02	-34.16	-35.94	-15.1	-21.0	-19.9	-19.3
500.00	-27.78	-29.65	-29.87	-13.3	-17.6	-17.0	-16.3
600.00	-23.94	-24.64	-23.08	-11.5	-13.7	-13.5	-12.7
700.00	-19.69	-19.34	-16.61	-8.9	-9.5	-9.4	-8.6
800.00	-15.15	-13.95	-10.59	-5.1	-4.9	-4.9	-4.1
900.00	-10.26	-8.43	-4.80	-.7	.0	.0	.7
1000.00	-5.18	-2.74	.89	4.1	5.1	5.1	5.8

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 of formation for the isomer group relative to the elements at 298.15 K. This quantity allows the direct calculation of heat effects when the reactants and products are at different temperatures.

The increments per carbon atom are of interest because they indicate the extent to which we can estimate thermodynamic properties of isomer groups of higher carbon numbers.

5. Equilibrium Mole Fractions Within Alkanol Isomer Groups

The equilibrium mole fractions within isomer groups calculated from standard Gibbs energies of formation are given in Table 9 for the alkanols in the ideal gas state. Since the uncertainties in $\Delta_f G^\circ(\mathrm{I})$ 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. The usual equation

Table 9. Equilibrium mole fractions within alkanol isomer groups

T/K	298.15	300	400	500	600	700	800	900	1000
C3H8O									
1-propanol	.0136	.0141	.0598	.1322	.2114	.2849	.3435	.3927	.4325
2-propanol	.9864	.9859	.9402	.8678	.7886	.7151	.6565	.6073	.5675
C4H10O									
1-butanol	.0000	.0000	.0008	.0057	.0182	.0371	.0587	.0812	.1026
2(RS)-butanol	.0138	.0146	.1003	.2681	.4342	.5491	.6136	.6460	.6603
2-methyl-1-propanol	.0003	.0003	.0038	.0146	.0297	.0441	.0551	.0641	.0708
2-methyl-2-propanol	.9859	.9851	.8951	.7116	.5178	.3698	.2726	.2088	.1663
C5H12O									
1-pentanol	.0000	.0000	.0004	.0025	.0073	.0145	.0233	.0329	.0426
2(RS)-pentanol	.0177	.0184	.0766	.1544	.2219	.2706	.3031	.3241	.3375
3-pentanol	.0089	.0092	.0383	.0772	.1110	.1353	.1515	.1621	.1688
2(RS)-methyl-1-butanol	.0001	.0001	.0013	.0055	.0124	.0209	.0296	.0379	.0454
2-methyl-2-butanol	.9202	.9180	.7588	.5841	.4449	.3462	.2779	.2299	.1953
3-methyl-2(RS)-butanol	.0522	.0534	.1211	.1690	.1904	.1954	.1926	.1868	.1801
3-methyl-1-butanol	.0000	.0000	.0007	.0027	.0062	.0105	.0148	.0189	.0227
2,2-dimethyl-1-propanol	.0009	.0009	.0027	.0046	.0059	.0067	.0072	.0075	.0076
C6H14O									
1-hexanol	.0000	.0000	.0001	.0009	.0028	.0060	.0102	.0150	.0200
2(RS)-hexanol	.0036	.0038	.0224	.0536	.0858	.1125	.1327	.1474	.1582
3(RS)-hexanol	.0036	.0038	.0224	.0536	.0858	.1125	.1327	.1474	.1582
2(RS)-methyl-1-pentanol	.0000	.0000	.0004	.0019	.0048	.0087	.0130	.0172	.0213
2-methyl-2-pentanol	.1892	.1905	.2213	.2030	.1721	.1439	.1216	.1046	.0915
2-methyl-3(RS)-pentanol	.0107	.0111	.0353	.0587	.0736	.0812	.0843	.0850	.0844
4-methyl-2(RS)-pentanol	.0107	.0111	.0353	.0587	.0736	.0812	.0843	.0850	.0844
4-methyl-1-pentanol	.0000	.0000	.0002	.0009	.0024	.0043	.0065	.0086	.0106
3(RS)-methyl-1-pentanol	.0000	.0000	.0004	.0019	.0048	.0087	.0130	.0172	.0213
3(RS)-methyl-2(RS)-pentanol	.0215	.0222	.0706	.1175	.1473	.1624	.1686	.1699	.1688
3-methyl-3-pentanol	.1892	.1905	.2213	.2030	.1721	.1439	.1216	.1046	.0915
2(RS),3-dimethyl-1-butanol	.0001	.0001	.0006	.0021	.0041	.0063	.0082	.0099	.0114
2,3-dimethyl-2-butanol	.5572	.5527	.3497	.2222	.1476	.1039	.0773	.0603	.0488
2-ethyl-1-butanol	.0000	.0000	.0002	.0009	.0024	.0043	.0065	.0086	.0106
2,2-dimethyl-1-butanol	.0000	.0000	.0003	.0010	.0018	.0026	.0034	.0042	.0048
3,3-dimethyl-2(RS)-butanol	.0141	.0142	.0193	.0197	.0182	.0164	.0149	.0137	.0127
3,3-dimethyl-1-butanol	.0000	.0000	.0001	.0003	.0006	.0009	.0011	.0014	.0016
C7H16O									
1-heptanol	.0000	.0000	.0000	.0003	.0010	.0024	.0043	.0065	.0089
2(RS)-heptanol	.0009	.0010	.0067	.0181	.0318	.0446	.0554	.0640	.0709
3(RS)-heptanol	.0009	.0010	.0067	.0181	.0318	.0446	.0554	.0640	.0709
4-heptanol	.0005	.0005	.0033	.0091	.0159	.0223	.0277	.0320	.0354
5-methyl-1-hexanol	.0000	.0000	.0001	.0003	.0009	.0017	.0027	.0037	.0048
5-methyl-2(RS)-hexanol	.0027	.0028	.0105	.0198	.0273	.0322	.0352	.0369	.0378

Table 9. Equilibrium mole fractions within alkanol isomer groups -- continued

T/K	298.15	300	400	500	600	700	800	900	1000
5-methyl-3(RS)-hexanol	.0027	.0028	.0105	.0198	.0273	.0322	.0352	.0369	.0378
2-methyl-3(RS)-hexanol	.0027	.0028	.0105	.0198	.0273	.0322	.0352	.0369	.0378
2-methyl-2-hexanol	.0473	.0478	.0660	.0685	.0637	.0571	.0508	.0454	.0410
2(RS)-methyl-1-hexanol	.0000	.0000	.0001	.0006	.0018	.0034	.0054	.0075	.0095
4(RS)-methyl-1-hexanol	.0000	.0000	.0001	.0006	.0018	.0034	.0054	.0075	.0095
4(RS)-methyl-2(RS)-hexanol	.0054	.0056	.0211	.0397	.0546	.0644	.0704	.0738	.0756
4(RS)-methyl-3(RS)-hexanol	.0054	.0056	.0211	.0397	.0546	.0644	.0704	.0738	.0756
3(RS)-methyl-3-hexanol	.0946	.0957	.1319	.1371	.1275	.1142	.1016	.0908	.0820
3(RS)-methyl-2(RS)-hexanol	.0054	.0056	.0211	.0397	.0546	.0644	.0704	.0738	.0756
3(RS)-methyl-1-hexanol	.0000	.0000	.0001	.0006	.0018	.0034	.0054	.0075	.0095
4,4-dimethyl-1-pentanol	.0000	.0000	.0000	.0001	.0002	.0003	.0005	.0006	.0007
4,4-dimethyl-2(RS)-pentanol	.0035	.0036	.0057	.0066	.0067	.0065	.0062	.0059	.0057
2,2-dimethyl-1-pentanol	.0035	.0036	.0057	.0066	.0067	.0065	.0062	.0059	.0057
2,2-dimethyl-1-pentanol	.0000	.0000	.0001	.0003	.0007	.0010	.0014	.0018	.0021
3,3-dimethyl-1-pentanol	.0000	.0000	.0001	.0003	.0007	.0010	.0014	.0018	.0021
3,3-dimethyl-2(RS)-pentanol	.0105	.0107	.0172	.0199	.0202	.0196	.0187	.0178	.0170
3(RS),4-dimethyl-1-pentanol	.0000	.0000	.0002	.0007	.0015	.0025	.0034	.0043	.0051
3(RS),4-dimethyl-2(RS)-pentanol	.0158	.0161	.0333	.0434	.0468	.0465	.0448	.0425	.0403
2(RS),3(RS)-dimethyl-1-pentanol	.0000	.0000	.0004	.0014	.0031	.0050	.0069	.0086	.0102
2,3(RS)-dimethyl-2-pentanol	.2787	.2775	.2085	.1501	.1094	.0824	.0646	.0524	.0437
2,3(RS)-dimethyl-3-pentanol	.2787	.2775	.2085	.1501	.1094	.0824	.0646	.0524	.0437
2(RS),4-dimethyl-1-pentanol	.0000	.0000	.0002	.0007	.0015	.0025	.0034	.0043	.0051
2,4-dimethyl-2-pentanol	.1394	.1388	.1042	.0750	.0547	.0412	.0323	.0262	.0219
2,4-dimethyl-3-pentanol	.0040	.0040	.0083	.0109	.0117	.0116	.0112	.0106	.0101
2(RS)-ethyl-1-pentanol	.0000	.0000	.0001	.0006	.0018	.0034	.0054	.0075	.0095
3-ethyl-1-pentanol	.0000	.0000	.0001	.0003	.0009	.0017	.0027	.0037	.0048
3-ethyl-2(RS)-pentanol	.0027	.0028	.0105	.0198	.0273	.0322	.0352	.0369	.0378
3-ethyl-3-pentanol	.0473	.0478	.0660	.0685	.0637	.0571	.0508	.0454	.0410
2-ethyl-2-methyl-1-butanol	.0000	.0000	.0001	.0003	.0007	.0010	.0014	.0018	.0021
2(RS)-ethyl-3-methyl-1-butanol	.0000	.0000	.0002	.0007	.0015	.0025	.0034	.0043	.0051
2(RS),3,3-trimethyl-1-butanol	.0000	.0000	.0000	.0001	.0002	.0003	.0004	.0004	.0005
2,3,3-trimethyl-2-butanol	.0473	.0465	.0208	.0112	.0069	.0047	.0035	.0027	.0022
2,2,3-trimethyl-1-butanol	.0000	.0000	.0001	.0002	.0003	.0004	.0006	.0007	.0008
C8H18O									
1-octanol	.0000	.0000	.0000	.0001	.0004	.0010	.0019	.0030	.0042
2(RS)-octanol	.0003	.0003	.0024	.0071	.0132	.0194	.0249	.0295	.0334
3(RS)-octanol	.0003	.0003	.0024	.0071	.0132	.0194	.0249	.0295	.0334
4(RS)-octanol	.0003	.0003	.0024	.0071	.0132	.0194	.0249	.0295	.0334
2(RS)-methyl-1-heptanol	.0000	.0000	.0000	.0003	.0007	.0015	.0024	.0035	.0045
2-methyl-2-heptanol	.0149	.0151	.0236	.0267	.0264	.0248	.0228	.0210	.0193
2-methyl-3(RS)-heptanol	.0008	.0009	.0038	.0077	.0113	.0140	.0158	.0170	.0178
2-methyl-4(RS)-heptanol	.0008	.0009	.0038	.0077	.0113	.0140	.0158	.0170	.0178
6-methyl-3(RS)-heptanol	.0008	.0009	.0038	.0077	.0113	.0140	.0158	.0170	.0178
6-methyl-2(RS)-heptanol	.0008	.0009	.0038	.0077	.0113	.0140	.0158	.0170	.0178
6-methyl-1-heptanol	.0000	.0000	.0000	.0001	.0004	.0007	.0012	.0017	.0022
3(RS)-methyl-1-heptanol	.0000	.0000	.0000	.0003	.0007	.0015	.0024	.0035	.0045
3(RS)-methyl-2(RS)-heptanol	.0017	.0018	.0075	.0155	.0226	.0280	.0316	.0341	.0356
3(RS)-methyl-3-heptanol	.0298	.0302	.0473	.0535	.0529	.0496	.0456	.0419	.0386
3(RS)-methyl-4(RS)-heptanol	.0017	.0018	.0075	.0155	.0226	.0280	.0316	.0341	.0356
5(RS)-methyl-3(RS)-heptanol	.0017	.0018	.0075	.0155	.0226	.0280	.0316	.0341	.0356
5(RS)-methyl-2(RS)-heptanol	.0017	.0018	.0075	.0155	.0226	.0280	.0316	.0341	.0356
5(RS)-methyl-1-heptanol	.0000	.0000	.0000	.0003	.0007	.0015	.0024	.0035	.0045
4(RS)-methyl-1-heptanol	.0000	.0000	.0000	.0003	.0007	.0015	.0024	.0035	.0045

Table 9. Equilibrium mole fractions within alkanol isomer groups -- continued

T/K	298.15	300	400	500	600	700	800	900	1000
4(RS)-methyl-2(RS)-heptanol	.0017	.0018	.0075	.0155	.0226	.0280	.0316	.0341	.0356
4(RS)-methyl-3(RS)-heptanol	.0017	.0018	.0075	.0155	.0226	.0280	.0316	.0341	.0356
4-methyl-4-heptanol	.0149	.0151	.0235	.0267	.0264	.0248	.0228	.0210	.0193
2,2-dimethyl-1-hexanol	.0000	.0000	.0000	.0001	.0003	.0005	.0006	.0008	.0010
2,2-dimethyl-3(RS)-hexanol	.0011	.0011	.0021	.0026	.0028	.0028	.0028	.0027	.0027
5,5-dimethyl-3(RS)-hexanol	.0011	.0011	.0021	.0026	.0028	.0028	.0028	.0027	.0027
5,5-dimethyl-2(RS)-hexanol	.0011	.0011	.0021	.0026	.0028	.0028	.0028	.0027	.0027
5,5-dimethyl-1-hexanol	.0000	.0000	.0000	.0000	.0001	.0002	.0002	.0003	.0003
3,3-dimethyl-1-hexanol	.0000	.0000	.0000	.0001	.0003	.0005	.0006	.0008	.0010
3,3-dimethyl-2(RS)-hexanol	.0033	.0034	.0062	.0078	.0084	.0085	.0084	.0082	.0080
4,4-dimethyl-3(RS)-hexanol	.0033	.0034	.0062	.0078	.0084	.0085	.0084	.0082	.0080
4,4-dimethyl-2(RS)-hexanol	.0033	.0034	.0062	.0078	.0084	.0085	.0084	.0082	.0080
4,4-dimethyl-1-hexanol	.0000	.0000	.0000	.0001	.0003	.0005	.0006	.0008	.0010
4(RS),5-dimethyl-1-hexanol	.0000	.0000	.0001	.0003	.0006	.0011	.0015	.0020	.0024
4(RS),5-dimethyl-2(RS)-hexanol	.0050	.0051	.0119	.0170	.0194	.0202	.0201	.0196	.0190
4(RS),5-dimethyl-3(RS)-hexanol	.0050	.0051	.0119	.0170	.0194	.0202	.0201	.0196	.0190
2,3-dimethyl-3(RS)-hexanol	.0878	.0877	.0747	.0586	.0454	.0358	.0290	.0242	.0206
2,3(RS)-dimethyl-2-hexanol	.0878	.0877	.0747	.0586	.0454	.0358	.0290	.0242	.0206
2(RS),3(RS)-dimethyl-1-hexanol	.0000	.0000	.0001	.0005	.0013	.0022	.0031	.0040	.0048
3(RS),5-dimethyl-1-hexanol	.0000	.0000	.0001	.0003	.0006	.0011	.0015	.0020	.0024
3(RS),5-dimethyl-2(RS)-hexanol	.0050	.0051	.0119	.0170	.0194	.0202	.0201	.0196	.0190
3(RS),5-dimethyl-3-hexanol	.0878	.0877	.0747	.0586	.0454	.0358	.0290	.0242	.0206
2,4(RS)-dimethyl-3(RS)-hexanol	.0050	.0051	.0119	.0170	.0194	.0202	.0201	.0196	.0190
2,4(RS)-dimethyl-2-hexanol	.0878	.0877	.0747	.0586	.0454	.0358	.0290	.0242	.0206
2(RS),4(RS)-dimethyl-1-hexanol	.0000	.0000	.0001	.0005	.0013	.0022	.0031	.0040	.0048
2(RS),5-dimethyl-1-hexanol	.0000	.0000	.0001	.0003	.0006	.0011	.0015	.0020	.0024
2,5-dimethyl-2-hexanol	.0439	.0438	.0374	.0293	.0227	.0179	.0145	.0121	.0103
2,5-dimethyl-3(RS)-hexanol	.0025	.0026	.0060	.0085	.0097	.0101	.0101	.0098	.0095
3(RS),4(RS)-dimethyl-1-hexanol	.0000	.0000	.0001	.0005	.0013	.0022	.0031	.0040	.0048
3(RS),4(RS)-dimethyl-2(RS)-hexanol	.0100	.0102	.0239	.0339	.0388	.0404	.0402	.0393	.0380
3(RS),4(RS)-dimethyl-3-hexanol	.1756	.1754	.1494	.1171	.0908	.0716	.0580	.0483	.0412
2(RS)-ethyl-1-hexanol	.0000	.0000	.0000	.0003	.0007	.0015	.0024	.0035	.0045
3(RS)-ethyl-1-hexanol	.0000	.0000	.0000	.0003	.0007	.0015	.0024	.0035	.0045
3(RS)-ethyl-2(RS)-hexanol	.0017	.0018	.0075	.0155	.0226	.0280	.0316	.0341	.0356
3-ethyl-3-hexanol	.0149	.0151	.0236	.0267	.0264	.0248	.0228	.0210	.0193
4-ethyl-3(RS)-hexanol	.0008	.0009	.0038	.0077	.0113	.0140	.0158	.0170	.0178
4-ethyl-2(RS)-hexanol	.0008	.0009	.0038	.0077	.0113	.0140	.0158	.0170	.0178
4-ethyl-1-hexanol	.0000	.0000	.0000	.0001	.0004	.0007	.0012	.0017	.0022
2(RS)-ethyl-2-methyl-1-pentanol	.0000	.0000	.0001	.0003	.0005	.0009	.0013	.0017	.0020
2(RS)-isopropyl-1-pentanol	.0000	.0000	.0001	.0003	.0006	.0011	.0015	.0020	.0024
2(RS)-ethyl-4-methyl-1-pentanol	.0000	.0000	.0001	.0003	.0006	.0011	.0015	.0020	.0024
3(RS),4,4-trimethyl-1-pentanol	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0002	.0002
3(RS),4,4-trimethyl-2(RS)-pentanol	.0017	.0017	.0024	.0025	.0025	.0023	.0021	.0020	.0019
2,2,3(RS)-trimethyl-3-pentanol	.0298	.0294	.0149	.0088	.0057	.0041	.0031	.0025	.0021
2,2,3(RS)-trimethyl-1-pentanol	.0000	.0000	.0000	.0001	.0002	.0004	.0005	.0006	.0007
2(RS),4,4-trimethyl-1-pentanol	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0002	.0002
2,4,4-trimethyl-2-pentanol	.0149	.0147	.0075	.0044	.0029	.0020	.0016	.0012	.0010
2,2,4-trimethyl-3(RS)-pentanol	.0008	.0009	.0012	.0013	.0012	.0012	.0011	.0010	.0010
2,2,4-trimethyl-1-pentanol	.0000	.0000	.0000	.0001	.0001	.0002	.0002	.0003	.0004
3,3,4-trimethyl-1-pentanol	.0000	.0000	.0000	.0001	.0001	.0002	.0002	.0003	.0004
3,3,4-trimethyl-2(RS)-pentanol	.0025	.0026	.0036	.0038	.0037	.0035	.0032	.0030	.0029
2,3,3-trimethyl-2-pentanol	.0447	.0441	.0224	.0132	.0086	.0061	.0047	.0037	.0031
2(RS),3,3-trimethyl-1-pentanol	.0000	.0000	.0000	.0001	.0002	.0004	.0005	.0006	.0007
3-ethyl-3-methyl-1-pentanol	.0000	.0000	.0000	.0001	.0003	.0005	.0006	.0008	.0010
3-ethyl-3-methyl-2(RS)-pentanol	.0033	.0034	.0062	.0078	.0084	.0085	.0084	.0082	.0080

Table 9. Equilibrium mole fractions within alkanol isomer groups -- continued

T/K	298.15	300	400	500	600	700	800	900	1000
2(RS)-ethyl-3(RS)-methyl-1-pentanol	.0000	.0000	.0001	.0005	.0013	.0022	.0031	.0040	.0048
2(RS),3(RS),4-trimethyl-1-pentanol	.0000	.0000	.0001	.0003	.0006	.0009	.0012	.0015	.0017
2,3(RS),4-trimethyl-2-pentanol	.0670	.0665	.0432	.0287	.0199	.0145	.0111	.0089	.0073
2,3,4-trimethyl-3-pentanol	.0335	.0332	.0216	.0143	.0100	.0073	.0056	.0044	.0037
2-propyl-1-pentanol	.0000	.0000	.0000	.0001	.0004	.0007	.0012	.0017	.0022
3(RS)-ethyl-4-methyl-1-pentanol	.0000	.0000	.0001	.0003	.0006	.0011	.0015	.0020	.0024
3(RS)-ethyl-4-methyl-2(RS)-pentanol	.0050	.0051	.0119	.0170	.0194	.0202	.0201	.0196	.0190
3-ethyl-2-methyl-3-pentanol	.0439	.0438	.0374	.0293	.0227	.0179	.0145	.0121	.0103
3-ethyl-2-methyl-2-pentanol	.0439	.0438	.0374	.0293	.0227	.0179	.0145	.0121	.0103
3-ethyl-2(RS)-methyl-1-pentanol	.0000	.0000	.0001	.0003	.0006	.0011	.0015	.0020	.0024
2(RS)-ethyl-3,3-dimethyl-1-butanol	.0000	.0000	.0000	.0000	.0001	.0001	.0002	.0002	.0002
2(RS)-ethyl-2-methyl-3-methyl-1-butanol	.0000	.0000	.0000	.0001	.0002	.0004	.0005	.0006	.0007
2,2-diethyl-1-butanol	.0000	.0000	.0000	.0001	.0003	.0005	.0006	.0008	.0010
2,2,3,3-tetramethyl-1-butanol	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
2-isopropyl-3-methyl-1-butanol	.0000	.0000	.0000	.0001	.0001	.0002	.0003	.0004	.0004

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

Compounds are named in tables according to the IUPAC Revised and Collected Recommendations for the Nomenclature of Organic Chemistry, 1979.[18]

6. Standard Thermodynamic Properties of Individual Alkanol Species

The values of C_P°, S°, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ for all the alkanol species through $C_8H_{18}O$ are given in Tables 10–13 in SI units for a standard state pressure of 1 bar. The values for CH_4O through $C_4H_{10}O$ have been converted from the tables of Stull, Westrum, and Sinke[9] and the values for $C_5H_{12}O$ through $C_8H_{18}O$ have been calculated using the Benson method.[10] The values for chiral forms are for the racemates.

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

T/K	298.15	300	400	500	600	700	800	900	1000
CH4O									
methanol	43.89	44.02	51.42	59.50	67.03	73.72	79.66	84.89	89.45
C2H6O									
ethanol	65.44	65.73	81.00	95.27	107.49	117.95	126.90	134.68	141.54
C3H8O									
1-propanol	87.11	87.49	108.20	127.65	144.50	159.12	171.71	182.63	192.17
2-propanol	88.74	89.16	112.05	133.43	149.52	164.05	176.27	186.73	195.89
C4H10O									
1-butanol	110.00	110.50	137.24	160.08	183.58	202.13	218.03	231.79	243.76
2(RS)-butanol	113.30	113.80	141.00	166.10	187.11	205.10	220.41	233.80	245.27
2-methyl-1-propanol	109.43	109.97	137.83	162.81	184.91	204.12	220.45	233.90	244.46
2-methyl-2-propanol	113.39	113.93	142.93	168.49	189.83	207.69	223.09	236.06	247.53
C5H12O									
1-pentanol	133.5	134.1	167.2	197.0	223.4	246.4	266.1	282.5	295.5
2(RS)-pentanol	135.8	136.4	170.1	200.2	226.8	249.7	269.2	285.1	297.4
3-pentanol	135.8	136.4	170.1	200.2	226.8	249.7	269.2	285.1	297.4
2(RS)-methyl-1-butanol	132.4	133.1	166.9	197.2	224.0	247.2	267.0	283.3	296.0
2-methyl-2-butanol	136.9	137.6	171.5	201.8	228.4	251.4	270.7	286.4	298.5
3-methyl-2(RS)-butanol	134.7	135.4	169.8	200.4	227.4	250.6	270.1	285.9	297.9
3-methyl-1-butanol	132.4	133.1	166.9	197.2	224.0	247.2	267.0	283.3	296.0
2,2-dimethyl-1-propanol	134.8	135.5	171.0	202.6	230.2	253.7	273.3	289.0	300.6
C6H14O									
1-hexanol	156.5	157.2	196.3	231.3	262.4	289.5	312.7	331.8	347.0
2(RS)-hexanol	158.8	159.5	199.2	234.6	265.8	292.9	315.7	334.4	348.9
3(RS)-hexanol	158.8	159.5	199.2	234.6	265.8	292.9	315.7	334.4	348.9
2(RS)-methyl-1-pentanol	155.4	156.2	195.9	231.6	263.0	290.4	313.6	332.6	347.5
2-methyl-2-pentanol	159.9	160.7	200.5	236.1	267.4	294.5	317.3	335.8	350.0
2-methyl-3(RS)-pentanol	157.7	158.5	198.8	234.8	266.4	293.7	316.6	335.2	349.4
4-methyl-2(RS)-pentanol	157.7	158.5	198.8	234.8	266.4	293.7	316.6	335.2	349.4
4-methyl-1-pentanol	155.4	156.2	195.9	231.6	263.0	290.4	313.6	332.6	347.5
3(RS)-methyl 1-pentanol	155.4	156.2	195.9	231.6	263.0	290.4	313.6	332.6	347.5
3(RS)-methyl-2(RS)-pentanol	157.7	158.5	198.8	234.8	266.4	293.7	316.6	335.2	349.4
3-methyl-3-pentanol	159.9	160.7	200.5	236.1	267.4	294.5	317.3	335.8	350.0
2(RS),3-dimethyl-1-butanol	154.4	155.1	195.6	231.8	263.6	291.2	314.5	333.4	348.1
2,3-dimethyl-2-butanol	158.8	159.6	200.2	236.3	268.0	295.3	318.2	336.6	350.5
2-ethyl-1-butanol	155.4	156.2	195.9	231.6	263.0	290.4	313.6	332.6	347.5
2,2-dimethyl-1-butanol	157.8	158.6	200.1	237.0	269.2	296.9	319.9	338.3	352.1
3,3-dimethyl-2(RS)-butanol	160.1	160.9	203.0	240.2	272.6	300.2	323.0	340.9	354.0
3,3-dimethyl-1-butanol	157.8	158.6	200.1	237.0	269.2	296.9	319.9	338.3	352.1
C7H16O									
1-heptanol	179.5	180.3	225.3	265.7	301.5	332.6	359.2	381.2	398.5
2(RS)-heptanol	181.8	182.7	228.2	268.9	304.9	336.0	362.3	383.8	400.4
3(RS)-heptanol	181.8	182.7	228.2	268.9	304.9	336.0	362.3	383.8	400.4
4-heptanol	181.8	182.7	228.2	268.9	304.9	336.0	362.3	383.8	400.4

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

T/K	298.15	300	400	500	600	700	800	900	1000
5-methyl-1-hexanol	178.4	179.3	225.0	265.9	302.1	333.5	360.1	382.0	399.1
5-methyl-2(RS)-hexanol	180.7	181.6	227.9	269.2	305.5	336.8	363.2	384.6	401.0
5-methyl-3(RS)-hexanol	180.7	181.6	227.9	269.2	305.5	336.8	363.2	384.6	401.0
2-methyl-3(RS)-hexanol	180.7	181.6	227.9	269.2	305.5	336.8	363.2	384.6	401.0
2-methyl-2-hexanol	182.9	183.8	229.6	270.5	306.5	337.6	363.8	385.1	401.5
2(RS)-methyl-1-hexanol	178.4	179.3	225.0	265.9	302.1	333.5	360.1	382.0	399.1
4(RS)-methyl-1-hexanol	178.4	179.3	225.0	265.9	302.1	333.5	360.1	382.0	399.1
4(RS)-methyl-2(RS)-hexanol	180.7	181.6	227.9	269.2	305.5	336.8	363.2	384.6	401.0
4(RS)-methyl-3(RS)-hexanol	180.7	181.6	227.9	269.2	305.5	336.8	363.2	384.6	401.0
3(RS)-methyl-3-hexanol	182.9	183.8	229.6	270.5	306.5	337.6	363.8	385.1	401.5
3(RS)-methyl-2(RS)-hexanol	180.7	181.6	227.9	269.2	305.5	336.8	363.2	384.6	401.0
3(RS)-methyl-1-hexanol	178.4	179.3	225.0	265.9	302.1	333.5	360.1	382.0	399.1
4,4-dimethyl-1-pentanol	180.8	181.7	229.1	271.3	308.3	340.0	366.5	387.7	403.7
4,4-dimethyl-2(RS)-pentanol	183.1	184.0	232.0	274.6	311.7	343.3	369.5	390.3	405.6
2,2-dimethyl-1-pentanol	183.1	184.0	232.0	274.6	311.7	343.3	369.5	390.3	405.6
2,2-dimethyl-1-pentanol,	180.8	181.7	229.1	271.3	308.3	340.0	366.5	387.7	403.7
3,3-dimethyl-1-pentanol	180.8	181.7	229.1	271.3	308.3	340.0	366.5	387.7	403.7
3,3-dimethyl-2(RS)-pentanol	183.1	184.0	232.0	274.6	311.7	343.3	369.5	390.3	405.6
3(RS),4-dimethyl-1-pentanol	177.3	178.2	224.7	266.1	302.7	334.3	361.0	382.8	399.6
3(RS),4-dimethyl-2(RS)-pentanol	179.6	180.6	227.5	269.4	306.1	337.7	364.1	385.4	401.5
2(RS),3(RS)-dimethyl-1-pentanol	177.3	178.2	224.7	266.1	302.7	334.3	361.0	382.8	399.6
2,3(RS)-dimethyl-2-pentanol	181.8	182.7	229.3	270.7	307.1	338.4	364.7	385.9	402.1
2,3(RS)-dimethyl-3-pentanol	181.8	182.7	229.3	270.7	307.1	338.4	364.7	385.9	402.1
2(RS),4-dimethyl-1-pentanol	177.3	178.2	224.7	266.1	302.7	334.3	361.0	382.8	399.6
2,4-dimethyl-2-pentanol	181.8	182.7	229.3	270.7	307.1	338.4	364.7	385.9	402.1
2,4-dimethyl-3-pentanol	179.6	180.6	227.5	269.4	306.1	337.7	364.1	385.4	401.5
2(RS)-ethyl-1-pentanol	178.4	179.3	225.0	265.9	302.1	333.5	360.1	382.0	399.1
3-ethyl-1-pentanol	178.4	179.3	225.0	265.9	302.1	333.5	360.1	382.0	399.1
3-ethyl-2(RS)-pentanol	180.7	181.6	227.9	269.2	305.5	336.8	363.2	384.6	401.0
3-ethyl-3-pentanol	182.9	183.8	229.6	270.5	306.5	337.6	363.8	385.1	401.5
2-ethyl-2-methyl-1-butanol	180.8	181.7	229.1	271.3	308.3	340.0	366.5	387.7	403.7
2(RS)-ethyl-3-methyl-1-butanol	177.3	178.2	224.7	266.1	302.7	334.3	361.0	382.8	399.6
2(RS),3,3-trimethyl-1-butanol	179.7	180.6	228.8	271.5	308.9	340.8	367.3	388.5	404.2
2,3,3-trimethyl-2-butanol	184.2	185.1	233.4	276.1	313.3	344.9	371.0	391.6	406.6
2,2,3-trimethyl-1-butanol	179.7	180.6	228.8	271.5	308.9	340.8	367.3	388.5	404.2
C8H18O									
1-octanol	202.5	203.4	254.4	300.1	340.5	375.8	405.8	430.5	450.1
2(RS)-octanol	204.8	205.8	257.3	303.3	343.9	379.1	408.8	433.1	452.0
3(RS)-octanol	204.8	205.8	257.3	303.3	343.9	379.1	408.8	433.1	452.0
4(RS)-octanol	204.8	205.8	257.3	303.3	343.9	379.1	408.8	433.1	452.0
2(RS)-methyl-1-heptanol	201.4	202.4	254.0	300.3	341.1	376.6	406.7	431.3	450.6
2-methyl-2-heptanol	205.9	206.9	258.6	304.9	345.6	380.7	410.4	434.5	453.1
2-methyl-3(RS)-heptanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
2-methyl-4(RS)-heptanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
6-methyl-3(RS)-heptanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
6-methyl-2(RS)-heptanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
6-methyl-1-heptanol	201.4	202.4	254.0	300.3	341.1	376.6	406.7	431.3	450.6
3(RS)-methyl-1-heptanol	201.4	202.4	254.0	300.3	341.1	376.6	406.7	431.3	450.6
3(RS)-methyl-2(RS)-heptanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
3(RS)-methyl-3-heptanol	205.9	206.9	258.6	304.9	345.6	380.7	410.4	434.5	453.1
3(RS)-methyl-4(RS)-heptanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
5(RS)-methyl-3(RS)-heptanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
5(RS)-methyl-2(RS)-heptanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
5(RS)-methyl-1-heptanol	201.4	202.4	254.0	300.3	341.1	376.6	406.7	431.3	450.6

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

T/K	298.15	300	400	500	600	700	800	900	1000
4(RS)-methyl-1-heptanol	201.4	202.4	254.0	300.3	341.1	376.6	406.7	431.3	450.6
4(RS)-methyl-2(RS)-heptanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
4(RS)-methyl-3(RS)-heptanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
4-methyl-4-heptanol	205.9	206.9	258.6	304.9	345.6	380.7	410.4	434.5	453.1
2,2-dimethyl-1-hexanol	203.7	204.8	258.2	305.7	347.3	383.1	413.0	437.0	455.2
2,2-dimethyl-3(RS)-hexanol	206.0	207.1	261.1	308.9	350.7	386.4	416.1	439.6	457.1
5,5-dimethyl-3(RS)-hexanol	206.0	207.1	261.1	308.9	350.7	386.4	416.1	439.6	457.1
5,5-dimethyl-2(RS)-hexanol	206.0	207.1	261.1	308.9	350.7	386.4	416.1	439.6	457.1
5,5-dimethyl-1-hexanol	203.7	204.8	258.2	305.7	347.3	383.1	413.0	437.0	455.2
3,3-dimethyl-1-hexanol	203.7	204.8	258.2	305.7	347.3	383.1	413.0	437.0	455.2
3,3-dimethyl-2(RS)-hexanol	206.0	207.1	261.1	308.9	350.7	386.4	416.1	439.6	457.1
4,4-dimethyl-3(RS)-hexanol	206.0	207.1	261.1	308.9	350.7	386.4	416.1	439.6	457.1
4,4-dimethyl-2(RS)-hexanol	206.0	207.1	261.1	308.9	350.7	386.4	416.1	439.6	457.1
4,4-dimethyl-1-hexanol	203.7	204.8	258.2	305.7	347.3	383.1	413.0	437.0	455.2
4(RS),5-dimethyl-1-hexanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
4(RS),5-dimethyl-2(RS)-hexanol	202.6	203.7	256.6	303.8	345.1	380.8	410.6	434.7	453.1
4(RS),5-dimethyl-3(RS)-hexanol	202.6	203.7	256.6	303.8	345.1	380.8	410.6	434.7	453.1
2,3-dimethyl-3(RS)-hexanol	204.8	205.8	258.3	305.1	346.2	381.6	411.3	435.3	453.6
2,3(RS)-dimethyl-2-hexanol	204.8	205.8	258.3	305.1	346.2	381.6	411.3	435.3	453.6
2(RS),3(RS)-dimethyl-1-hexanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
3(RS),5-dimethyl-1-hexanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
3(RS),5-dimethyl-2(RS)-hexanol	202.6	203.7	256.6	303.8	345.1	380.8	410.6	434.7	453.1
3(RS),5-dimethyl-3-hexanol	204.8	205.8	258.3	305.1	346.2	381.6	411.3	435.3	453.6
2,4(RS)-dimethyl-3(RS)-hexanol	202.6	203.7	256.6	303.8	345.1	380.8	410.6	434.7	453.1
2,4(RS)-dimethyl-2-hexanol	204.8	205.8	258.3	305.1	346.2	381.6	411.3	435.3	453.6
2(RS),4(RS)-dimethyl-1-hexanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
2(RS),5-dimethyl-1-hexanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
2,5-dimethyl-2-hexanol	204.8	205.8	258.3	305.1	346.2	381.6	411.3	435.3	453.6
2,5-dimethyl-3(RS)-hexanol	202.6	203.7	256.6	303.8	345.1	380.8	410.6	434.7	453.1
3(RS),4(RS)-dimethyl-1-hexanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
3(RS),4(RS)-dimethyl-2(RS)-hexanol	202.6	203.7	256.6	303.8	345.1	380.8	410.6	434.7	453.1
3(RS),4(RS)-dimethyl-3-hexanol	204.8	205.8	258.3	305.1	346.2	381.6	411.3	435.3	453.6
2(RS)-ethyl-1-hexanol	201.4	202.4	254.0	300.3	341.1	376.6	406.7	431.3	450.6
3(RS)-ethyl-1-hexanol	201.4	202.4	254.0	300.3	341.1	376.6	406.7	431.3	450.6
3(RS)-ethyl-2(RS)-hexanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
3-ethyl-3-hexanol	205.9	206.9	258.6	304.9	345.6	380.7	410.4	434.5	453.1
4-ethyl-3(RS)-hexanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
4-ethyl-2(RS)-hexanol	203.7	204.7	256.9	303.5	344.5	379.9	409.7	433.9	452.5
4-ethyl-1-hexanol	201.4	202.4	254.0	300.3	341.1	376.6	406.7	431.3	450.6
2(RS)-ethyl-2-methyl-1-pentanol	203.7	204.8	258.2	305.7	347.3	383.1	413.0	437.0	455.2
2(RS)-isopropyl-1-pentanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
2(RS)-ethyl-4-methyl-1-pentanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
3(RS),4,4-trimethyl-1-pentanol	202.7	203.7	257.8	305.9	347.9	383.9	413.9	437.8	455.7
3(RS),4,4-trimethyl-2(RS)-pentanol	205.0	206.1	260.7	309.2	351.3	387.3	417.0	440.4	457.6
2,2,3(RS)-trimethyl-3-pentanol	207.2	208.2	262.4	310.5	352.4	388.1	417.6	441.0	458.2
2,2,3(RS)-trimethyl-1-pentanol	202.7	203.7	257.8	305.9	347.9	383.9	413.9	437.8	455.7
2(RS),4,4-trimethyl-1-pentanol	202.7	203.7	257.8	305.9	347.9	383.9	413.9	437.8	455.7
2,4,4-trimethyl-2-pentanol	207.2	208.2	262.4	310.5	352.4	388.1	417.6	441.0	458.2
2,2,4-trimethyl-3(RS)-pentanol	205.0	206.1	260.7	309.2	351.3	387.3	417.0	440.4	457.6
2,2,4-trimethyl-1-pentanol	202.7	203.7	257.8	305.9	347.9	383.9	413.9	437.8	455.7
3,3,4-trimethyl-1-pentanol	202.7	203.7	257.8	305.9	347.9	383.9	413.9	437.8	455.7
3,3,4-trimethyl-2(RS)-pentanol	205.0	206.1	260.7	309.2	351.3	387.3	417.0	440.4	457.6
2,3,3-trimethyl-2-pentanol	207.2	208.2	262.4	310.5	352.4	388.1	417.6	441.0	458.2
2(RS),3,3-trimethyl-1-pentanol	202.7	203.7	257.8	305.9	347.9	383.9	413.9	437.8	455.7
3-ethyl-3-methyl-1-pentanol	203.7	204.8	258.2	305.7	347.3	383.1	413.0	437.0	455.2

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

T/K	298.15	300	400	500	600	700	800	900	1000
3-ethyl-3-methyl-2(RS)-pentanol	206.0	207.1	261.1	308.9	350.7	386.4	416.1	439.6	457.1
2(RS)-ethyl-3(RS)-methyl-1-pentanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
2(RS),3(RS),4-trimethyl-1-pentanol	199.3	200.3	253.4	300.7	342.4	378.3	408.5	432.9	451.7
2,3(RS),4-trimethyl-2-pentanol	203.8	204.8	258.0	305.3	346.8	382.4	412.2	436.1	454.1
2,3,4-trimethyl-3-pentanol	203.8	204.8	258.0	305.3	346.8	382.4	412.2	436.1	454.1
2-propyl-1-pentanol	201.4	202.4	254.0	300.3	341.1	376.6	406.7	431.3	450.6
3(RS)-ethyl-4-methyl-1-pentanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
3(RS)-ethyl-4-methyl-2(RS)-pentanol	202.6	203.7	256.6	303.8	345.1	380.8	410.6	434.7	453.1
3-ethyl-2-methyl-3-pentanol	204.8	205.8	258.3	305.1	346.2	381.6	411.3	435.3	453.6
3-ethyl-2-methyl-2-pentanol	204.8	205.8	258.3	305.1	346.2	381.6	411.3	435.3	453.6
3-ethyl-2(RS)-methyl-1-pentanol	200.3	201.4	253.7	300.5	341.8	377.4	407.6	432.1	451.1
2(RS)-ethyl-3,3-dimethyl-1-butanol	202.7	203.7	257.8	305.9	347.9	383.9	413.9	437.8	455.7
2(RS)-ethyl-2-methyl-3-methyl-1-butanol	202.7	203.7	257.8	305.9	347.9	383.9	413.9	437.8	455.7
2,2-diethyl-1-butanol	203.7	204.8	258.2	305.7	347.3	383.1	413.0	437.0	455.2
2,2,3,3-tetramethyl-1-butanol	205.0	206.1	262.0	311.3	354.1	390.4	420.2	443.5	460.3
2-isopropyl-3-methyl-1-butanol	199.3	200.3	253.4	300.7	342.4	378.3	408.5	432.9	451.7

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

T/K	298.15	300	400	500	600	700	800	900	1000
CH4O									
methanol	239.81	240.10	253.74	266.13	277.63	288.47	298.72	308.43	317.59
C2H6O									
ethanol	282.70	283.12	304.16	323.78	342.28	359.64	376.00	391.40	405.96
C3H8O									
1-propanol	324.91	325.46	353.49	379.81	404.62	428.01	450.10	470.98	490.73
2-propanol	310.02	310.60	339.39	366.80	392.61	416.75	439.47	460.85	481.02
C4H10O									
1-butanol	363.28	363.99	399.47	432.86	464.37	494.07	522.15	548.63	573.69
2(RS)-butanol	359.14	359.85	396.38	430.60	462.82	493.03	521.44	548.17	573.44
2-methyl-1-propanol	348.44	349.12	384.64	418.14	449.82	479.80	508.16	534.93	560.14
2-methyl-2-propanol	326.38	327.09	363.95	398.64	431.31	461.94	490.73	517.75	543.24
C5H12O									
1-pentanol	399.1	399.9	443.1	483.7	522.0	558.2	592.4	624.7	655.2
2(RS)-pentanol	396.5	397.3	441.3	482.6	521.5	558.2	592.8	625.5	656.2
3-pentanol	390.7	391.6	435.5	476.8	515.7	552.4	587.1	619.7	650.4
2(RS)-methyl-1-butanol	393.6	394.4	437.4	478.0	516.4	552.7	587.0	619.5	650.0
2-methyl-2-butanol	375.0	375.9	420.2	461.8	501.0	538.0	572.8	605.6	636.5
3-methyl-2(RS)-butanol	385.3	386.1	429.9	471.1	510.1	546.9	581.7	614.5	645.2
3-methyl-1-butanol	387.9	388.7	431.7	472.2	510.6	546.9	581.3	613.7	644.2
2,2-dimethyl-1-propanol	361.1	361.9	405.8	447.4	486.9	524.2	559.4	592.5	623.6
C6H14O									
1-hexanol	438.5	439.5	490.1	537.8	582.8	625.3	665.5	703.5	739.3
2(RS)-hexanol	435.9	436.9	488.3	536.6	582.2	625.3	666.0	704.3	740.3
3(RS)-hexanol	435.9	436.9	488.3	536.6	582.2	625.3	666.0	704.3	740.3
2(RS)-methyl-1-pentanol	433.0	434.0	484.5	532.1	577.2	619.8	660.1	698.2	734.1
2-methyl-2-pentanol	414.5	415.4	467.2	515.9	561.8	605.1	645.9	684.4	720.6
2-methyl-3(RS)-pentanol	424.7	425.7	476.9	525.2	570.9	614.0	654.8	693.2	729.3
4-methyl-2(RS)-pentanol	424.7	425.7	476.9	525.2	570.9	614.0	654.8	693.2	729.3
4-methyl-1-pentanol	427.3	428.2	478.7	526.3	571.4	614.0	654.4	692.5	728.3
3(RS)-methyl-1-pentanol	433.0	434.0	484.5	532.1	577.2	619.8	660.1	698.2	734.1
3(RS)-methyl-2(RS)-pentanol	430.5	431.4	482.7	531.0	576.6	619.8	660.6	699.0	735.1
3-methyl-3-pentanol	414.5	415.4	467.2	515.9	561.8	605.1	645.9	684.4	720.6
2(RS),3-dimethyl-1-butanol	421.8	422.8	473.0	520.7	565.8	608.6	649.0	687.2	723.1
2,3-dimethyl-2-butanol	403.2	404.2	455.8	504.4	550.4	593.8	634.8	673.4	709.6
2-ethyl-1-butanol	427.3	428.2	478.7	526.3	571.4	614.0	654.4	692.5	728.3
2,2-dimethyl-1-butanol	409.6	410.6	462.0	510.7	556.8	600.4	641.6	680.4	716.8
3,3-dimethyl-2(RS)-butanol	397.9	398.9	451.0	500.4	547.2	591.3	632.9	672.1	708.7
3,3-dimethyl-1-butanol	400.5	401.4	452.9	501.5	547.7	591.3	632.5	671.3	707.7
C7H16O									
1-heptanol	477.9	479.0	537.2	591.9	643.6	692.4	738.6	782.3	823.4
2(RS)-heptanol	475.3	476.5	535.4	590.7	643.0	692.4	739.1	783.0	824.4
3(RS)-heptanol	475.3	476.5	535.4	590.7	643.0	692.4	739.1	783.0	824.4
4-heptanol	469.6	470.7	529.6	585.0	637.3	686.7	733.3	777.3	818.6

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

T/K	298.15	300	400	500	600	700	800	900	1000
5-methyl-1-hexanol	466.7	467.8	525.7	580.4	632.2	681.2	727.5	771.2	812.4
5-methyl-2(RS)-hexanol	464.1	465.2	523.9	579.3	631.7	681.2	727.9	772.0	813.4
5-methyl-3(RS)-hexanol	464.1	465.2	523.9	579.3	631.7	681.2	727.9	772.0	813.4
2-methyl-3(RS)-hexanol	464.1	465.2	523.9	579.3	631.7	681.2	727.9	772.0	813.4
2-methyl-2-hexanol	453.9	455.0	514.3	570.0	622.6	672.2	719.0	763.2	804.6
2(RS)-methyl-1-hexanol	472.4	473.6	531.5	586.2	637.9	686.9	733.3	777.0	818.1
4(RS)-methyl-1-hexanol	472.4	473.6	531.5	586.2	637.9	686.9	733.3	777.0	818.1
4(RS)-methyl-2(RS)-hexanol	469.9	471.0	529.7	585.1	637.4	686.9	733.7	777.7	819.2
4(RS)-methyl-3(RS)-hexanol	469.9	471.0	529.7	585.1	637.4	686.9	733.7	777.7	819.2
3(RS)-methyl-3-hexanol	459.6	460.8	520.0	575.7	628.3	678.0	724.8	768.9	810.4
3(RS)-methyl-2(RS)-hexanol	469.9	471.0	529.7	585.1	637.4	686.9	733.7	777.7	819.2
3(RS)-methyl-1-hexanol	472.4	473.6	531.5	586.2	637.9	686.9	733.3	777.0	818.1
4,4-dimethyl-1-pentanol	439.9	441.0	499.9	555.6	608.5	658.4	705.6	750.1	791.8
4,4-dimethyl-2(RS)-pentanol	437.3	438.4	498.1	554.5	607.9	658.4	706.0	750.8	792.8
2,2-dimethyl-1-pentanol	437.3	438.4	498.1	554.5	607.9	658.4	706.0	750.8	792.8
2,2-dimethyl-1-pentanol	449.0	450.1	509.0	564.8	617.6	667.6	714.7	759.2	800.9
3,3-dimethyl-1-pentanol	449.0	450.1	509.0	564.8	617.6	667.6	714.7	759.2	800.9
3,3-dimethyl-2(RS)-pentanol	446.4	447.6	507.2	563.7	617.1	667.6	715.2	760.0	801.9
3(RS),4-dimethyl-1-pentanol	461.2	462.3	520.1	574.8	626.6	675.7	722.1	765.9	807.2
3(RS),4-dimethyl-2(RS)-pentanol	458.6	459.8	518.3	573.6	626.1	675.7	722.5	766.7	808.2
2(RS),3(RS)-dimethyl-1-pentanol	467.0	468.1	525.8	580.5	632.3	681.4	727.9	771.7	812.9
2,3(RS)-dimethyl-2-pentanol	448.4	449.5	508.6	564.3	616.9	666.7	713.7	757.9	799.4
2,3(RS)-dimethyl-3-pentanol	448.4	449.5	508.6	564.3	616.9	666.7	713.7	757.9	799.4
2(RS),4-dimethyl-1-pentanol	461.2	462.3	520.1	574.8	626.6	675.7	722.1	765.9	807.2
2,4-dimethyl-2-pentanol	442.6	443.8	502.8	558.5	611.2	660.9	707.9	752.1	793.7
2,4-dimethyl-3-pentanol	447.1	448.2	506.7	562.1	614.5	664.2	711.0	755.2	796.7
2(RS)-ethyl-1-pentanol	472.4	473.6	531.5	586.2	637.9	686.9	733.3	777.0	818.1
3-ethyl-1-pentanol	466.7	467.8	525.7	580.4	632.2	681.2	727.5	771.2	812.4
3-ethyl-2(RS)-pentanol	464.1	465.2	523.9	579.3	631.7	681.2	727.9	772.0	813.4
3-ethyl-3-pentanol	453.9	455.0	514.3	570.0	622.6	672.2	719.0	763.2	804.6
2-ethyl-2-methyl-1-butanol	449.0	450.1	509.0	564.8	617.6	667.6	714.7	759.2	800.9
2(RS)-ethyl-3-methyl-1-butanol	461.2	462.3	520.1	574.8	626.6	675.7	722.1	765.9	807.2
2(RS),3,3-trimethyl-1-butanol	434.4	435.5	494.2	550.0	602.9	652.9	700.2	744.8	786.6
2,3,3-trimethyl-2-butanol	415.8	417.0	477.0	533.7	587.5	638.2	686.0	731.0	773.1
2,2,3-trimethyl-1-butanol	437.8	438.9	497.6	553.3	606.2	656.3	703.6	748.2	789.9
C8H18O									
1-octanol	517.3	518.6	584.2	646.0	704.3	759.5	811.7	861.0	907.4
2(RS)-octanol	514.7	516.0	582.4	644.8	703.8	759.5	812.2	861.8	908.4
3(RS)-octanol	514.7	516.0	582.4	644.8	703.8	759.5	812.2	861.8	908.4
4(RS)-octanol	514.7	516.0	582.4	644.8	703.8	759.5	812.2	861.8	908.4
2(RS)-methyl-1-heptanol	511.9	513.1	578.5	640.3	698.7	754.1	806.4	855.7	902.2
2-methyl-2-heptanol	493.3	494.6	561.3	624.1	683.3	739.3	792.2	841.9	888.7
2-methyl-3(RS)-heptanol	503.5	504.8	571.0	633.4	692.5	748.3	801.0	850.7	897.5
2-methyl-4(RS)-heptanol	503.5	504.8	571.0	633.4	692.5	748.3	801.0	850.7	897.5
6-methyl-3(RS)-heptanol	503.5	504.8	571.0	633.4	692.5	748.3	801.0	850.7	897.5
6-methyl-2(RS)-heptanol	503.5	504.8	571.0	633.4	692.5	748.3	801.0	850.7	897.5
6-methyl-1-heptanol	506.1	507.3	572.8	634.5	693.0	748.3	800.6	850.0	896.5
3(RS)-methyl-1-heptanol	511.9	513.1	578.5	640.3	698.7	754.1	806.4	855.7	902.2
3(RS)-methyl-2(RS)-heptanol	509.3	510.5	576.7	639.2	698.2	754.1	806.8	856.5	903.2
3(RS)-methyl-3-heptanol	499.0	500.3	567.1	629.8	689.1	745.1	797.9	847.7	894.5
3(RS)-methyl-4(RS)-heptanol	509.3	510.5	576.7	639.2	698.2	754.1	806.8	856.5	903.2
5(RS)-methyl-3(RS)-heptanol	509.3	510.5	576.7	639.2	698.2	754.1	806.8	856.5	903.2
5(RS)-methyl-2(RS)-heptanol	509.3	510.5	576.7	639.2	698.2	754.1	806.8	856.5	903.2
5(RS)-methyl-1-heptanol	511.9	513.1	578.5	640.3	698.7	754.1	806.4	855.7	902.2

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

T/K	298.15	300	400	500	600	700	800	900	1000
4(RS)-methyl-1-heptanol	511.9	513.1	578.5	640.3	698.7	754.1	806.4	855.7	902.2
4(RS)-methyl-2(RS)-heptanol	509.3	510.5	576.7	639.2	698.2	754.1	806.8	856.5	903.2
4(RS)-methyl-3(RS)-heptanol	509.3	510.5	576.7	639.2	698.2	754.1	806.8	856.5	903.2
4-methyl-4-heptanol	493.3	494.6	561.3	624.1	683.3	739.3	792.2	841.9	888.7
2,2-dimethyl-1-hexanol	488.4	489.7	556.1	618.9	678.4	734.7	787.9	838.0	885.0
2,2-dimethyl-3(RS)-hexanol	476.7	478.0	545.1	608.6	668.7	725.6	779.2	829.6	876.9
5,5-dimethyl-3(RS)-hexanol	476.7	478.0	545.1	608.6	668.7	725.6	779.2	829.6	876.9
5,5-dimethyl-2(RS)-hexanol	476.7	478.0	545.1	608.6	668.7	725.6	779.2	829.6	876.9
5,5-dimethyl-1-hexanol	479.3	480.6	546.9	609.7	669.2	725.6	778.7	828.8	875.9
3,3-dimethyl-1-hexanol	488.4	489.7	556.1	618.9	678.4	734.7	787.9	838.0	885.0
3,3-dimethyl-2(RS)-hexanol	485.9	487.1	554.2	617.8	677.9	734.7	788.3	838.7	886.0
4,4-dimethyl-3(RS)-hexanol	485.9	487.1	554.2	617.8	677.9	734.7	788.3	838.7	886.0
4,4-dimethyl-2(RS)-hexanol	485.9	487.1	554.2	617.8	677.9	734.7	788.3	838.7	886.0
4,4-dimethyl-1-hexanol	488.4	489.7	556.1	618.9	678.4	734.7	787.9	838.0	885.0
4(RS),5-dimethyl-1-hexanol	500.6	501.9	567.1	628.8	687.4	742.8	795.2	844.7	891.3
4(RS),5-dimethyl-2(RS)-hexanol	498.1	499.3	565.3	627.7	686.8	742.8	795.7	845.5	892.3
4(RS),5-dimethyl-3(RS)-hexanol	498.1	499.3	565.3	627.7	686.8	742.8	795.7	845.5	892.3
2,3-dimethyl-3(RS)-hexanol	487.8	489.1	555.6	618.4	677.7	733.8	786.8	836.7	883.5
2,3(RS)-dimethyl-2-hexanol	487.8	489.1	555.6	618.4	677.7	733.8	786.8	836.7	883.5
2(RS),3(RS)-dimethyl-1-hexanol	506.4	507.6	572.9	634.6	693.1	748.6	801.0	850.5	897.0
3(RS),5-dimethyl-1-hexanol	500.6	501.9	567.1	628.8	687.4	742.8	795.2	844.7	891.3
3(RS),5-dimethyl-2(RS)-hexanol	498.1	499.3	565.3	627.7	686.8	742.8	795.7	845.5	892.3
3(RS),5-dimethyl-3-hexanol	487.8	489.1	555.6	618.4	677.7	733.8	786.8	836.7	883.5
2,4(RS)-dimethyl-3(RS)-hexanol	498.1	499.3	565.3	627.7	686.8	742.8	795.7	845.5	892.3
2,4(RS)-dimethyl-2-hexanol	487.8	489.1	555.6	618.4	677.7	733.8	786.8	836.7	883.5
2(RS),4(RS)-dimethyl-1-hexanol	506.4	507.6	572.9	634.6	693.1	748.6	801.0	850.5	897.0
2(RS),5-dimethyl-1-hexanol	500.6	501.9	567.1	628.8	687.4	742.8	795.2	844.7	891.3
2,5-dimethyl-2-hexanol	482.1	483.3	549.9	612.6	672.0	728.1	781.0	830.9	877.8
2,5-dimethyl-3(RS)-hexanol	492.3	493.6	559.5	622.0	681.1	737.0	789.9	839.7	886.5
3(RS),4(RS)-dimethyl-1-hexanol	506.4	507.6	572.9	634.6	693.1	748.6	801.0	850.5	897.0
3(RS),4(RS)-dimethyl-2(RS)-hexanol	503.8	505.1	571.1	633.5	692.6	748.6	801.4	851.2	898.0
3(RS),4(RS)-dimethyl-3-hexanol	493.6	494.9	561.4	624.2	683.5	739.6	792.5	842.4	889.3
2(RS)-ethyl-1-hexanol	511.9	513.1	578.5	640.3	698.7	754.1	806.4	855.7	902.2
3(RS)-ethyl-1-hexanol	511.9	513.1	578.5	640.3	698.7	754.1	806.4	855.7	902.2
3(RS)-ethyl-2(RS)-hexanol	509.3	510.5	576.7	639.2	698.2	754.1	806.8	856.5	903.2
3-ethyl-3-hexanol	493.3	494.6	561.3	624.1	683.3	739.3	792.2	841.9	888.7
4-ethyl-3(RS)-hexanol	503.5	504.8	571.0	633.4	692.5	748.3	801.0	850.7	897.5
4-ethyl-2(RS)-hexanol	503.5	504.8	571.0	633.4	692.5	748.3	801.0	850.7	897.5
4-ethyl-1-hexanol	506.1	507.3	572.8	634.5	693.0	748.3	800.6	850.0	896.5
2(RS)-ethyl-2-methyl-1-pentanol	494.2	495.5	561.8	624.6	684.1	740.5	793.6	843.7	890.8
2(RS)-isopropyl-1-pentanol	500.6	501.9	567.1	628.8	687.4	742.8	795.2	844.7	891.3
2(RS)-ethyl-4-methyl-1-pentanol	500.6	501.9	567.1	628.8	687.4	742.8	795.2	844.7	891.3
3(RS),4,4-trimethyl-1-pentanol	473.8	475.1	541.3	604.1	663.6	720.1	773.4	823.5	870.7
3(RS),4,4-trimethyl-2(RS)-pentanol	471.3	472.5	539.4	602.9	663.1	720.1	773.8	824.3	871.7
2,2,3(RS)-trimethyl-3-pentanol	461.0	462.3	529.8	593.6	654.0	711.1	764.9	815.5	862.9
2,2,3(RS)-trimethyl-1-pentanol	483.0	484.2	550.4	613.2	672.8	729.2	782.5	832.7	879.8
2(RS),4,4-trimethyl-1-pentanol	473.8	475.1	541.3	604.1	663.6	720.1	773.4	823.5	870.7
2,4,4-trimethyl-2-pentanol	455.2	456.5	524.0	587.8	648.2	705.3	759.1	809.7	857.1
2,2,4-trimethyl-3(RS)-pentanol	465.5	466.8	533.7	597.2	657.4	714.3	768.0	818.5	865.9
2,2,4-trimethyl-1-pentanol	477.2	478.5	544.6	607.4	667.0	723.4	776.7	826.9	874.0
3,3,4-trimethyl-1-pentanol	477.2	478.5	544.6	607.4	667.0	723.4	776.7	826.9	874.0
3,3,4-trimethyl-2(RS)-pentanol	474.6	475.9	542.8	606.3	666.5	723.4	777.2	827.7	875.0
2,3,3-trimethyl-2-pentanol	464.4	465.7	533.1	597.0	657.4	714.5	768.3	818.9	866.3
2(RS),3,3-trimethyl-1-pentanol	483.0	484.2	550.4	613.2	672.8	729.2	782.5	832.7	879.8
3-ethyl-3-methyl-1-pentanol	488.4	489.7	556.1	618.9	678.4	734.7	787.9	838.0	885.0

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

T/K	298.15	300	400	500	600	700	800	900	1000
3-ethyl-3-methyl-2(RS)-pentanol	485.9	487.1	554.2	617.8	677.9	734.7	788.3	838.7	886.0
2(RS)-ethyl-3(RS)-methyl-1-pentanol	506.4	507.6	572.9	634.6	693.1	748.6	801.0	850.5	897.0
2(RS),3(RS),4-trimethyl-1-pentanol	495.2	496.4	561.4	623.2	681.8	737.3	789.9	839.4	886.1
2,3(RS),4-trimethyl-2-pentanol	476.6	477.9	544.2	607.0	666.4	722.6	775.6	825.6	872.6
2,3,4-trimethyl-3-pentanol	470.8	472.1	538.4	601.2	660.6	716.8	769.9	819.9	866.8
2-propyl-1-pentanol	506.1	507.3	572.8	634.5	693.0	748.3	800.6	850.0	896.5
3(RS)-ethyl-4-methyl-1-pentanol	500.6	501.9	567.1	628.8	687.4	742.8	795.2	844.7	891.3
3(RS)-ethyl-4-methyl-2(RS)-pentanol	498.1	499.3	565.3	627.7	686.8	742.8	795.7	845.5	892.3
3-ethyl-2-methyl-3-pentanol	482.1	483.3	549.9	612.6	672.0	728.1	781.0	830.9	877.8
3-ethyl-2-methyl-2-pentanol	482.1	483.3	549.9	612.6	672.0	728.1	781.0	830.9	877.8
3-ethyl-2(RS)-methyl-1-pentanol	500.6	501.9	567.1	628.8	687.4	742.8	795.2	844.7	891.3
2(RS)-ethyl-3,3-dimethyl-1-butanol	473.8	475.1	541.3	604.1	663.6	720.1	773.4	823.5	870.7
2(RS)-ethyl-2-methyl-3-methyl-1-butanol	483.0	484.2	550.4	613.2	672.8	729.2	782.5	832.7	879.8
2,2-diethyl-1-butanol	488.4	489.7	556.1	618.9	678.4	734.7	787.9	838.0	885.0
2,2,3,3-tetramethyl-1-butanol	450.4	451.7	518.8	582.6	643.3	700.7	754.8	805.8	853.4
2-isopropyl-3-methyl-1-butanol	483.6	484.9	549.9	611.6	670.2	725.8	778.3	827.9	874.5

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

T/K	298.15	300	400	500	600	700	800	900	1000
CH4O									
methanol	-201.17	-201.25	-204.81	-207.94	-210.62	-212.88	-214.68	-216.15	-217.28
C2H6O									
ethanol	-234.81	-234.89	-239.83	-243.97	-247.32	-250.04	-252.17	-253.76	-254.93
C3H8O									
1-propanol	-257.53	-257.65	-264.05	-269.45	-273.88	-277.36	-280.08	-282.04	-283.38
2-propanol	-272.59	-272.71	-278.86	-283.76	-287.61	-290.62	-292.84	-294.39	-295.31
C4H10O									
1-butanol	-274.43	-274.60	-282.34	-288.82	-294.05	-298.11	-301.25	-303.47	-304.85
2(RS)-butanol	-292.29	-292.46	-299.83	-305.93	-310.79	-314.55	-317.40	-319.36	-320.62
2-methyl-1-propanol	-285.77	-285.93	-293.60	-300.00	-305.12	-309.06	-311.93	-313.92	-315.21
2-methyl-2-propanol	-312.63	-312.80	-320.08	-325.93	-330.54	-334.05	-336.60	-338.36	-339.36
C5H12O									
1-pentanol	-297.0	-297.2	-306.1	-313.6	-319.6	-324.2	-327.5	-329.8	-331.3
2(RS)-pentanol	-315.3	-315.5	-324.1	-331.3	-337.0	-341.2	-344.3	-346.3	-347.5
3-pentanol	-315.3	-315.5	-324.1	-331.3	-337.0	-341.2	-344.3	-346.3	-347.5
2(RS)-methyl-1-butanol	-303.0	-303.2	-312.2	-319.7	-325.6	-330.2	-333.4	-335.6	-337.0
2-methyl-2-butanol	-331.5	-331.7	-340.2	-347.2	-352.7	-356.8	-359.7	-361.5	-362.6
3-methyl-2(RS)-butanol	-321.3	-321.5	-330.2	-337.4	-343.0	-347.2	-350.2	-352.1	-353.2
3-methyl-1-butanol	-303.0	-303.2	-312.2	-319.7	-325.6	-330.2	-333.4	-335.6	-337.0
2,2-dimethyl-1-propanol	-318.4	-318.6	-327.2	-334.2	-339.6	-343.5	-346.1	-347.7	-348.6
C6H14O									
1-hexanol	-317.6	-317.9	-328.1	-336.6	-343.5	-348.7	-352.4	-354.9	-356.4
2(RS)-hexanol	-335.9	-336.1	-346.1	-354.4	-360.8	-365.7	-369.1	-371.3	-372.6
3(RS)-hexanol	-335.9	-336.1	-346.1	-354.4	-360.8	-365.7	-369.1	-371.3	-372.6
2(RS)-methyl-1-pentanol	-323.7	-323.9	-334.2	-342.7	-349.5	-354.7	-358.3	-360.7	-362.1
2-methyl-2-pentanol	-352.1	-352.3	-362.2	-370.3	-376.6	-381.3	-384.5	-386.6	-387.8
2-methyl-3(RS)-pentanol	-342.0	-342.2	-352.2	-360.5	-366.9	-371.7	-375.0	-377.1	-378.3
4-methyl-2(RS)-pentanol	-342.0	-342.2	-352.2	-360.5	-366.9	-371.7	-375.0	-377.1	-378.3
4-methyl-1-pentanol	-323.7	-323.9	-334.2	-342.7	-349.5	-354.7	-358.3	-360.7	-362.1
3(RS)-methyl-1-pentanol	-323.7	-323.9	-334.2	-342.7	-349.5	-354.7	-358.3	-360.7	-362.1
3(RS)-methyl-2(RS)-pentanol	-342.0	-342.2	-352.2	-360.5	-366.9	-371.7	-375.0	-377.1	-378.3
3-methyl-3-pentanol	-352.1	-352.3	-362.2	-370.3	-376.6	-381.3	-384.5	-386.6	-387.8
2(RS),3-dimethyl-1-butanol	-329.7	-329.9	-340.3	-348.8	-355.6	-360.6	-364.2	-366.5	-367.9
2,3-dimethyl-2-butanol	-358.2	-358.4	-368.3	-376.4	-382.6	-387.3	-390.4	-392.4	-393.5
2-ethyl-1-butanol	-323.7	-323.9	-334.2	-342.7	-349.5	-354.7	-358.3	-360.7	-362.1
2,2-dimethyl-1-butanol	-332.3	-332.6	-342.5	-350.6	-356.8	-361.3	-364.3	-366.1	-367.0
3,3-dimethyl-2(RS)-butanol	-350.6	-350.8	-360.5	-368.3	-374.2	-378.3	-381.0	-382.5	-383.2
3,3-dimethyl-1-butanol	-332.3	-332.6	-342.5	-350.6	-356.8	-361.3	-364.3	-366.1	-367.0
C7H16O									
1-heptanol	-338.3	-338.5	-350.1	-359.7	-367.3	-373.1	-377.2	-380.0	-381.5
2(RS)-heptanol	-356.6	-356.8	-368.1	-377.4	-384.7	-390.2	-394.0	-396.4	-397.7
3(RS)-heptanol	-356.6	-356.8	-368.1	-377.4	-384.7	-390.2	-394.0	-396.4	-397.7
4-heptanol	-356.6	-356.8	-368.1	-377.4	-384.7	-390.2	-394.0	-396.4	-397.7

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

T/K	298.15	300	400	500	600	700	800	900	1000
5-methyl-1-hexanol	-344.3	-344.5	-356.2	-365.8	-373.4	-379.1	-383.1	-385.8	-387.3
5-methyl-2(RS)-hexanol	-362.6	-362.8	-374.2	-383.5	-390.8	-396.2	-399.9	-402.2	-403.5
5-methyl-3(RS)-hexanol	-362.6	-362.8	-374.2	-383.5	-390.8	-396.2	-399.9	-402.2	-403.5
2-methyl-3(RS)-hexanol	-362.6	-362.8	-374.2	-383.5	-390.8	-396.2	-399.9	-402.2	-403.5
2-methyl-2-hexanol	-372.8	-373.0	-384.1	-393.3	-400.5	-405.8	-409.4	-411.7	-412.9
2(RS)-methyl-1-hexanol	-344.3	-344.5	-356.2	-365.8	-373.4	-379.1	-383.1	-385.8	-387.3
4(RS)-methyl-1-hexanol	-344.3	-344.5	-356.2	-365.8	-373.4	-379.1	-383.1	-385.8	-387.3
4(RS)-methyl-2(RS)-hexanol	-362.6	-362.8	-374.2	-383.5	-390.8	-396.2	-399.9	-402.2	-403.5
4(RS)-methyl-3(RS)-hexanol	-362.6	-362.8	-374.2	-383.5	-390.8	-396.2	-399.9	-402.2	-403.5
3(RS)-methyl-3-hexanol	-372.8	-373.0	-384.1	-393.3	-400.5	-405.8	-409.4	-411.7	-412.9
3(RS)-methyl-2(RS)-hexanol	-362.6	-362.8	-374.2	-383.5	-390.8	-396.2	-399.9	-402.2	-403.5
3(RS)-methyl-1-hexanol	-344.3	-344.5	-356.2	-365.8	-373.4	-379.1	-383.1	-385.8	-387.3
4,4-dimethyl-1-pentanol	-353.0	-353.2	-364.5	-373.6	-380.6	-385.7	-389.1	-391.1	-392.1
4,4-dimethyl-2(RS)-pentanol	-371.2	-371.5	-382.5	-391.3	-398.0	-402.8	-405.8	-407.6	-408.3
2,2-dimethyl-1-pentanol	-371.2	-371.5	-382.5	-391.3	-398.0	-402.8	-405.8	-407.6	-408.3
2,2-dimethyl-1-pentanol	-353.0	-353.2	-364.5	-373.6	-380.6	-385.7	-389.1	-391.1	-392.1
3,3-dimethyl-1-pentanol	-353.0	-353.2	-364.5	-373.6	-380.6	-385.7	-389.1	-391.1	-392.1
3,3-dimethyl-2(RS)-pentanol	-371.2	-371.5	-382.5	-391.3	-398.0	-402.8	-405.8	-407.6	-408.3
3(RS),4-dimethyl-1-pentanol	-350.3	-350.6	-362.3	-371.9	-379.4	-385.1	-389.0	-391.6	-393.0
3(RS),4-dimethyl-2(RS)-pentanol	-368.6	-368.9	-380.3	-389.6	-396.8	-402.1	-405.8	-408.0	-409.2
2(RS),3(RS)-dimethyl-1-pentanol	-350.3	-350.6	-362.3	-371.9	-379.4	-385.1	-389.0	-391.6	-393.0
2,3(RS)-dimethyl-2-pentanol	-378.8	-379.0	-390.2	-399.4	-406.5	-411.8	-415.3	-417.5	-418.7
2,3(RS)-dimethyl-3-pentanol	-378.8	-379.0	-390.2	-399.4	-406.5	-411.8	-415.3	-417.5	-418.7
2(RS),4-dimethyl-1-pentanol	-350.3	-350.6	-362.3	-371.9	-379.4	-385.1	-389.0	-391.6	-393.0
2,4-dimethyl-2-pentanol	-378.8	-379.0	-390.2	-399.4	-406.5	-411.8	-415.3	-417.5	-418.7
2,4-dimethyl-3-pentanol	-368.6	-368.9	-380.3	-389.6	-396.8	-402.1	-405.8	-408.0	-409.2
2(RS)-ethyl-1-pentanol	-344.3	-344.5	-356.2	-365.8	-373.4	-379.1	-383.1	-385.8	-387.3
3-ethyl-1-pentanol	-344.3	-344.5	-356.2	-365.8	-373.4	-379.1	-383.1	-385.8	-387.3
3-ethyl-2(RS)-pentanol	-362.6	-362.8	-374.2	-383.5	-390.8	-396.2	-399.9	-402.2	-403.5
3-ethyl-3-pentanol	-372.8	-373.0	-384.1	-393.3	-400.5	-405.8	-409.4	-411.7	-412.9
2-ethyl-2-methyl-1-butanol	-353.0	-353.2	-364.5	-373.6	-380.6	-385.7	-389.1	-391.1	-392.1
2(RS)-ethyl-3-methyl-1-butanol	-350.3	-350.6	-362.3	-371.9	-379.4	-385.1	-389.0	-391.6	-393.0
2(RS),3,3-trimethyl-1-butanol	-355.6	-355.9	-367.2	-376.4	-383.4	-388.4	-391.7	-393.6	-394.5
2,3,3-trimethyl-2-butanol	-384.1	-384.3	-395.2	-403.9	-410.4	-415.0	-417.9	-419.5	-420.2
2,2,3-trimethyl-1-butanol	-355.6	-355.9	-367.2	-376.4	-383.4	-388.4	-391.7	-393.6	-394.5
C8H18O									
1-octanol	-358.9	-359.2	-372.0	-382.7	-391.2	-397.6	-402.1	-405.0	-406.7
2(RS)-octanol	-377.2	-377.5	-390.0	-400.4	-408.6	-414.6	-418.8	-421.5	-422.9
3(RS)-octanol	-377.2	-377.5	-390.0	-400.4	-408.6	-414.6	-418.8	-421.5	-422.9
4(RS)-octanol	-377.2	-377.5	-390.0	-400.4	-408.6	-414.6	-418.8	-421.5	-422.9
2(RS)-methyl-1-heptanol	-364.9	-365.2	-378.1	-388.8	-397.3	-403.6	-408.0	-410.8	-412.4
2-methyl-2-heptanol	-393.4	-393.6	-406.1	-416.4	-424.3	-430.2	-434.3	-436.7	-438.1
2-methyl-3(RS)-heptanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
2-methyl-4(RS)-heptanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
6-methyl-3(RS)-heptanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
6-methyl-2(RS)-heptanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
6-methyl-1-heptanol	-364.9	-365.2	-378.1	-388.8	-397.3	-403.6	-408.0	-410.8	-412.4
3(RS)-methyl-1-heptanol	-364.9	-365.2	-378.1	-388.8	-397.3	-403.6	-408.0	-410.8	-412.4
3(RS)-methyl-2(RS)-heptanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
3(RS)-methyl-3-heptanol	-393.4	-393.6	-406.1	-416.4	-424.3	-430.2	-434.3	-436.7	-438.1
3(RS)-methyl-4(RS)-heptanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
5(RS)-methyl-3(RS)-heptanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
5(RS)-methyl-2(RS)-heptanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
5(RS)-methyl-1-heptanol	-364.9	-365.2	-378.1	-388.8	-397.3	-403.6	-408.0	-410.8	-412.4

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

T/K	298.15	300	400	500	600	700	800	900	1000
4(RS)-methyl-1-heptanol	-364.9	-365.2	-378.1	-388.8	-397.3	-403.6	-408.0	-410.8	-412.4
4(RS)-methyl-2(RS)-heptanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
4(RS)-methyl-3(RS)-heptanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
4-methyl-4-heptanol	-393.4	-393.6	-406.1	-416.4	-424.3	-430.2	-434.3	-436.7	-438.1
2,2-dimethyl-1-hexanol	-373.6	-373.9	-386.5	-396.7	-404.5	-410.2	-414.0	-416.2	-417.3
2,2-dimethyl-3(RS)-hexanol	-391.9	-392.1	-404.5	-414.4	-421.9	-427.2	-430.7	-432.6	-433.5
5,5-dimethyl-3(RS)-hexanol	-391.9	-392.1	-404.5	-414.4	-421.9	-427.2	-430.7	-432.6	-433.5
5,5-dimethyl-2(RS)-hexanol	-391.9	-392.1	-404.5	-414.4	-421.9	-427.2	-430.7	-432.6	-433.5
5,5-dimethyl-1-hexanol	-373.6	-373.9	-386.5	-396.7	-404.5	-410.2	-414.0	-416.2	-417.3
3,3-dimethyl-1-hexanol	-373.6	-373.9	-386.5	-396.7	-404.5	-410.2	-414.0	-416.2	-417.3
3,3-dimethyl-2(RS)-hexanol	-391.9	-392.1	-404.5	-414.4	-421.9	-427.2	-430.7	-432.6	-433.5
4,4-dimethyl-3(RS)-hexanol	-391.9	-392.1	-404.5	-414.4	-421.9	-427.2	-430.7	-432.6	-433.5
4,4-dimethyl-2(RS)-hexanol	-391.9	-392.1	-404.5	-414.4	-421.9	-427.2	-430.7	-432.6	-433.5
4,4-dimethyl-1-hexanol	-373.6	-373.9	-386.5	-396.7	-404.5	-410.2	-414.0	-416.2	-417.3
4(RS),5-dimethyl-1-hexanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
4(RS),5-dimethyl-2(RS)-hexanol	-389.2	-389.5	-402.2	-412.6	-420.7	-426.6	-430.6	-433.1	-434.4
4(RS),5-dimethyl-3(RS)-hexanol	-389.2	-389.5	-402.2	-412.6	-420.7	-426.6	-430.6	-433.1	-434.4
2,3-dimethyl-3(RS)-hexanol	-399.4	-399.7	-412.2	-422.5	-430.4	-436.2	-440.2	-442.6	-443.8
2,3(RS)-dimethyl-2-hexanol	-399.4	-399.7	-412.2	-422.5	-430.4	-436.2	-440.2	-442.6	-443.8
2(RS),3(RS)-dimethyl-1-hexanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
3(RS),5-dimethyl-1-hexanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
3(RS),5-dimethyl-2(RS)-hexanol	-389.2	-389.5	-402.2	-412.6	-420.7	-426.6	-430.6	-433.1	-434.4
3(RS),5-dimethyl-3-hexanol	-399.4	-399.7	-412.2	-422.5	-430.4	-436.2	-440.2	-442.6	-443.8
2,4(RS)-dimethyl-3(RS)-hexanol	-389.2	-389.5	-402.2	-412.6	-420.7	-426.6	-430.6	-433.1	-434.4
2,4(RS)-dimethyl-2-hexanol	-399.4	-399.7	-412.2	-422.5	-430.4	-436.2	-440.2	-442.6	-443.8
2(RS),4(RS)-dimethyl-1-hexanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
2(RS),5-dimethyl-1-hexanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
2,5-dimethyl-2-hexanol	-399.4	-399.7	-412.2	-422.5	-430.4	-436.2	-440.2	-442.6	-443.8
2,5-dimethyl-3(RS)-hexanol	-389.2	-389.5	-402.2	-412.6	-420.7	-426.6	-430.6	-433.1	-434.4
3(RS),4(RS)-dimethyl-1-hexanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
3(RS),4(RS)-dimethyl-2(RS)-hexanol	-389.2	-389.5	-402.2	-412.6	-420.7	-426.6	-430.6	-433.1	-434.4
3(RS),4(RS)-dimethyl-3-hexanol	-399.4	-399.7	-412.2	-422.5	-430.4	-436.2	-440.2	-442.6	-443.8
2(RS)-ethyl-1-hexanol	-364.9	-365.2	-378.1	-388.8	-397.3	-403.6	-408.0	-410.8	-412.4
3(RS)-ethyl-1-hexanol	-364.9	-365.2	-378.1	-388.8	-397.3	-403.6	-408.0	-410.8	-412.4
3(RS)-ethyl-2(RS)-hexanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
3-ethyl-3-hexanol	-393.4	-393.6	-406.1	-416.4	-424.3	-430.2	-434.3	-436.7	-438.1
4-ethyl-3(RS)-hexanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
4-ethyl-2(RS)-hexanol	-383.2	-383.5	-396.1	-406.5	-414.6	-420.6	-424.7	-427.3	-428.6
4-ethyl-1-hexanol	-364.9	-365.2	-378.1	-388.8	-397.3	-403.6	-408.0	-410.8	-412.4
2(RS)-ethyl-2-methyl-1-pentanol	-373.6	-373.9	-386.5	-396.7	-404.5	-410.2	-414.0	-416.2	-417.3
2(RS)-isopropyl-1-pentanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
2(RS)-ethyl-4-methyl-1-pentanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
3(RS),4,4-trimethyl-1-pentanol	-376.3	-376.5	-389.2	-399.4	-407.2	-412.8	-416.5	-418.7	-419.7
3(RS),4,4-trimethyl-2(RS)-pentanol	-394.6	-394.8	-407.2	-417.1	-424.6	-429.9	-433.2	-435.1	-435.9
2,2,3(RS)-trimethyl-3-pentanol	-404.7	-405.0	-417.2	-426.9	-434.3	-439.5	-442.8	-444.6	-445.3
2,2,3(RS)-trimethyl-1-pentanol	-376.3	-376.5	-389.2	-399.4	-407.2	-412.8	-416.5	-418.7	-419.7
2(RS),4,4-trimethyl-1-pentanol	-376.3	-376.5	-389.2	-399.4	-407.2	-412.8	-416.5	-418.7	-419.7
2,4,4-trimethyl-2-pentanol	-404.7	-405.0	-417.2	-426.9	-434.3	-439.5	-442.8	-444.6	-445.3
2,2,4-trimethyl-3(RS)-pentanol	-394.6	-394.8	-407.2	-417.1	-424.6	-429.9	-433.2	-435.1	-435.9
2,2,4-trimethyl-1-pentanol	-376.3	-376.5	-389.2	-399.4	-407.2	-412.8	-416.5	-418.7	-419.7
3,3,4-trimethyl-1-pentanol	-376.3	-376.5	-389.2	-399.4	-407.2	-412.8	-416.5	-418.7	-419.7
3,3,4-trimethyl-2(RS)-pentanol	-394.6	-394.8	-407.2	-417.1	-424.6	-429.9	-433.2	-435.1	-435.9
2,3,3-trimethyl-2-pentanol	-404.7	-405.0	-417.2	-426.9	-434.3	-439.5	-442.8	-444.6	-445.3
2(RS),3,3-trimethyl-1-pentanol	-376.3	-376.5	-389.2	-399.4	-407.2	-412.8	-416.5	-418.7	-419.7
3-ethyl-3-methyl-1-pentanol	-373.6	-373.9	-386.5	-396.7	-404.5	-410.2	-414.0	-416.2	-417.3

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

T/K	298.15	300	400	500	600	700	800	900	1000
3-ethyl-3-methyl-2(RS)-pentanol	-391.9	-392.1	-404.5	-414.4	-421.9	-427.2	-430.7	-432.6	-433.5
2(RS)-ethyl-3(RS)-methyl-1-pentanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
2(RS),3(RS),4-trimethyl-1-pentanol	-373.6	-373.9	-387.0	-397.7	-406.0	-412.2	-416.4	-419.1	-420.6
2,3(RS),4-trimethyl-2-pentanol	-402.1	-402.4	-415.0	-425.2	-433.1	-438.9	-442.7	-445.0	-446.2
2,3,4-trimethyl-3-pentanol	-402.1	-402.4	-415.0	-425.2	-433.1	-438.9	-442.7	-445.0	-446.2
2-propyl-1-pentanol	-364.9	-365.2	-378.1	-388.8	-397.3	-403.6	-408.0	-410.8	-412.4
3(RS)-ethyl-4-methyl-1-pentanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
3(RS)-ethyl-4-methyl-2(RS)-pentanol	-389.2	-389.5	-402.2	-412.6	-420.7	-426.6	-430.6	-433.1	-434.4
3-ethyl-2-methyl-3-pentanol	-399.4	-399.7	-412.2	-422.5	-430.4	-436.2	-440.2	-442.6	-443.8
3-ethyl-2-methyl-2-pentanol	-399.4	-399.7	-412.2	-422.5	-430.4	-436.2	-440.2	-442.6	-443.8
3-ethyl-2(RS)-methyl-1-pentanol	-371.0	-371.2	-384.2	-394.9	-403.3	-409.6	-413.9	-416.6	-418.2
2(RS)-ethyl-3,3-dimethyl-1-butanol	-376.3	-376.5	-389.2	-399.4	-407.2	-412.8	-416.5	-418.7	-419.7
2(RS)-ethyl-2-methyl-3-methyl-1-butanol	-376.3	-376.5	-389.2	-399.4	-407.2	-412.8	-416.5	-418.7	-419.7
2,2-diethyl-1-butanol	-373.6	-373.9	-386.5	-396.7	-404.5	-410.2	-414.0	-416.2	-417.3
2,2,3,3-tetramethyl-1-butanol	-381.6	-381.9	-394.2	-403.9	-411.1	-416.1	-419.2	-420.7	-421.2
2-isopropyl-3-methyl-1-butanol	-373.6	-373.9	-387.0	-397.7	-406.0	-412.2	-416.4	-419.1	-420.6

Table 13. Standard Gibbs energy of formation for alkanols ir kJ/mol

T/K	298.15	300	400	500	600	700	800	900	1000
CH4O									
methanol	-162.46	-162.21	-148.63	-134.27	-119.23	-103.82	-88.15	-72.24	-56.15
C2H6O									
ethanol	-168.20	-167.82	-144.66	-120.36	-95.36	-69.81	-43.92	-17.75	8.56
C3H8O									
1-propanol	-162.85	-162.27	-129.47	-95.16	-59.90	-23.96	12.44	49.13	86.03
2-propanol	-173.48	-172.85	-138.63	-102.99	-66.46	-29.31	8.13	45.87	83.77
C4H10O									
1-butanol	-150.52	-149.77	-106.96	-62.35	-16.53	30.05	77.13	124.58	172.24
2(RS)-butanol	-167.17	-166.42	-123.19	-78.33	-32.34	14.36	61.52	109.06	156.76
2-methyl-1-propanol	-157.42	-156.62	-112.31	-66.23	-18.96	29.04	77.56	126.35	175.33
2-methyl-2-propanol	-177.76	-176.92	-130.47	-82.39	-33.22	16.66	66.92	117.51	168.23
C5H12O									
1-pentanol	-143.1	-142.1	-89.1	-33.9	22.6	80.0	138.0	196.4	254.9
2(RS)-pentanol	-160.6	-159.7	-106.3	-51.0	5.6	63.0	121.0	179.2	237.7
3-pentanol	-158.9	-157.9	-104.0	-48.2	9.0	67.0	125.6	184.4	243.4
2(RS)-methyl-1-butanol	-147.5	-146.5	-92.9	-37.2	19.9	77.9	136.5	195.3	254.4
2-methyl-2-butanol	-170.4	-169.4	-114.0	-56.6	2.1	61.6	121.6	181.8	242.2
3-methyl-2(RS)-butanol	-163.3	-162.3	-107.9	-51.4	6.3	64.9	124.0	183.4	242.9
3-methyl-1-butanol	-145.8	-144.8	-90.6	-34.3	23.4	81.9	141.1	200.5	260.1
2,2-dimethyl-1-propanol	-153.1	-152.1	-95.3	-36.4	23.7	84.5	145.9	207.5	269.2
C6H14O									
1-hexanol	-134.8	-133.7	-70.7	-5.3	61.7	129.6	198.2	267.2	336.3
2(RS)-hexanol	-152.3	-151.2	-88.0	-22.4	44.6	112.6	181.1	250.0	319.1
3(RS)-hexanol	-152.3	-151.2	-88.0	-22.4	44.6	112.6	181.1	250.0	319.1
2(RS)-methyl-1-pentanol	-139.2	-138.1	-74.5	-8.6	59.0	127.5	196.6	266.1	335.8
2-methyl-2-pentanol	-162.1	-160.9	-95.6	-28.0	41.1	111.1	181.7	252.6	323.7
2-methyl-3(RS)-pentanol	-155.0	-153.8	-89.5	-22.8	45.4	114.5	184.2	254.2	324.4
4-methyl-2(RS)-pentanol	-155.0	-153.8	-89.5	-22.8	45.4	114.5	184.2	254.2	324.4
4-methyl-1-pentanol	-137.5	-136.3	-72.2	-5.7	62.4	131.5	201.2	271.3	341.6
3(RS)-methyl-1-pentanol	-139.2	-138.1	-74.5	-8.6	59.0	127.5	196.6	266.1	335.8
3(RS)-methyl-2(RS)-pentanol	-156.7	-155.6	-91.8	-25.7	41.9	110.4	179.5	249.0	318.6
3-methyl-3-pentanol	-162.1	-160.9	-95.6	-28.0	41.1	111.1	181.7	252.6	323.7
2(RS),3-dimethyl-1-butanol	-141.9	-140.7	-76.0	-8.9	59.7	129.4	199.6	270.2	341.0
2,3-dimethyl-2-butanol	-164.8	-163.6	-97.1	-28.3	41.9	113.0	184.7	256.7	328.9
2-ethyl-1-butanol	-137.5	-136.3	-72.2	-5.7	62.4	131.5	201.2	271.3	341.6
2,2-dimethyl-1-butanol	-140.9	-139.7	-73.8	-5.7	63.9	134.4	205.4	276.7	348.2
3,3-dimethyl-2(RS)-butanol	-155.7	-154.5	-87.5	-18.3	52.3	123.7	195.7	267.8	340.1
3,3-dimethyl-1-butanol	-138.1	-136.9	-70.2	-1.1	69.4	140.8	212.7	285.0	357.3
C7H16O									
1-heptanol	-126.5	-125.2	-52.3	23.3	100.7	179.1	258.4	337.9	417.8
2(RS)-heptanol	-144.0	-142.7	-69.6	6.2	83.6	162.1	241.3	320.8	400.6
3(RS)-heptanol	-144.0	-142.7	-69.6	6.2	83.6	162.1	241.3	320.8	400.6
4-heptanol	-142.3	-141.0	-67.3	9.0	87.1	166.1	245.9	326.0	406.3

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

T/K	298.15	300	400	500	600	700	800	900	1000
5-methyl-1-hexanol	-129.2	-127.9	-53.8	22.9	101.5	181.0	261.4	342.1	423.0
5-methyl-2(RS)-hexanol	-146.7	-145.4	-71.1	5.8	84.4	164.0	244.3	324.9	405.8
5-methyl-3(RS)-hexanol	-146.7	-145.4	-71.1	5.8	84.4	164.0	244.3	324.9	405.8
2-methyl-3(RS)-hexanol	-146.7	-145.4	-71.1	5.8	84.4	164.0	244.3	324.9	405.8
2-methyl-2-hexanol	-153.8	-152.5	-77.2	.6	80.2	160.7	241.9	323.4	405.1
2(RS)-methyl-1-hexanol	-130.9	-129.6	-56.1	20.1	98.0	177.0	256.8	336.9	417.3
4(RS)-methyl-1-hexanol	-130.9	-129.6	-56.1	20.1	98.0	177.0	256.8	336.9	417.3
4(RS)-methyl-2(RS)-hexanol	-148.4	-147.1	-73.4	2.9	80.9	160.0	239.7	319.8	400.0
4(RS)-methyl-3(RS)-hexanol	-148.4	-147.1	-73.4	2.9	80.9	160.0	239.7	319.8	400.0
3(RS)-methyl-3-hexanol	-155.5	-154.2	-79.5	-2.2	76.7	156.6	237.3	318.2	399.4
3(RS)-methyl-2(RS)-hexanol	-148.4	-147.1	-73.4	2.9	80.9	160.0	239.7	319.8	400.0
3(RS)-methyl-1-hexanol	-130.9	-129.6	-56.1	20.1	98.0	177.0	256.8	336.9	417.3
4,4-dimethyl-1-pentanol	-129.9	-128.5	-51.8	27.5	108.4	190.3	272.9	355.7	438.8
4,4-dimethyl-2(RS)-pentanol	-147.4	-146.0	-69.1	10.3	91.4	173.3	255.8	338.6	421.6
2,2-dimethyl-1-pentanol	-147.4	-146.0	-69.1	10.3	91.4	173.3	255.8	338.6	421.6
2,2-dimethyl-1-pentanol	-132.6	-131.2	-55.4	22.9	102.9	183.9	265.6	347.5	429.6
3,3-dimethyl-1-pentanol	-132.6	-131.2	-55.4	22.9	102.9	183.9	265.6	347.5	429.6
3,3-dimethyl-2(RS)-pentanol	-150.1	-148.7	-72.7	5.8	85.9	166.9	248.5	330.4	412.4
3(RS),4-dimethyl-1-pentanol	-133.6	-132.2	-57.6	19.7	98.8	178.9	259.8	341.0	422.5
3(RS),4-dimethyl-2(RS)-pentanol	-151.1	-149.8	-74.9	2.5	81.7	161.9	242.7	323.9	405.3
2(RS),3(RS)-dimethyl-1-pentanol	-135.3	-134.0	-59.9	16.8	95.3	174.9	255.2	335.8	416.7
2,3(RS)-dimethyl-2-pentanol	-158.2	-156.8	-81.0	-2.6	77.5	158.5	240.3	322.3	404.6
2,3(RS)-dimethyl-3-pentanol	-158.2	-156.8	-81.0	-2.6	77.5	158.5	240.3	322.3	404.6
2(RS),4-dimethyl-1-pentanol	-133.6	-132.2	-57.6	19.7	98.8	178.9	259.8	341.0	422.5
2,4-dimethyl-2-pentanol	-156.5	-155.1	-78.7	.3	80.9	162.6	244.9	327.5	410.4
2,4-dimethyl-3-pentanol	-147.7	-146.3	-70.3	8.3	88.6	169.9	251.9	334.3	416.8
2(RS)-ethyl-1-pentanol	-130.9	-129.6	-56.1	20.1	98.0	177.0	256.8	336.9	417.3
3-ethyl-1-pentanol	-129.2	-127.9	-53.8	22.9	101.5	181.0	261.4	342.1	423.0
3-ethyl-2(RS)-pentanol	-146.7	-145.4	-71.1	5.8	84.4	164.0	244.3	324.9	405.8
3-ethyl-3-pentanol	-153.8	-152.5	-77.2	.6	80.2	160.7	241.9	323.4	405.1
2-ethyl-2-methyl-1-butanol	-132.6	-131.2	-55.4	22.9	102.9	183.9	265.6	347.5	429.6
2(RS)-ethyl-3-methyl-1-butanol	-133.6	-132.2	-57.6	19.7	98.8	178.9	259.8	341.0	422.5
2(RS),3,3-trimethyl-1-butanol	-130.9	-129.5	-52.3	27.6	109.1	191.5	274.7	358.0	441.6
2,3,3-trimethyl-2-butanol	-153.8	-152.4	-73.3	8.2	91.2	175.2	259.8	344.5	429.5
2,2,3-trimethyl-1-butanol	-131.9	-130.5	-53.6	25.9	107.1	189.2	272.0	355.0	438.2
C8H18O									
1-octanol	-118.2	-116.7	-33.9	51.9	139.7	228.7	318.5	408.7	499.2
2(RS)-octanol	-135.7	-134.2	-51.2	34.8	122.6	211.7	301.5	391.6	482.0
3(RS)-octanol	-135.7	-134.2	-51.2	34.8	122.6	211.7	301.5	391.6	482.0
4(RS)-octanol	-135.7	-134.2	-51.2	34.8	122.6	211.7	301.5	391.6	482.0
2(RS)-methyl-1-heptanol	-122.6	-121.1	-37.7	48.7	137.0	226.6	316.9	407.7	498.7
2-methyl-2-heptanol	-145.5	-144.0	-58.8	29.2	119.2	210.2	302.0	394.2	486.6
2-methyl-3(RS)-heptanol	-138.4	-136.9	-52.7	34.4	123.4	213.6	304.5	395.7	487.3
2-methyl-4(RS)-heptanol	-138.4	-136.9	-52.7	34.4	123.4	213.6	304.5	395.7	487.3
6-methyl-3(RS)-heptanol	-138.4	-136.9	-52.7	34.4	123.4	213.6	304.5	395.7	487.3
6-methyl-2(RS)-heptanol	-138.4	-136.9	-52.7	34.4	123.4	213.6	304.5	395.7	487.3
6-methyl-1-heptanol	-120.9	-119.4	-35.4	51.5	140.5	230.6	321.5	412.9	504.5
3(RS)-methyl-1-heptanol	-122.6	-121.1	-37.7	48.7	137.0	226.6	316.9	407.7	498.7
3(RS)-methyl-2(RS)-heptanol	-140.1	-138.6	-55.0	31.5	120.0	209.5	299.9	390.6	481.5
3(RS)-methyl-3-heptanol	-147.2	-145.7	-61.1	26.4	115.7	206.2	297.4	389.0	480.8
3(RS)-methyl-4(RS)-heptanol	-140.1	-138.6	-55.0	31.5	120.0	209.5	299.9	390.6	481.5
5(RS)-methyl-3(RS)-heptanol	-140.1	-138.6	-55.0	31.5	120.0	209.5	299.9	390.6	481.5
5(RS)-methyl-2(RS)-heptanol	-140.1	-138.6	-55.0	31.5	120.0	209.5	299.9	390.6	481.5
5(RS)-methyl-1-heptanol	-122.6	-121.1	-37.7	48.7	137.0	226.6	316.9	407.7	498.7

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

T/K	298.15	300	400	500	600	700	800	900	1000
4(RS)-methyl-1-heptanol	-122.6	-121.1	-37.7	48.7	137.0	226.6	316.9	407.7	498.7
4(RS)-methyl-2(RS)-heptanol	-140.1	-138.6	-55.0	31.5	120.0	209.5	299.9	390.6	481.5
4(RS)-methyl-3(RS)-heptanol	-140.1	-138.6	-55.0	31.5	120.0	209.5	299.9	390.6	481.5
4-methyl-4-heptanol	-145.5	-144.0	-58.8	29.2	119.2	210.2	302.0	394.2	486.6
2,2-dimethyl-1-hexanol	-124.3	-122.7	-37.0	51.5	142.0	233.5	325.8	418.3	511.1
2,2-dimethyl-3(RS)-hexanol	-139.1	-137.5	-50.7	38.9	130.4	222.9	316.0	409.4	503.0
5,5-dimethyl-3(RS)-hexanol	-139.1	-137.5	-50.7	38.9	130.4	222.9	316.0	409.4	503.0
5,5-dimethyl-2(RS)-hexanol	-139.1	-137.5	-50.7	38.9	130.4	222.9	316.0	409.4	503.0
5,5-dimethyl-1-hexanol	-121.6	-120.0	-33.4	56.1	147.4	239.9	333.1	426.5	520.2
3,3-dimethyl-1-hexanol	-124.3	-122.7	-37.0	51.5	142.0	233.5	325.8	418.3	511.1
3,3-dimethyl-2(RS)-hexanol	-141.8	-140.3	-54.3	34.4	124.9	216.5	308.7	401.2	493.9
4,4-dimethyl-3(RS)-hexanol	-141.8	-140.3	-54.3	34.4	124.9	216.5	308.7	401.2	493.9
4,4-dimethyl-2(RS)-hexanol	-141.8	-140.3	-54.3	34.4	124.9	216.5	308.7	401.2	493.9
4,4-dimethyl-1-hexanol	-124.3	-122.7	-37.0	51.5	142.0	233.5	325.8	418.3	511.1
4(RS),5-dimethyl-1-hexanol	-125.3	-123.8	-39.2	48.3	137.8	228.5	319.9	411.8	503.9
4(RS),5-dimethyl-2(RS)-hexanol	-142.8	-141.3	-56.5	31.1	120.7	211.4	302.9	394.7	486.7
4(RS),5-dimethyl-3(RS)-hexanol	-142.8	-141.3	-56.5	31.1	120.7	211.4	302.9	394.7	486.7
2,3-dimethyl-3(RS)-hexanol	-149.9	-148.4	-62.6	26.0	116.5	208.1	300.4	393.1	486.0
2,3(RS)-dimethyl-2-hexanol	-149.9	-148.4	-62.6	26.0	116.5	208.1	300.4	393.1	486.0
2(RS),3(RS)-dimethyl-1-hexanol	-127.0	-125.5	-41.5	45.4	134.3	224.4	315.3	406.6	498.2
3(RS),5-dimethyl-1-hexanol	-125.3	-123.8	-39.2	48.3	137.8	228.5	319.9	411.8	503.9
3(RS),5-dimethyl-2(RS)-hexanol	-142.8	-141.3	-56.5	31.1	120.7	211.4	302.9	394.7	486.7
3(RS),5-dimethyl-3-hexanol	-149.9	-148.4	-62.6	26.0	116.5	208.1	300.4	393.1	486.0
2,4(RS)-dimethyl-3(RS)-hexanol	-142.8	-141.3	-56.5	31.1	120.7	211.4	302.9	394.7	486.7
2,4(RS)-dimethyl-2-hexanol	-149.9	-148.4	-62.6	26.0	116.5	208.1	300.4	393.1	486.0
2(RS),4(RS)-dimethyl-1-hexanol	-127.0	-125.5	-41.5	45.4	134.3	224.4	315.3	406.6	498.2
2(RS),5-dimethyl-1-hexanol	-125.3	-123.8	-39.2	48.3	137.8	228.5	319.9	411.8	503.9
2,5-dimethyl-2-hexanol	-148.2	-146.6	-60.3	28.9	119.9	212.1	305.1	398.3	491.8
2,5-dimethyl-3(RS)-hexanol	-141.1	-139.6	-54.2	34.0	124.2	215.5	307.5	399.9	492.5
3(RS),4(RS)-dimethyl-1-hexanol	-127.0	-125.5	-41.5	45.4	134.3	224.4	315.3	406.6	498.2
3(RS),4(RS)-dimethyl-2(RS)-hexanol	-144.5	-143.0	-58.8	28.3	117.3	207.4	298.3	389.5	480.9
3(RS),4(RS)-dimethyl-3-hexanol	-151.6	-150.1	-64.9	23.1	113.0	204.1	295.8	387.9	480.3
2(RS)-ethyl-1-hexanol	-122.6	-121.1	-37.7	48.7	137.0	226.6	316.9	407.7	498.7
3(RS)-ethyl-1-hexanol	-122.6	-121.1	-37.7	48.7	137.0	226.6	316.9	407.7	498.7
3(RS)-ethyl-2(RS)-hexanol	-140.1	-138.6	-55.0	31.5	120.0	209.5	299.9	390.6	481.5
3-ethyl-3-hexanol	-145.5	-144.0	-58.8	29.2	119.2	210.2	302.0	394.2	486.6
4-ethyl-3(RS)-hexanol	-138.4	-136.9	-52.7	34.4	123.4	213.6	304.5	395.7	487.3
4-ethyl-2(RS)-hexanol	-138.4	-136.9	-52.7	34.4	123.4	213.6	304.5	395.7	487.3
4-ethyl-1-hexanol	-120.9	-119.4	-35.4	51.5	140.5	230.6	321.5	412.9	504.5
2(RS)-ethyl-2-methyl-1-pentanol	-126.0	-124.5	-39.3	48.6	138.5	229.5	321.1	413.1	505.3
2(RS)-isopropyl-1-pentanol	-125.3	-123.8	-39.2	48.3	137.8	228.5	319.9	411.8	503.9
2(RS)-ethyl-4-methyl-1-pentanol	-125.3	-123.8	-39.2	48.3	137.8	228.5	319.9	411.8	503.9
3(RS),4,4-trimethyl-1-pentanol	-122.6	-121.0	-33.9	56.2	148.1	241.1	334.8	428.8	523.0
3(RS),4,4-trimethyl-2(RS)-pentanol	-140.1	-138.6	-51.2	39.0	131.0	224.1	317.8	411.7	505.8
2,2,3(RS)-trimethyl-3-pentanol	-147.2	-145.6	-57.3	33.9	126.8	220.7	315.3	410.1	505.1
2,2,3(RS)-trimethyl-1-pentanol	-125.3	-123.8	-37.5	51.6	142.6	234.7	327.5	420.6	513.9
2(RS),4,4-trimethyl-1-pentanol	-122.6	-121.0	-33.9	56.2	148.1	241.1	334.8	428.8	523.0
2,4,4-trimethyl-2-pentanol	-145.5	-143.9	-55.0	36.8	130.3	224.8	319.9	415.3	510.9
2,2,4-trimethyl-3(RS)-pentanol	-138.4	-136.8	-48.9	41.9	134.5	228.1	322.4	416.9	511.6
2,2,4-trimethyl-1-pentanol	-123.6	-122.1	-35.2	54.5	146.1	238.7	332.1	425.8	519.7
3,3,4-trimethyl-1-pentanol	-123.6	-122.1	-35.2	54.5	146.1	238.7	332.1	425.8	519.7
3,3,4-trimethyl-2(RS)-pentanol	-141.1	-139.6	-52.5	37.3	129.0	221.7	315.1	408.7	502.4
2,3,3-trimethyl-2-pentanol	-148.2	-146.7	-58.6	32.2	124.8	218.4	312.6	407.1	501.8
2(RS),3,3-trimethyl-1-pentanol	-125.3	-123.8	-37.5	51.6	142.6	234.7	327.5	420.6	513.9
3-ethyl-3-methyl-1-pentanol	-124.3	-122.7	-37.0	51.5	142.0	233.5	325.8	418.3	511.1

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

T/K	298.15	300	400	500	600	700	800	900	1000
3-ethyl-3-methyl-2(RS)-pentanol	-141.8	-140.3	-54.3	34.4	124.9	216.5	308.7	401.2	493.9
2(RS)-ethyl-3(RS)-methyl-1-pentanol	-127.0	-125.5	-41.5	45.4	134.3	224.4	315.3	406.6	498.2
2(RS),3(RS),4-trimethyl-1-pentanol	-126.3	-124.8	-39.7	48.4	138.4	229.7	321.7	414.1	506.7
2,3(RS),4-trimethyl-2-pentanol	-149.2	-147.7	-60.8	29.0	120.6	213.3	306.8	400.6	494.6
2,3,4-trimethyl-3-pentanol	-147.5	-146.0	-58.5	31.8	124.1	217.4	311.4	405.8	500.4
2-propyl-1-pentanol	-120.9	-119.4	-35.4	51.5	140.5	230.6	321.5	412.9	504.5
3(RS)-ethyl-4-methyl-1-pentanol	-125.3	-123.8	-39.2	48.3	137.8	228.5	319.9	411.8	503.9
3(RS)-ethyl-4-methyl-2(RS)-pentanol	-142.8	-141.3	-56.5	31.1	120.7	211.4	302.9	394.7	486.7
3-ethyl-2-methyl-3-pentanol	-148.2	-146.6	-60.3	28.9	119.9	212.1	305.1	398.3	491.8
3-ethyl-2-methyl-2-pentanol	-148.2	-146.6	-60.3	28.9	119.9	212.1	305.1	398.3	491.8
3-ethyl-2(RS)-methyl-1-pentanol	-125.3	-123.8	-39.2	48.3	137.8	228.5	319.9	411.8	503.9
2(RS)-ethyl-3,3-dimethyl-1-butanol	-122.6	-121.0	-33.9	56.2	148.1	241.1	334.8	428 8	523.0
2(RS)-ethyl-2-methyl-3-methyl-1-butanol	-125.3	-123.8	-37.5	51.6	142.6	234.7	327.5	420 6	513.9
2,2-diethyl-1-butanol	-124.3	-122.7	-37.0	51.5	142.0	233.5	325.8	418 3	511.1
2,2,3,3-tetramethyl-1-butanol	-120.9	-119.3	-29.9	62.4	156.4	251.4	347.0	442 8	538.8
2-isopropyl-3-methyl-1-butanol	-122.9	-121.3	-35.1	54.1	145.3	237.7	330.9	424.5	518.3

Table 14. Log K for the formation of an alkanol isomer group and water (reaction 4)

T/K	C2H6O	C3H8O	C4H10O	C5H12O	C6H14O	C7H16O	C8H18O
298.15	1.361	1.352	1.219	.271	-.043	.377	.326
300.00	1.322	1.292	1.158	.220	-.096	.325	.275
400.00	-.677	-.924	-1.227	-1.801	-2.107	-1.722	-1.768
500.00	-1.890	-2.239	-2.614	-2.974	-3.262	-2.926	-2.970
600.00	-2.703	-3.092	-3.478	-3.727	-4.004	-3.704	-3.745
700.00	-3.285	-3.683	-4.048	-4.241	-4.505	-4.239	-4.278
800.00	-3.723	-4.111	-4.449	-4.620	-4.872	-4.627	-4.664
900.00	-4.061	-4.435	-4.745	-4.898	-5.138	-4.917	-4.952
1000.00	-4.326	-4.686	-4.971	-5.114	-5.343	-5.142	-5.175

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. This is illustrated by Table 14 which gives log K for the gas reaction

$$C_nH_{2n}\,(\text{alkene isomer group}) + H_2O = C_nH_{2n+2}O\,(\text{alkanol isomer group}), \quad (4)$$

where the reference pressure is 1 bar and ideality is assumed. It is of interest to observe that the dependence of the equilibrium constant for this reaction on temperature is greater at high carbon numbers than at low carbon numbers. The values of $\Delta_f G^\circ(\mathrm{I})$ for the alkene isomer groups are from Alberty and Gehrig,[4] and the values of $\Delta_f G^\circ$ for $H_2O(g)$ are from Stull and Prophet.[17]

8. Nomenclature

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

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

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

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

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

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

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

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

n = number of carbon atoms in a molecule

N_I = number of isomers in an isomer group

OPT = number of optical isomers

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

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

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

TSN = total symmetry number

y_i = mole fraction of isomer i within the isomer group

y_I = mole fraction of isomer group I in a mixture

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