Standard Chemical Thermodynamic Properties of Alkanethiol Isomer Groups

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The chemical thermodynamic properties of alkanethiol (RSH where R is an alkyl group) isomer groups from CH_4S to $C_4H_{10}S$ 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 $C_5H_{12}S$ to $C_8H_{18}S$ 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 alkanethiols from CH_4S to $C_8H_{18}S$ in SI units for a standard state pressure of 1 bar.

Key words: alkanethiols; 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] and alkynes.[7] This paper presents data on the alkanethiols. Chemical thermodynamic properties are given in Stull, Westrum, and Sinke[8] for all isomers in this series only through $C_4H_{10}S$. It has therefore been of interest to extend these data to $C_8H_{18}S$ by use of the Benson

group method,[9] 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 Alkanethiol Isomer Groups

When isomers are in chemical equilibrium it has been known for some time[10,11] 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

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

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

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

where y_I is the sum of the mole fractions of the individual isomers. The corresponding equations for the other standard thermodynamic properties $C_P^\circ(I)$, $S^\circ(\mathrm{I})$, 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 alkanethiols, the standard chemical thermodynamic properties for an isomer group are interrelated by

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

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. Fortunately, the numbers of stereoisomeric and nonstereoisomeric monosubstitution products of paraffins were calculated by Blair and Henze[12] in 1932. Their table was very helpful in identifying all the isomers through $C_8H_{18}S$. An expanded version of their table through $C_8H_{18}S$ is given in Table 1. The isomers are classified according to whether sulfur is bonded to a primary, secondary, or tertiary carbon and according to the numbers of chiral centers (none, one, two, or three).

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 alkanethiols 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. Therefore, the numbers of lines in tables in this article is smaller than the total numbers of isomers.

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

	Chiral Centers	Primary	Secondary	Tertiary	Total
CH4S	None	1			1
C2H6S	None	1			1
C3H8S	None	1	1		2
C4H10S	None	2		1	3
	One		1		1
	Total	2	1	1	4
C5H12S	None	3	1	1	5
	One	2	4		6
	Total	5	5	1	11
C6H14S	None	5		3	8
	One	6	10		16
	Two		4		4
	Total	11	14	3	28
C7H16S	None	8	2	4	14
	One	16	18	6	40
	Two	4	16		20
	Total	28	36	10	74
C8H18S	None	14		9	23
	One	40	38	14	92
	Two	20	52	4	76
	Three		8		8
	Total	74	98	27	199

All of the references used by Stull, Westrum, and Sinke,[8] while compiling the data for their tables on the alkanethiols, are too numerous to mention here. Scott and McCullough[13] developed the original thermodynamic tables on the alkanethiols. El-Sabban and Scott[14] published tables for eight alkanethiols, but their values have not been used here because their values for $\Delta_f H^\circ$ (298.15 K) differ by about 50 kJ mol^{-1} from those of Stull, Westrum, and Sinke,[8] and Cox and Pilcher.[15]

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

Since data are available for all of the isomers of the alkanethiols only through $C_4H_{10}S$, 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 $C_8H_{18}S$ in the ideal gas state.

In order to make these calculations, the structure of each alkanethiol species was divided into the following Benson groups; $C(H)_3(C)$, $C(H)_2(C)_2$, $C(H)(C)_3$, $C(C)_4$, $C(H)_3S$, $C(C)(H)_2S$, $C(C)_2(H)S$, $C(C)_3S$, $S(C)(H)$, and gauche corrections. In addition, the total symmetry number (TSN) and number of optical isomers (OPT) 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[16] was very helpful.

The assignment of Benson groups was checked by multiplying the matrix of numbers of groups by a matrix which had in its first column the number of carbon atoms in the group, in the second column the number of hydrogen atoms in each group, and in the third column the number of sulfur 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, hy-

Table 2. Root mean square deviations between alkanethiol 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								
CH4S	.02	.00	.00	.00	.00	.01	.01	.00	.00
C2H6S	.04	.04	.18	.63	1.35	2.21	3.17	4.20	5.22
C3H8S	.57	.55	.63	.61	.49	.35	.18	.16	.32
C4H10S	.54	.55	.88	.59	.84	1.94	3.33	4.83	6.30
	Standard entropy in J/K mol								
CH4S	.01	.04	.04	.05	.05	.05	.06	.06	.04
C2H6S	.28	.27	.25	.35	.52	.81	1.16	1.59	2.08
C3H8S	1.13	1.12	1.07	1.09	1.09	1.12	1.10	1.09	1.05
C4H10S	2.19	2.18	2.08	2.05	2.05	2.09	2.19	2.40	2.78
	Standard enthalpy of formation in kJ/mol								
CH4S	.13	.13	.15	.13	.14	.16	.13	.14	.11
C2H6S	.88	.90	.86	.79	.69	.54	.24	.10	.56
C3H8S	.62	.62	.62	.65	.64	.67	.71	.71	.72
C4H10S	1.07	1.06	1.08	1.12	1.14	1.20	1.27	1.48	1.88
	Standard Gibbs energy of formation in kJ/mol								
CH4S	.14	.15	.17	.17	.18	.20	.19	.21	.17
C2H6S	.95	.97	.94	.95	.99	1.09	1.14	1.30	1.49
C3H8S	.95	.95	1.04	1.16	1.23	1.35	1.45	1.55	1.65
C4H10S	1.60	1.59	1.74	1.90	2.07	2.27	2.45	2.63	2.86

drogen atoms, and sulfur 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]

The matrix of numbers of contributions was then multiplied by the matrix of the Benson values to obtain for each species the sum of the contributions to $\Delta_f H^\circ_{298}$, $S^\circ_{\text{int}298}$, C°_{P298}, C°_{P300}, C°_{P500}, C°_{P700}, and C°_{P1000}. In further steps in the calculation the heat capacity values were fit to the equation

$$C^\circ_P = a + \frac{b}{\sqrt{T}} + \frac{c}{T^2} + \frac{d}{T}, \tag{4}$$

and the values of a, b, c, and d were used to calculate C°_P, S°, and $\Delta_f H^\circ$ from 298.15 to 3000 K.

$$S^\circ = S^\circ_0 + a \ln T - 2bT^{-1/2} - (c/2)T^{-2} - d/T - R \ln \text{TSN}, \tag{5}$$

$$\Delta_f H^\circ = \Delta_f H^\circ_0 + aT + 2bT^{1/2} - c/T + d \ln T - n(H^\circ - H^\circ_{298})_{\text{graph}} - (n+1)(H^\circ - H^\circ_{298})\text{H}_2 - (H^\circ - H^\circ_{298})_S, \tag{6}$$

where n is the number of carbon atoms. The values of $\Delta_f G^\circ$ at various temperatures were then calculated using Eq. (3). The values of $H^\circ - H^\circ_{298}$ and S° for graphite, $H_2(g)$, and sulfur in its standard state were obtained from the JANAF[17] tables.

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

T/K	CH4S	C2H6S	C3H8S	C4H10S	C5H12S	C6H14S	C7H16S	C8H18S
298.15	50.25	72.68	106.38	164.09	169.0	202.7	218.7	236.1
300.00	50.42	72.97	106.83	164.93	169.6	203.1	219.4	237.0
400.00	58.74	88.20	127.70	186.31	197.7	228.6	257.4	284.2
500.00	66.57	101.92	144.58	195.08	221.7	256.4	292.1	326.2
600.00	73.51	113.85	159.37	207.30	243.1	282.4	322.7	362.1
700.00	79.62	124.18	172.60	221.05	262.4	305.6	349.6	393.0
800.00	85.02	133.18	184.59	234.68	279.6	326.1	373.2	420.0
900.00	89.79	141.04	195.45	247.62	295.0	344.3	394.1	443.6
1000.00	94.06	148.03	205.24	259.60	308.8	360.5	412.6	464.5

Table 3a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	22.43	33.70	57.71	4.9	33.7	15.9	17.5
300.00	22.55	33.86	58.10	4.6	33.6	16.2	17.6
400.00	29.46	39.50	58.61	11.4	31.0	28.8	26.8
500.00	35.35	42.66	50.50	26.6	34.8	35.6	34.1
600.00	40.33	45.52	47.93	35.8	39.3	40.3	39.4
700.00	44.56	48.42	48.45	41.3	43.3	44.0	43.4
800.00	48.16	51.41	50.09	44.9	46.6	47.1	46.8
900.00	51.25	54.41	52.17	47.4	49.3	49.7	49.6
1000.00	53.97	57.21	54.36	49.2	51.7	52.0	52.0

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

T/K	CH4S	C2H6S	C3H8S	C4H10S	C5H12S	C6H14S	C7H16S	C8H18S
298.15	255.17	296.21	329.13	350.76	405.4	446.9	490.8	536.0
300.00	255.50	296.67	329.83	351.78	406.5	448.1	492.1	537.4
400.00	271.15	319.81	363.55	403.04	459.2	509.9	560.5	612.1
500.00	285.12	340.98	393.94	445.52	506.0	564.0	621.7	680.2
600.00	297.89	360.65	421.59	482.12	548.3	613.0	677.7	742.9
700.00	309.68	378.97	447.17	515.11	587.2	658.4	729.6	801.1
800.00	320.69	396.17	471.04	545.51	623.4	700.5	777.8	855.4
900.00	330.98	412.32	493.40	573.91	657.3	740.0	823.0	906.2
1000.00	340.65	427.55	514.51	600.62	689.1	777.2	865.5	954.1

Table 4a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	41.05	32.92	21.63	54.7	41.5	43.9	45.2
300.00	41.17	33.15	21.96	54.7	41.7	44.0	45.3
400.00	48.66	43.74	39.49	56.2	50.7	50.6	51.6
500.00	55.86	52.96	51.58	60.4	58.0	57.8	58.4
600.00	62.76	60.95	60.53	66.2	64.7	64.7	65.1
700.00	69.29	68.20	67.94	72.1	71.1	71.2	71.5
800.00	75.48	74.88	74.46	77.9	77.1	77.3	77.6
900.00	81.34	81.08	80.51	83.4	82.8	83.0	83.2
1000.00	86.90	86.96	86.11	88.4	88.1	88.3	88.6

Table 2 shows how well the chemical thermodynamic properties calculated using the Benson method agree with the values from Stull, Westrum, and Sinke[8] for CH_4S through $C_4H_{10}S$. 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_4S, C_2H_6S, and C_3H_8S this yields the magnitudes of the deviations, and for $C_4H_{10}S$ it yields the root-mean-square deviations at various temperatures.

4. Tables of Standard Thermodynamic Properties of Alkanethiol 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.[18]

The remaining tables in this paper have all been calculated using values from Stull, Westrum, and Sinke for CH_4S to $C_4H_{10}S$ and values calculated using the Benson method for $C_5H_{12}S$, $C_6H_{14}S$, $C_7H_{16}S$, and $C_8H_{18}S$ species. Tables 3–8 give isomer group properties and the increments per carbon atom. Table 7 gives $H°(I,T) - H°(I,298.15\ K)$, the standard enthalpy for an isomer group relative to the isomer group at 298.15 K. Table 8 gives values for $H°(I,T) - H°(I, 298.15\ K) + \Delta_f H°(I,298.15\ K)$, 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.

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

T/K	CH4S	C2H6S	C3H8S	C4H10S	C5H12S	C6H14S	C7H16S	C8H18S
298.15	-22.97	-46.11	-75.16	-106.39	-125.6	-148.7	-171.4	-193.5
300.00	-23.05	-46.19	-75.27	-106.48	-125.7	-148.8	-171.6	-193.7
400.00	-29.04	-53.51	-82.80	-111.86	-134.4	-158.3	-182.7	-206.4
500.00	-33.85	-59.37	-88.76	-116.68	-141.5	-166.4	-191.8	-216.7
600.00	-37.87	-64.10	-93.64	-121.14	-147.3	-173.0	-199.1	-224.8
700.00	-41.21	-67.86	-97.42	-124.84	-151.9	-178.2	-204.8	-230.9
800.00	-98.62	-125.56	-154.98	-182.35	-209.9	-236.6	-263.5	-290.0
900.00	-99.70	-126.65	-155.80	-183.10	-211.1	-237.9	-265.0	-291.7
1000.00	-100.46	-127.28	-155.96	-183.05	-211.3	-238.3	-265.4	-292.2

Table 5a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-23.14	-29.06	-31.23	-19.2	-23.1	-22.7	-22.0
300.00	-23.14	-29.08	-31.21	-19.2	-23.1	-22.8	-22.1
400.00	-24.48	-29.29	-29.06	-22.6	-23.9	-24.4	-23.7
500.00	-25.52	-29.39	-27.92	-24.9	-24.9	-25.4	-24.8
600.00	-26.23	-29.54	-27.50	-26.2	-25.7	-26.1	-25.6
700.00	-26.65	-29.56	-27.41	-27.0	-26.3	-26.6	-26.2
800.00	-26.94	-29.42	-27.38	-27.6	-26.7	-26.9	-26.5
900.00	-26.94	-29.16	-27.30	-28.0	-26.9	-27.1	-26.7
1000.00	-26.82	-28.68	-27.09	-28.3	-26.9	-27.1	-26.8

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

T/K	CH4S	C2H6S	C3H8S	C4H10S	C5H12S	C6H14S	C7H16S	C8H18S
298.15	-9.90	-4.60	-2.80	.19	5.4	10.6	15.4	20.7
300.00	-9.83	-4.33	-2.36	.83	6.2	11.6	16.6	22.0
400.00	-4.78	10.45	22.83	37.14	51.3	66.3	80.8	95.6
500.00	1.86	27.10	49.92	74.91	98.5	123.4	147.8	172.4
600.00	9.39	44.86	78.11	113.66	147.1	182.0	216.4	251.0
700.00	17.62	63.46	107.17	153.20	196.7	241.6	286.2	330.9
800.00	20.94	77.10	131.28	187.83	241.4	296.6	351.4	406.2
900.00	35.93	102.52	167.13	234.11	297.9	363.3	428.3	493.3
1000.00	51.09	128.03	203.04	280.50	354.5	430.1	505.3	580.6

Table 6a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	5.30	1.80	2.99	5.2	5.2	4.8	5.3
300.00	5.50	1.97	3.19	5.4	5.4	5.0	5.4
400.00	15.23	12.38	14.31	14.1	15.0	14.6	14.8
500.00	25.24	22.82	24.99	23.6	24.8	24.4	24.6
600.00	35.47	33.25	35.55	33.5	34.8	34.4	34.6
700.00	45.85	43.70	46.03	43.5	45.0	44.6	44.7
800.00	56.17	54.18	56.55	53.6	55.2	54.8	54.8
900.00	66.59	64.61	66.98	63.8	65.4	65.0	65.0
1000.00	76.94	75.02	77.46	74.0	75.7	75.2	75.2

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

T/K	CH4S	C2H6S	C3H8S	C4H10S	C5H12S	C6H14S	C7H16S	C8H18S
298.15	.00	.00	.00	.00	.0	.0	.0	.0
300.00	.08	.15	.20	.29	.3	.4	.4	.4
400.00	5.53	8.18	11.95	18.11	18.7	21.9	24.3	26.6
500.00	11.82	17.68	25.59	37.15	39.7	46.2	51.8	57.2
600.00	18.82	28.48	40.75	57.23	63.0	73.1	82.5	91.7
700.00	26.47	40.42	57.38	78.66	88.3	102.6	116.2	129.5
800.00	34.74	53.27	75.25	101.44	115.4	134.2	152.4	170.2
900.00	43.47	67.01	94.26	125.54	144.1	167.7	190.7	213.4
1000.00	52.69	81.49	114.34	150.96	174.3	203.0	231.1	258.8

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	.05	.09	.0	.1	.0	.0
400.00	2.66	3.76	6.17	.6	3.2	2.3	2.3
500.00	5.86	7.91	11.56	2.6	6.5	5.6	5.4
600.00	9.66	12.27	16.49	5.7	10.2	9.4	9.1
700.00	13.95	16.96	21.28	9.6	14.3	13.6	13.3
800.00	18.53	21.98	26.19	13.9	18.8	18.2	17.8
900.00	23.54	27.25	31.28	18.6	23.6	23.0	22.6
1000.00	28.80	32.85	36.62	23.4	28.7	28.1	27.7

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

T/K	CH4S	C2H6S	C3H8S	C4H10S	C5H12S	C6H14S	C7H16S	C8H18S
298.15	-22.97	-46.11	-75.16	-106.39	-125.6	-148.7	-171.4	-193.5
300.00	-22.89	-45.95	-74.96	-106.10	-125.3	-148.3	-171.0	-193.0
400.00	-17.44	-37.92	-60.22	-88.28	-106.9	-126.8	-147.2	-166.9
500.00	-11.15	-28.43	-49.58	-69.25	-85.9	-102.5	-119.7	-136.3
600.00	-4.15	-17.63	-34.42	-49.16	-62.6	-75.5	-88.9	-101.8
700.00	3.50	-5.69	-17.78	-27.73	-37.3	-46.1	-55.3	-64.0
800.00	11.77	7.16	.08	-4.95	-10.2	-14.5	-19.1	-23.3
900.00	20.50	20.90	19.10	19.15	18.5	19.0	19.3	19.9
1000.00	29.72	35.38	39.17	44.56	48.7	54.3	59.6	65.4

Table 8a. Increments per carbon atom

T/K	C2-C1	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-23.14	-29.06	-31.23	-19.2	-23.1	-22.7	-22.0
300.00	-23.07	-29.01	-31.14	-19.2	-23.1	-22.7	-22.0
400.00	-20.48	-25.29	-25.06	-18.6	-19.9	-20.4	-19.7
500.00	-17.28	-21.15	-19.67	-16.6	-16.7	-17.2	-16.6
600.00	-13.48	-16.79	-14.74	-13.4	-12.9	-13.3	-12.9
700.00	-9.19	-12.09	-9.95	-9.6	-8.8	-9.1	-8.7
800.00	-4.61	-7.08	-5.04	-5.2	-4.3	-4.6	-4.2
900.00	.41	-1.81	.05	-.6	.5	.3	.6
1000.00	5.66	3.80	5.39	4.2	5.5	5.4	5.7

Table 9. Equilibrium mole fractions within alkanethiol isomer groups

T/K	298.15	300	400	500	600	700	800	900	1000
C3H8S									
1-propanethiol	.1277	.1301	.2550	.3604	.4329	.4896	.5320	.5634	.5896
2-propanethiol	.8723	.8699	.7450	.6396	.5671	.5104	.4680	.4366	.4104
C4H10S									
1-butanethiol	.0118	.0124	.0624	.1277	.1889	.2397	.2824	.3186	.3537
2(RS)-butanethiol	.1147	.1176	.2625	.3372	.3616	.3648	.3614	.3547	.3449
2-methyl-1-propanethiol	.1082	.1107	.2218	.2675	.2742	.2695	.2586	.2474	.2341
2-methyl-2-propanethiol	.7653	.7593	.4532	.2675	.1752	.1259	.0975	.0793	.0672
C5H12S									
1-pentanethiol	.0036	.0038	.0178	.0395	.0629	.0851	.1051	.1229	.1389
2(RS)-pentanethiol	.0987	.1005	.1843	.2335	.2578	.2687	.2728	.2732	.2715
3-pentanethiol	.0493	.0502	.0922	.1167	.1289	.1344	.1364	.1366	.1357
2(RS)-methyl-1-butanethiol	.0214	.0219	.0563	.0864	.1080	.1229	.1336	.1417	.1482
2-methyl-2-butanethiol	.3174	.3153	.2150	.1526	.1161	.0939	.0794	.0693	.0618
3-methyl-2(RS)-butanethiol	.2906	.2915	.2912	.2556	.2213	.1942	.1735	.1576	.1449
3-methyl-1-butanethiol	.0107	.0110	.0282	.0432	.0540	.0615	.0668	.0709	.0741
2,2-dimethyl-1-propanethiol	.2083	.2059	.1150	.0724	.0511	.0394	.0324	.0279	.0249
C6H14S									
1-hexanethiol	.0010	.0011	.0064	.0158	.0271	.0386	.0496	.0598	.0692
2(RS)-hexanethiol	.0282	.0289	.0659	.0934	.1111	.1221	.1288	.1329	.1352
3(RS)-hexanethiol	.0282	.0289	.0659	.0934	.1111	.1221	.1288	.1329	.1352
2(RS)-methyl-1-pentanethiol	.0061	.0063	.0201	.0346	.0465	.0558	.0631	.0689	.0738
2-methyl-2-pentanethiol	.0908	.0907	.0768	.0611	.0501	.0426	.0375	.0337	.0308
2-methyl-3(RS)-pentanethiol	.0831	.0839	.1040	.1023	.0954	.0882	.0819	.0766	.0722
4-methyl-2(RS)-pentanethiol	.0831	.0839	.1040	.1023	.0954	.0882	.0819	.0766	.0722
4-methyl-1-pentanethiol	.0031	.0032	.0101	.0173	.0233	.0279	.0315	.0345	.0369
3(RS)-methyl-1-pentanethiol	.0061	.0063	.0201	.0346	.0465	.0558	.0631	.0689	.0738
3(RS)-methyl-2(RS)-pentanethiol	.1662	.1677	.2081	.2046	.1907	.1764	.1639	.1533	.1443
3-methyl-3-pentanethiol	.0908	.0907	.0768	.0611	.0501	.0426	.0375	.0337	.0308
2(RS),3-dimethyl-1-butanethiol	.0180	.0183	.0318	.0379	.0399	.0403	.0401	.0398	.0394
2,3-dimethyl-2-butanethiol	.2674	.2632	.1213	.0669	.0430	.0308	.0238	.0194	.0164
2-ethyl-1-butanethiol	.0031	.0032	.0101	.0173	.0233	.0279	.0315	.0345	.0369
2,2-dimethyl-1-butanethiol	.0120	.0121	.0165	.0174	.0173	.0170	.0168	.0166	.0166
3,3-dimethyl-2(RS)-butanethiol	.1089	.1075	.0567	.0343	.0236	.0179	.0145	.0123	.0108
3,3-dimethyl-1-butanethiol	.0040	.0040	.0055	.0058	.0058	.0057	.0056	.0055	.0055
C7H16S									
1-heptanethiol	.0003	.0003	.0020	.0058	.0108	.0164	.0221	.0275	.0327
2(RS)-heptanethiol	.0070	.0072	.0207	.0340	.0444	.0519	.0573	.0611	.0638
3(RS)-heptanethiol	.0070	.0072	.0207	.0340	.0444	.0519	.0573	.0611	.0638
4-heptanethiol	.0035	.0036	.0104	.0170	.0222	.0260	.0286	.0306	.0319
5-methyl-1-hexanethiol	.0008	.0008	.0032	.0063	.0093	.0119	.0140	.0159	.0174
5-methyl-2(RS)-hexanethiol	.0206	.0209	.0328	.0372	.0381	.0375	.0364	.0353	.0341
5-methyl-3(RS)-hexanethiol	.0206	.0209	.0328	.0372	.0381	.0375	.0364	.0353	.0341
2-methyl-3(RS)-hexanethiol	.0206	.0209	.0328	.0372	.0381	.0375	.0364	.0353	.0341
2-methyl-2-hexanethiol	.0226	.0227	.0242	.0222	.0200	.0181	.0167	.0155	.0145
2(RS)-methyl-1-hexanethiol	.0015	.0016	.0063	.0126	.0186	.0237	.0281	.0317	.0349
4(RS)-methyl-1-hexanethiol	.0015	.0016	.0063	.0126	.0186	.0237	.0281	.0317	.0349
4(RS)-methyl-2(RS)-hexanethiol	.0413	.0419	.0656	.0745	.0762	.0750	.0729	.0705	.0682
4(RS)-methyl-3(RS)-hexanethiol	.0413	.0419	.0656	.0745	.0762	.0750	.0729	.0705	.0682
3(RS)-methyl-3-hexanethiol	.0451	.0453	.0484	.0445	.0400	.0363	.0333	.0310	.0291
3(RS)-methyl-2(RS)-hexanethiol	.0413	.0419	.0656	.0745	.0762	.0750	.0729	.0705	.0682
3(RS)-methyl-1-hexanethiol	.0015	.0016	.0063	.0126	.0186	.0237	.0281	.0317	.0349
4,4-dimethyl-1-pentanethiol	.0010	.0010	.0017	.0021	.0023	.0024	.0025	.0026	.0026
4,4-dimethyl-2(RS)-pentanethiol	.0270	.0269	.0179	.0125	.0094	.0076	.0065	.0057	.0051
2,2-dimethyl-1-pentanethiol	.0270	.0269	.0179	.0125	.0094	.0076	.0065	.0057	.0051
2,2-dimethyl-1-pentanethiol	.0030	.0030	.0052	.0063	.0069	.0072	.0075	.0077	.0079
3,3-dimethyl-1-pentanethiol	.0030	.0030	.0052	.0063	.0069	.0072	.0075	.0077	.0079
3,3-dimethyl-2(RS)-pentanethiol	.0811	.0806	.0536	.0374	.0283	.0228	.0194	.0170	.0154
3(RS),4-dimethyl-1-pentanethiol	.0045	.0046	.0100	.0138	.0160	.0172	.0179	.0183	.0186
3(RS),4-dimethyl-2(RS)-pentanethiol	.1216	.1216	.1036	.0816	.0654	.0542	.0464	.0407	.0364
2(RS),3(RS)-dimethyl-1-pentanethiol	.0089	.0091	.0200	.0276	.0319	.0343	.0357	.0366	.0372
2,3(RS)-dimethyl-2-pentanethiol	.1328	.1315	.0764	.0487	.0343	.0262	.0212	.0179	.0155
2,3(RS)-dimethyl-3-pentanethiol	.1328	.1315	.0764	.0487	.0343	.0262	.0212	.0179	.0155
2(RS),4-dimethyl-1-pentanethiol	.0045	.0046	.0100	.0138	.0160	.0172	.0179	.0183	.0186
2,4-dimethyl-2-pentanethiol	.0664	.0657	.0382	.0243	.0172	.0131	.0106	.0089	.0078
2,4-dimethyl-3-pentanethiol	.0304	.0304	.0259	.0204	.0163	.0135	.0116	.0102	.0091
2(RS)-ethyl-1-pentanethiol	.0015	.0016	.0063	.0126	.0186	.0237	.0281	.0317	.0349
3-ethyl-1-pentanethiol	.0008	.0008	.0032	.0063	.0093	.0119	.0140	.0159	.0174
3-ethyl-2(RS)-pentanethiol	.0206	.0209	.0328	.0372	.0381	.0375	.0364	.0353	.0341
3-ethyl-3-pentanethiol	.0226	.0227	.0242	.0222	.0200	.0181	.0167	.0155	.0145
2-ethyl-2-methyl-1-butanethiol	.0030	.0030	.0052	.0063	.0069	.0072	.0075	.0077	.0079
2(RS)-ethyl-3-methyl-1-butanethiol	.0045	.0046	.0100	.0138	.0160	.0172	.0179	.0183	.0186
2(RS),3,3-trimethyl-1-butanethiol	.0015	.0015	.0020	.0021	.0020	.0020	.0019	.0019	.0019
2,3,3-trimethyl-2-butanethiol	.0225	.0220	.0076	.0036	.0022	.0015	.0011	.0009	.0008
2,2,3-trimethyl-1-butanethiol	.0023	.0023	.0030	.0031	.0030	.0029	.0029	.0028	.0028
C8H18S									
1-octanethiol	.0001	.0001	.0007	.0022	.0045	.0071	.0099	.0127	.0155
2(RS)-octanethiol	.0021	.0021	.0071	.0130	.0182	.0225	.0258	.0283	.0302
3(RS)-octanethiol	.0021	.0021	.0071	.0130	.0182	.0225	.0258	.0283	.0302
4(RS)-octanethiol	.0021	.0021	.0071	.0130	.0182	.0225	.0258	.0283	.0302
2(RS)-methyl-1-heptanethiol	.0004	.0005	.0022	.0048	.0076	.0103	.0126	.0147	.0165
2-methyl-2-heptanethiol	.0066	.0067	.0083	.0085	.0082	.0079	.0075	.0072	.0069
2-methyl-3(RS)-heptanethiol	.0061	.0062	.0112	.0142	.0157	.0162	.0164	.0163	.0161
2-methyl-4(RS)-heptanethiol	.0061	.0062	.0112	.0142	.0157	.0162	.0164	.0163	.0161
6-methyl-3(RS)-heptanethiol	.0061	.0062	.0112	.0142	.0157	.0162	.0164	.0163	.0161
6-methyl-2(RS)-heptanethiol	.0061	.0062	.0112	.0142	.0157	.0162	.0164	.0163	.0161
6-methyl-1-heptanethiol	.0002	.0002	.0011	.0024	.0038	.0051	.0063	.0073	.0083
3(RS)-methyl-1-heptanethiol	.0004	.0005	.0022	.0048	.0076	.0103	.0126	.0147	.0165
3(RS)-methyl-2(RS)-heptanethiol	.0121	.0123	.0225	.0285	.0313	.0325	.0328	.0327	.0323
3(RS)-methyl-3-heptanethiol	.0132	.0134	.0166	.0170	.0164	.0157	.0150	.0144	.0138
3(RS)-methyl-4(RS)-heptanethiol	.0121	.0123	.0225	.0285	.0313	.0325	.0328	.0327	.0323
5(RS)-methyl-3(RS)-heptanethiol	.0121	.0123	.0225	.0285	.0313	.0325	.0328	.0327	.0323
5(RS)-methyl-2(RS)-heptanethiol	.0121	.0123	.0225	.0285	.0313	.0325	.0328	.0327	.0323
5(RS)-methyl-1-heptanethiol	.0004	.0005	.0022	.0048	.0076	.0103	.0126	.0147	.0165
4(RS)-methyl-1-heptanethiol	.0004	.0005	.0022	.0048	.0076	.0103	.0126	.0147	.0165

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

T/K	298.15	300	400	500	600	700	800	900	1000
4(RS)-methyl-2(RS)-heptanethiol	.0121	.0123	.0225	.0285	.0313	.0325	.0328	.0327	.0323
4(RS)-methyl-3(RS)-heptanethiol	.0121	.0123	.0225	.0285	.0313	.0325	.0328	.0327	.0323
4-methyl-4-heptanethiol	.0066	.0067	.0083	.0085	.0082	.0079	.0075	.0072	.0069
2,2-dimethyl-1-hexanethiol	.0009	.0009	.0018	.0024	.0028	.0031	.0034	.0035	.0037
2,2-dimethyl-3(RS)-hexanethiol	.0079	.0079	.0061	.0048	.0039	.0033	.0029	.0026	.0024
5,5-dimethyl-3(RS)-hexanethiol	.0079	.0079	.0061	.0048	.0039	.0033	.0029	.0026	.0024
5,5-dimethyl-2(RS)-hexanethiol	.0079	.0079	.0061	.0048	.0039	.0033	.0029	.0026	.0024
5,5-dimethyl-1-hexanethiol	.0003	.0003	.0006	.0008	.0009	.0010	.0011	.0012	.0012
3,3-dimethyl-1-hexanethiol	.0009	.0009	.0018	.0024	.0028	.0031	.0034	.0035	.0037
3,3-dimethyl-2(RS)-hexanethiol	.0238	.0237	.0184	.0143	.0116	.0099	.0087	.0079	.0073
4,4-dimethyl-3(RS)-hexanethiol	.0238	.0237	.0184	.0143	.0116	.0099	.0087	.0079	.0073
4,4-dimethyl-2(RS)-hexanethiol	.0238	.0237	.0184	.0143	.0116	.0099	.0087	.0079	.0073
4,4-dimethyl-1-hexanethiol	.0009	.0009	.0018	.0024	.0028	.0031	.0034	.0035	.0037
4(RS),5-dimethyl-1-hexanethiol	.0013	.0013	.0034	.0053	.0066	.0074	.0080	.0085	.0088
4(RS),5-dimethyl-2(RS)-hexanethiol	.0357	.0358	.0355	.0312	.0269	.0235	.0209	.0188	.0172
4(RS),5-dimethyl-3(RS)-hexanethiol	.0357	.0358	.0355	.0312	.0269	.0235	.0209	.0188	.0172
2,3-dimethyl-3(RS)-hexanethiol	.0390	.0387	.0262	.0186	.0141	.0113	.0095	.0083	.0073
2,3(RS)-dimethyl-2-hexanethiol	.0390	.0387	.0262	.0186	.0141	.0113	.0095	.0083	.0073
2(RS),3(RS)-dimethyl-1-hexanethiol	.0026	.0027	.0069	.0105	.0131	.0149	.0161	.0169	.0176
3(RS),5-dimethyl-1-hexanethiol	.0013	.0013	.0034	.0053	.0066	.0074	.0080	.0085	.0088
3(RS),5-dimethyl-2(RS)-hexanethiol	.0357	.0358	.0355	.0312	.0269	.0235	.0209	.0188	.0172
3(RS),5-dimethyl-3-hexanethiol	.0390	.0387	.0262	.0186	.0141	.0113	.0095	.0083	.0073
2,4(RS)-dimethyl-3(RS)-hexanethiol	.0357	.0358	.0355	.0312	.0269	.0235	.0209	.0188	.0172
2,4(RS)-dimethyl-2-hexanethiol	.0390	.0387	.0262	.0186	.0141	.0113	.0095	.0083	.0073
2(RS),4(RS)-dimethyl-1-hexanethiol	.0026	.0027	.0069	.0105	.0131	.0149	.0161	.0169	.0176
2(RS),5-dimethyl-1-hexanethiol	.0013	.0013	.0034	.0053	.0066	.0074	.0080	.0085	.0088
2,5-dimethyl-2-hexanethiol	.0195	.0194	.0131	.0093	.0071	.0057	.0048	.0041	.0037
2,5-dimethyl-3(RS)-hexanethiol	.0179	.0179	.0178	.0156	.0134	.0117	.0104	.0094	.0086
3(RS),4(RS)-dimethyl-1-hexanethiol	.0026	.0027	.0069	.0105	.0131	.0149	.0161	.0169	.0176
3(RS),4(RS)-dimethyl-2(RS)-hexanethiol	.0714	.0716	.0711	.0623	.0538	.0469	.0417	.0377	.0345
3(RS),4(RS)-dimethyl-3-hexanethiol	.0780	.0775	.0525	.0372	.0282	.0227	.0191	.0166	.0147
2(RS)-ethyl-1-hexanethiol	.0004	.0005	.0022	.0048	.0076	.0103	.0126	.0147	.0165
3(RS)-ethyl-1-hexanethiol	.0004	.0005	.0022	.0048	.0076	.0103	.0126	.0147	.0165
3(RS)-ethyl-2(RS)-hexanethiol	.0121	.0123	.0225	.0285	.0313	.0325	.0328	.0327	.0323
3-ethyl-3-hexanethiol	.0066	.0067	.0083	.0085	.0082	.0079	.0075	.0072	.0069
4-ethyl-3(RS)-hexanethiol	.0061	.0062	.0112	.0142	.0157	.0162	.0164	.0163	.0161
4-ethyl-2(RS)-hexanethiol	.0061	.0062	.0112	.0142	.0157	.0162	.0164	.0163	.0161
4-ethyl-1-hexanethiol	.0002	.0002	.0011	.0024	.0038	.0051	.0063	.0073	.0083
2(RS)-ethyl-2-methyl-1-pentanethiol	.0018	.0018	.0036	.0048	.0057	.0063	.0067	.0071	.0074
2(RS)-isopropyl-1-pentanethiol	.0013	.0013	.0034	.0053	.0066	.0074	.0080	.0085	.0088
2(RS)-ethyl-4-methyl-1-pentanethiol	.0013	.0013	.0034	.0053	.0066	.0074	.0080	.0085	.0088
3(RS),4,4-trimethyl-1-pentanethiol	.0004	.0005	.0007	.0008	.0008	.0008	.0009	.0009	.0009
3(RS),4,4-trimethyl-2(RS)-pentanethiol	.0121	.0120	.0071	.0047	.0034	.0027	.0022	.0019	.0017
2,2,3(RS)-trimethyl-3-pentanethiol	.0132	.0130	.0052	.0028	.0018	.0013	.0010	.0009	.0007
2,2,3(RS)-trimethyl-1-pentanethiol	.0013	.0014	.0021	.0024	.0025	.0025	.0026	.0026	.0027
2(RS),4,4-trimethyl-1-pentanethiol	.0004	.0005	.0007	.0008	.0008	.0008	.0009	.0009	.0009
2,4,4-trimethyl-2-pentanethiol	.0066	.0065	.0026	.0014	.0009	.0006	.0005	.0004	.0004
2,2,4-trimethyl-3(RS)-pentanethiol	.0061	.0060	.0035	.0023	.0017	.0013	.0011	.0010	.0009
2,2,4-trimethyl-1-pentanethiol	.0007	.0007	.0010	.0012	.0012	.0013	.0013	.0013	.0013
3,3,4-trimethyl-1-pentanethiol	.0007	.0007	.0010	.0012	.0012	.0013	.0013	.0013	.0013
3,3,4-trimethyl-2(RS)-pentanethiol	.0182	.0180	.0106	.0070	.0051	.0040	.0033	.0029	.0026
2,3,3-trimethyl-2-pentanethiol	.0199	.0195	.0078	.0042	.0027	.0019	.0015	.0013	.0011
2(RS),3,3-trimethyl-1-pentanethiol	.0013	.0014	.0021	.0024	.0025	.0025	.0026	.0026	.0027
3-ethyl-3-methyl-1-pentanethiol	.0009	.0009	.0018	.0024	.0028	.0031	.0034	.0035	.0037
3-ethyl-3-methyl-2(RS)-pentanethiol	.0238	.0237	.0184	.0143	.0116	.0099	.0087	.0079	.0073
2(RS)-ethyl-3(RS)-methyl-1-pentanethiol	.0026	.0027	.0069	.0105	.0131	.0149	.0161	.0169	.0176
2(RS),3(RS),4-trimethyl-1-pentanethiol	.0020	.0020	.0040	.0052	.0058	.0060	.0062	.0062	.0063
2,3(RS),4-trimethyl-2-pentanethiol	.0298	.0294	.0152	.0091	.0062	.0046	.0037	.0031	.0026
2,3,4-trimethyl-3-pentanethiol	.0149	.0147	.0076	.0046	.0031	.0023	.0018	.0015	.0013
2-propyl-1-pentanethiol	.0002	.0002	.0011	.0024	.0038	.0051	.0063	.0073	.0083
3(RS)-ethyl-4-methyl-1-pentanethiol	.0013	.0013	.0034	.0053	.0066	.0074	.0080	.0085	.0088
3(RS)-ethyl-4-methyl-2(RS)-pentanethiol	.0357	.0358	.0355	.0312	.0269	.0235	.0209	.0188	.0172
3-ethyl-2-methyl-3-pentanethiol	.0195	.0194	.0131	.0093	.0071	.0057	.0048	.0041	.0037
3-ethyl-2-methyl-2-pentanethiol	.0195	.0194	.0131	.0093	.0071	.0057	.0048	.0041	.0037
3-ethyl-2(RS)-methyl-1-pentanethiol	.0013	.0013	.0034	.0053	.0066	.0074	.0080	.0085	.0088
2(RS)-ethyl-3,3-dimethyl-1-butanethiol	.0004	.0005	.0007	.0008	.0008	.0008	.0009	.0009	.0009
2(RS)-ethyl-2-methyl-3-methyl-1-butanethiol	.0013	.0014	.0021	.0024	.0025	.0025	.0026	.0026	.0027
2,2-diethyl-1-butanethiol	.0009	.0009	.0018	.0024	.0028	.0031	.0034	.0035	.0037
2,2,3,3-tetramethyl-1-butanethiol	.0002	.0002	.0002	.0002	.0002	.0001	.0001	.0001	.0001
2-isopropyl-3-methyl-1-butanethiol	.0005	.0005	.0010	.0013	.0014	.0015	.0015	.0016	.0016

5. Equilibrium Mole Fractions Within Alkanethiol Isomer Groups

The equilibrium mole fractions within isomer groups calculated from standard Gibbs energies of formation are given in Table 9 for the alkanethiols in the ideal gas state. Since the uncertainties in $\Delta_f G°(I)$ and $\Delta_f G_i^\circ$ are about the same, the uncertainty in the difference is nearly independent of the relative values of the two parameters, but the absolute uncertainty does increase with temperature. 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, 1979.[19]

6. Standard Thermodynamic Properties of Individual Alkanethiol Species

The values of C_P°, $S°$, $\Delta_f H°$, and $\Delta_f G°$ for all the alkanethiol species through $C_8H_{18}S$ are given in Tables 10–13 in SI units for a standard state pressure of 1 bar. The values for CH_4S through $C_4H_{10}S$ have been converted from the tables of Stull, Westrum, and Sinke[8] and the values for $C_5H_{12}S$ through $C_8H_{18}S$ have been calculated using the Benson method.[9] The values for chiral forms are for the racemates.

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

T/K	298.15	300	400	500	600	700	800	900	1000
CH4S									
methanethiol	50.25	50.42	58.74	66.57	73.51	79.62	85.02	89.79	94.06
C2H6S									
ethanethiol	72.68	72.97	88.20	101.92	113.85	124.18	133.18	141.04	148.03
C3H8S									
1-propanethiol	94.77	95.19	116.57	136.23	153.64	168.91	182.42	194.43	205.06
2-propanethiol	95.98	96.40	118.62	138.32	154.89	168.95	181.00	191.38	200.50
C4H10S									
1-butanethiol	118.16	118.70	146.23	171.84	194.72	214.93	232.97	249.12	263.38
2(RS)-butanethiol	119.29	119.83	148.03	173.09	194.22	212.05	227.15	240.04	251.12
2-methyl-1-propanethiol	118.32	118.87	147.74	172.80	193.55	210.66	224.97	237.15	247.57
2-methyl-2-propanethiol	120.96	121.50	151.17	177.36	199.16	217.23	232.34	245.22	256.23
C5H12S									
1-pentanethiol	141.3	142.0	175.6	206.1	232.6	255.4	275.3	292.7	308.1
2(RS)-pentanethiol	142.0	142.6	176.9	207.5	233.3	255.0	273.5	289.5	303.4
3-pentanethiol	142.0	142.6	176.9	207.5	233.3	255.0	273.5	289.5	303.4
2(RS)-methyl-1-butanethiol	140.2	140.8	175.3	206.4	233.2	256.2	276.0	293.4	308.8
2-methyl-2-butanethiol	143.8	144.4	179.4	211.2	237.3	258.6	276.2	290.9	303.4
3-methyl-2(RS)-butanethiol	140.9	141.5	176.7	207.8	233.9	255.8	274.3	290.2	304.0
3-methyl-1-butanethiol	140.2	140.8	175.3	206.4	233.2	256.2	276.0	293.4	308.8
2,2-dimethyl-1-propanethiol	142.3	143.0	179.6	212.1	239.4	262.4	282.0	298.8	313.5
C6H14S									
1-hexanethiol	164.2	165.0	204.7	240.6	271.7	298.4	321.6	341.9	359.8
2(RS)-hexanethiol	164.9	165.6	206.0	242.0	272.4	298.0	319.8	338.6	355.0
3(RS)-hexanethiol	164.9	165.6	206.0	242.0	272.4	298.0	319.8	338.6	355.0
2(RS)-methyl-1-pentanethiol	163.1	163.9	204.4	240.9	272.3	299.2	322.3	342.6	360.4
2-methyl-2-pentanethiol	166.7	167.4	208.4	245.7	276.4	301.6	322.5	340.1	355.0
2-methyl-3(RS)-pentanethiol	163.8	164.5	205.7	242.3	273.0	298.8	320.6	339.3	355.6
4-methyl-2(RS)-pentanethiol	163.8	164.5	205.7	242.3	273.0	298.8	320.6	339.3	355.6
4-methyl-1-pentanethiol	163.1	163.9	204.4	240.9	272.3	299.2	322.3	342.6	360.4
3(RS)-methyl-1-pentanethiol	163.1	163.9	204.4	240.9	272.3	299.2	322.3	342.6	360.4
3(RS)-methyl-2(RS)-pentanethiol	163.8	164.5	205.7	242.3	273.0	298.8	320.6	339.3	355.6
3-methyl-3-pentanethiol	166.7	167.4	208.4	245.7	276.4	301.6	322.5	340.1	355.0
2(RS),3-dimethyl-1-butanethiol	162.0	162.7	204.1	241.3	272.9	299.9	323.1	343.3	361.0
2,3-dimethyl-2-butanethiol	165.6	166.3	208.2	246.0	277.0	302.4	323.3	340.8	355.7
2-ethyl-1-butanethiol	163.1	163.9	204.4	240.9	272.3	299.2	322.3	342.6	360.4
2,2-dimethyl-1-butanethiol	165.2	166.0	208.7	246.6	278.5	305.4	328.3	348.0	365.1
3,3-dimethyl-2(RS)-butanethiol	165.9	166.7	210.0	248.0	279.3	305.0	326.5	344.7	360.3
3,3-dimethyl-1-butanethiol	165.2	166.0	208.7	246.6	278.5	305.4	328.3	348.0	365.1
C7H16S									
1-heptanethiol	187.1	188.0	233.7	275.2	310.8	341.4	367.9	391.0	411.4
2(RS)-heptanethiol	187.8	188.7	235.1	276.5	311.5	341.0	366.1	387.8	406.6
3(RS)-heptanethiol	187.8	188.7	235.1	276.5	311.5	341.0	366.1	387.8	406.6
4-heptanethiol	187.8	188.7	235.1	276.5	311.5	341.0	366.1	387.8	406.6
5-methyl-1-hexanethiol	186.0	186.9	233.5	275.5	311.4	342.2	368.6	391.7	412.0
5-methyl-2(RS)-hexanethiol	186.7	187.5	234.8	276.8	312.1	341.8	366.9	388.5	407.2
5-methyl-3(RS)-hexanethiol	186.7	187.5	234.8	276.8	312.1	341.8	366.9	388.5	407.2
2-methyl-3(RS)-hexanethiol	186.7	187.5	234.8	276.8	312.1	341.8	366.9	388.5	407.2
2-methyl-2-hexanethiol	189.6	190.4	237.5	280.2	315.6	344.7	368.8	389.2	406.7
2(RS)-methyl-1-hexanethiol	186.0	186.9	233.5	275.5	311.4	342.2	368.6	391.7	412.0
4(RS)-methyl-1-hexanethiol	186.0	186.9	233.5	275.5	311.4	342.2	368.6	391.7	412.0
4(RS)-methyl-2(RS)-hexanethiol	186.7	187.5	234.8	276.8	312.1	341.8	366.9	388.5	407.2
4(RS)-methyl-3(RS)-hexanethiol	186.7	187.5	234.8	276.8	312.1	341.8	366.9	388.5	407.2
3(RS)-methyl-3-hexanethiol	189.6	190.4	237.5	280.2	315.6	344.7	368.8	389.2	406.7
3(RS)-methyl-2(RS)-hexanethiol	186.7	187.5	234.8	276.8	312.1	341.8	366.9	388.5	407.2
3(RS)-methyl-1-hexanethiol	186.0	186.9	233.5	275.5	311.4	342.2	368.6	391.7	412.0
4,4-dimethyl-1-pentanethiol	188.1	189.0	237.7	281.1	317.7	348.4	374.6	397.1	416.8
4,4-dimethyl-2(RS)-pentanethiol	188.8	189.7	239.1	282.5	318.4	348.0	372.8	393.9	412.0
2,2-dimethyl-1-pentanethiol	188.8	189.7	239.1	282.5	318.4	348.0	372.8	393.9	412.0
2,2-dimethyl-1-pentanethiol	188.1	189.0	237.7	281.1	317.7	348.4	374.6	397.1	416.8
3,3-dimethyl-1-pentanethiol	188.1	189.0	237.7	281.1	317.7	348.4	374.6	397.1	416.8
3,3-dimethyl-2(RS)-pentanethiol	188.8	189.7	239.1	282.5	318.4	348.0	372.8	393.9	412.0
3(RS),4-dimethyl-1-pentanethiol	184.9	185.7	233.2	275.8	312.0	342.9	369.4	392.4	412.6
3(RS),4-dimethyl-2(RS)-pentanethiol	185.5	186.4	234.5	277.1	312.8	342.5	367.6	389.2	407.8
2(RS),3(RS)-dimethyl-1-pentanethiol	184.9	185.7	233.2	275.8	312.0	342.9	369.4	392.4	412.6
2,3(RS)-dimethyl-2-pentanethiol	188.5	189.3	237.2	280.5	316.2	345.4	369.6	389.9	407.3
2,3(RS)-dimethyl-3-pentanethiol	188.5	189.3	237.2	280.5	316.2	345.4	369.6	389.9	407.3
2(RS),4-dimethyl-1-pentanethiol	184.9	185.7	233.2	275.8	312.0	342.9	369.4	392.4	412.6
2,4-dimethyl-2-pentanethiol	188.5	189.3	237.2	280.5	316.2	345.4	369.6	389.9	407.3
2,4-dimethyl-3-pentanethiol	185.5	186.4	234.5	277.1	312.8	342.5	367.6	389.2	407.8
2(RS)-ethyl-1-pentanethiol	186.0	186.9	233.5	275.5	311.4	342.2	368.6	391.7	412.0
3-ethyl-1-pentanethiol	186.0	186.9	233.5	275.5	311.4	342.2	368.6	391.7	412.0
3-ethyl-2(RS)-pentanethiol	186.7	187.5	234.8	276.8	312.1	341.8	366.9	388.5	407.2
3-ethyl-3-pentanethiol	189.6	190.4	237.5	280.2	315.6	344.7	368.8	389.2	406.7
2-ethyl-2-methyl-1-butanethiol	188.1	189.0	237.7	281.1	317.7	348.4	374.6	397.1	416.8
2(RS)-ethyl-3-methyl-1-butanethiol	184.9	185.7	233.2	275.8	312.0	342.9	369.4	392.4	412.6
2(RS),3,3-trimethyl-1-butanethiol	187.0	187.9	237.5	281.4	318.3	349.2	375.4	397.8	417.4
2,3,3-trimethyl-2-butanethiol	190.6	191.5	241.5	286.2	322.4	351.7	375.6	395.4	412.0
2,2,3-trimethyl-1-butanethiol	187.0	187.9	237.5	281.4	318.3	349.2	375.4	397.8	417.4
C8H18S									
1-octanethiol	210.1	211.0	262.8	309.7	349.9	384.4	414.2	440.2	463.1
2(RS)-octanethiol	210.7	211.7	264.1	311.1	350.7	384.0	412.4	436.9	458.3
3(RS)-octanethiol	210.7	211.7	264.1	311.1	350.7	384.0	412.4	436.9	458.3
4(RS)-octanethiol	210.7	211.7	264.1	311.1	350.7	384.0	412.4	436.9	458.3
2(RS)-methyl-1-heptanethiol	208.9	209.9	262.6	310.0	350.6	385.2	415.0	440.9	463.7
2-methyl-2-heptanethiol	212.5	213.4	266.6	314.7	354.7	387.7	415.2	438.4	458.3
2-methyl-3(RS)-heptanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
2-methyl-4(RS)-heptanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
6-methyl-3(RS)-heptanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
6-methyl-2(RS)-heptanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
6-methyl-1-heptanethiol	208.9	209.9	262.6	310.0	350.6	385.2	415.0	440.9	463.7
3(RS)-methyl-1-heptanethiol	208.9	209.9	262.6	310.0	350.6	385.2	415.0	440.9	463.7
3(RS)-methyl-2(RS)-heptanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
3(RS)-methyl-3-heptanethiol	212.5	213.4	266.6	314.7	354.7	387.7	415.2	438.4	458.3
3(RS)-methyl-4(RS)-heptanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
5(RS)-methyl-3(RS)-heptanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
5(RS)-methyl-2(RS)-heptanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
5(RS)-methyl-1-heptanethiol	208.9	209.9	262.6	310.0	350.6	385.2	415.0	440.9	463.7

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

T/K	298.15	300	400	500	600	700	800	900	1000
4(RS)-methyl-1-heptanethiol	208.9	209.9	262.6	310.0	350.6	385.2	415.0	440.9	463.7
4(RS)-methyl-2(RS)-heptanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
4(RS)-methyl-3(RS)-heptanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
4-methyl-4-heptanethiol	212.5	213.4	266.6	314.7	354.7	387.7	415.2	438.4	458.3
2,2-dimethyl-1-hexanethiol	211.1	212.1	266.8	315.6	356.8	391.4	420.9	446.3	468.4
2,2-dimethyl-3(RS)-hexanethiol	211.7	212.7	268.1	317.0	357.5	391.0	419.1	443.0	463.6
5,5-dimethyl-3(RS)-hexanethiol	211.7	212.7	268.1	317.0	357.5	391.0	419.1	443.0	463.6
5,5-dimethyl-2(RS)-hexanethiol	211.7	212.7	268.1	317.0	357.5	391.0	419.1	443.0	463.6
5,5-dimethyl-1-hexanethiol	211.1	212.1	266.8	315.6	356.8	391.4	420.9	446.3	468.4
3,3-dimethyl-1-hexanethiol	211.1	212.1	266.8	315.6	356.8	391.4	420.9	446.3	468.4
3,3-dimethyl-2(RS)-hexanethiol	211.7	212.7	268.1	317.0	357.5	391.0	419.1	443.0	463.6
4,4-dimethyl-3(RS)-hexanethiol	211.7	212.7	268.1	317.0	357.5	391.0	419.1	443.0	463.6
4,4-dimethyl-2(RS)-hexanethiol	211.7	212.7	268.1	317.0	357.5	391.0	419.1	443.0	463.6
4,4-dimethyl-1-hexanethiol	211.1	212.1	266.8	315.6	356.8	391.4	420.9	446.3	468.4
4(RS),5-dimethyl-1-hexanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
4(RS),5-dimethyl-2(RS)-hexanethiol	208.4	209.4	263.6	311.7	351.9	385.5	413.9	438.3	459.5
4(RS),5-dimethyl-3(RS)-hexanethiol	208.4	209.4	263.6	311.7	351.9	385.5	413.9	438.3	459.5
2,3-dimethyl-3(RS)-hexanethiol	211.4	212.3	266.3	315.0	355.3	388.4	415.9	439.1	458.9
2,3(RS)-dimethyl-2-hexanethiol	211.4	212.3	266.3	315.0	355.3	388.4	415.9	439.1	458.9
2(RS),3(RS)-dimethyl-1-hexanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
3(RS),5-dimethyl-1-hexanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
3(RS),5-dimethyl-2(RS)-hexanethiol	208.4	209.4	263.6	311.7	351.9	385.5	413.9	438.3	459.5
3(RS),5-dimethyl-3-hexanethiol	211.4	212.3	266.3	315.0	355.3	388.4	415.9	439.1	458.9
2,4(RS)-dimethyl-3(RS)-hexanethiol	208.4	209.4	263.6	311.7	351.9	385.5	413.9	438.3	459.5
2,4(RS)-dimethyl-2-hexanethiol	211.4	212.3	266.3	315.0	355.3	388.4	415.9	439.1	458.9
2(RS),4(RS)-dimethyl-1-hexanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
2(RS),5-dimethyl-1-hexanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
2,5-dimethyl-2-hexanethiol	211.4	212.3	266.3	315.0	355.3	388.4	415.9	439.1	458.9
2,5-dimethyl-3(RS)-hexanethiol	208.4	209.4	263.6	311.7	351.9	385.5	413.9	438.3	459.5
3(RS),4(RS)-dimethyl-1-hexanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
3(RS),4(RS)-dimethyl-2(RS)-hexanethiol	208.4	209.4	263.6	311.7	351.9	385.5	413.9	438.3	459.5
3(RS),4(RS)-dimethyl-3-hexanethiol	211.4	212.3	266.3	315.0	355.3	388.4	415.9	439.1	458.9
2(RS)-ethyl-1-hexanethiol	208.9	209.9	262.6	310.0	350.6	385.2	415.0	440.9	463.7
3(RS)-ethyl-1-hexanethiol	208.9	209.9	262.6	310.0	350.6	385.2	415.0	440.9	463.7
3(RS)-ethyl-2(RS)-hexanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
3-ethyl-3-hexanethiol	212.5	213.4	266.6	314.7	354.7	387.7	415.2	438.4	458.3
4-ethyl-3(RS)-hexanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
4-ethyl-2(RS)-hexanethiol	209.6	210.5	263.9	311.4	351.3	384.8	413.2	437.6	458.9
4-ethyl-1-hexanethiol	208.9	209.9	262.6	310.0	350.6	385.2	415.0	440.9	463.7
2(RS)-ethyl-2-methyl-1-pentanethiol	211.1	212.1	266.8	315.6	356.8	391.4	420.9	446.3	468.4
2(RS)-isopropyl-1-pentanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
2(RS)-ethyl-4-methyl-1-pentanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
3(RS),4,4-trimethyl-1-pentanethiol	209.9	210.9	266.5	316.0	357.4	392.2	421.7	447.0	469.0
3(RS),4,4-trimethyl-2(RS)-pentanethiol	210.6	211.6	267.9	317.3	358.1	391.8	419.9	443.7	464.2
2,2,3(RS)-trimethyl-3-pentanethiol	213.5	214.5	270.6	320.7	361.5	394.7	421.9	444.5	463.7
2,2,3(RS)-trimethyl-1-pentanethiol	209.9	210.9	266.5	316.0	357.4	392.2	421.7	447.0	469.0
2(RS),4,4-trimethyl-1-pentanethiol	209.9	210.9	266.5	316.0	357.4	392.2	421.7	447.0	469.0
2,4,4-trimethyl-2-pentanethiol	213.5	214.5	270.6	320.7	361.5	394.7	421.9	444.5	463.7
2,2,4-trimethyl-3(RS)-pentanethiol	210.6	211.6	267.9	317.3	358.1	391.8	419.9	443.7	464.2
2,2,4-trimethyl-1-pentanethiol	209.9	210.9	266.5	316.0	357.4	392.2	421.7	447.0	469.0
3,3,4-trimethyl-1-pentanethiol	209.9	210.9	266.5	316.0	357.4	392.2	421.7	447.0	469.0
3,3,4-trimethyl-2(RS)-pentanethiol	210.6	211.6	267.9	317.3	358.1	391.8	419.9	443.7	464.2
2,3,3-trimethyl-2-pentanethiol	213.5	214.5	270.6	320.7	361.5	394.7	421.9	444.5	463.7
2(RS),3,3-trimethyl-1-pentanethiol	209.9	210.9	266.5	316.0	357.4	392.2	421.7	447.0	469.0
3-ethyl-3-methyl-1-pentanethiol	211.1	212.1	266.8	315.6	356.8	391.4	420.9	446.3	468.4
3-ethyl-3-methyl-2(RS)-pentanethiol	211.7	212.7	268.1	317.0	357.5	391.0	419.1	443.0	463.6
2(RS)-ethyl-3(RS)-methyl-1-pentanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
2(RS),3(RS),4-trimethyl-1-pentanethiol	206.6	207.6	262.0	310.6	351.8	386.6	416.5	442.3	464.9
2,3(RS),4-trimethyl-2-pentanethiol	210.2	211.2	266.0	315.3	355.9	389.1	416.7	439.8	459.5
2,3,4-trimethyl-3-pentanethiol	210.2	211.2	266.0	315.3	355.9	389.1	416.7	439.8	459.5
2-propyl-1-pentanethiol	208.9	209.9	262.6	310.0	350.6	385.2	415.0	440.9	463.7
3(RS)-ethyl-4-methyl-1-pentanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
3(RS)-ethyl-4-methyl-2(RS)-pentanethiol	208.4	209.4	263.6	311.7	351.9	385.5	413.9	438.3	459.5
3-ethyl-2-methyl-3-pentanethiol	211.4	212.3	266.3	315.0	355.3	388.4	415.9	439.1	458.9
3-ethyl-2-methyl-2-pentanethiol	211.4	212.3	266.3	315.0	355.3	388.4	415.9	439.1	458.9
3-ethyl-2(RS)-methyl-1-pentanethiol	207.8	208.8	262.3	310.3	351.2	385.9	415.7	441.6	464.3
2(RS)-ethyl-3,3-dimethyl-1-butanethiol	209.9	210.9	266.5	316.0	357.4	392.2	421.7	447.0	469.0
2(RS)-ethyl-2-methyl-3-methyl-1-butanethiol	209.9	210.9	266.5	316.0	357.4	392.2	421.7	447.0	469.0
2,2-diethyl-1-butanethiol	211.1	212.1	266.8	315.6	356.8	391.4	420.9	446.3	468.4
2,2,3,3-tetramethyl-1-butanethiol	212.1	213.1	270.8	321.0	363.7	398.5	427.6	452.4	473.8
2-isopropyl-3-methyl-1-butanethiol	206.6	207.6	262.0	310.6	351.8	386.6	416.5	442.3	464.9

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

T/K	298.15	300	400	500	600	700	800	900	1000
CH4S									
methanethiol	255.17	255.50	271.15	285.12	297.89	309.68	320.69	330.98	340.65
C2H6S									
ethanethiol	296.21	296.67	319.81	340.98	360.65	378.97	396.17	412.32	427.55
C3H8S									
1-propanethiol	336.50	337.13	367.47	395.62	422.02	446.88	470.35	492.52	513.57
2-propanethiol	324.41	325.04	355.88	384.49	411.23	436.17	459.56	481.48	502.15
C4H10S									
1-butanethiol	375.33	376.08	414.03	449.47	482.86	514.45	544.32	572.73	599.72
2(RS)-butanethiol	366.84	367.59	406.00	441.81	475.29	506.58	535.91	563.44	589.30
2-methyl-1-propanethiol	362.99	363.74	401.98	437.71	471.10	502.27	531.35	558.59	584.11
2-methyl-2-propanethiol	338.14	338.89	378.01	414.62	448.97	481.06	511.06	539.18	565.62
C5H12S									
1-pentanethiol	414.7	415.6	461.1	503.6	543.6	581.2	616.6	650.1	681.7
2(RS)-pentanethiol	410.5	411.4	457.1	500.0	540.2	577.8	613.1	646.2	677.5
3-pentanethiol	404.7	405.6	451.4	494.2	534.4	572.0	607.3	640.5	671.7
2(RS)-methyl-1-butanethiol	409.3	410.1	455.4	498.0	538.0	575.7	611.3	644.8	676.5
2-methyl-2-butanethiol	386.8	387.7	434.0	477.5	518.4	556.7	592.4	625.8	657.1
3-methyl-2(RS)-butanethiol	399.3	400.1	445.7	488.5	528.8	566.6	602.0	635.2	666.5
3-methyl-1-butanethiol	403.5	404.4	449.6	492.2	532.3	570.0	605.5	639.0	670.8
2,2-dimethyl-1-propanethiol	376.7	377.6	423.8	467.4	508.6	547.3	583.6	617.8	650.1
C6H14S									
1-hexanethiol	454.1	455.2	508.1	557.7	604.4	648.4	689.7	728.8	765.8
2(RS)-hexanethiol	449.9	450.9	504.1	554.1	601.0	644.9	686.2	725.0	761.5
3(RS)-hexanethiol	449.9	450.9	504.1	554.1	601.0	644.9	686.2	725.0	761.5
2(RS)-methyl-1-pentanethiol	448.7	449.7	502.4	552.1	598.8	642.9	684.4	723.5	760.6
2-methyl-2-pentanethiol	426.2	427.2	481.0	531.6	579.2	623.8	665.5	704.5	741.1
2-methyl-3(RS)-pentanethiol	438.7	439.7	492.7	542.6	589.6	633.7	675.1	713.9	750.5
4-methyl-2(RS)-pentanethiol	438.7	439.7	492.7	542.6	589.6	633.7	675.1	713.9	750.5
4-methyl-1-pentanethiol	442.9	443.9	496.7	546.3	593.1	637.1	678.6	717.8	754.8
3(RS)-methyl-1-pentanethiol	448.7	449.7	502.4	552.1	598.8	642.9	684.4	723.5	760.6
3(RS)-methyl-2(RS)-pentanethiol	444.4	445.4	498.5	548.4	595.4	639.5	680.8	719.7	756.3
3-methyl-3-pentanethiol	426.2	427.2	481.0	531.6	579.2	623.8	665.5	704.5	741.1
2(RS),3-dimethyl-1-butanethiol	437.5	438.5	491.0	540.6	587.5	631.6	673.2	712.5	749.6
2,3-dimethyl-2-butanethiol	415.0	416.0	469.6	520.2	567.9	612.6	654.3	693.5	730.2
2-ethyl-1-butanethiol	442.9	443.9	496.7	546.3	593.1	637.1	678.6	717.8	754.8
2,2-dimethyl-1-butanethiol	425.2	426.3	479.9	530.7	578.5	623.6	665.9	705.7	743.3
3,3-dimethyl-2(RS)-butanethiol	411.9	412.9	466.8	517.9	566.0	611.0	653.2	692.7	729.9
3,3-dimethyl-1-butanethiol	416.1	417.1	470.8	521.5	569.4	614.4	656.7	696.6	734.1
C7H16S									
1-heptanethiol	493.6	494.7	555.1	611.8	665.2	715.5	762.9	807.5	849.8
2(RS)-heptanethiol	489.3	490.5	551.1	608.2	661.8	712.1	759.3	803.7	845.6
3(RS)-heptanethiol	489.3	490.5	551.1	608.2	661.8	712.1	759.3	803.7	845.6
4-heptanethiol	483.5	484.7	545.4	602.4	656.0	706.3	753.5	797.9	839.8
5-methyl-1-hexanethiol	482.3	483.5	543.7	600.4	653.9	704.3	751.7	796.5	838.8
5-methyl-2(RS)-hexanethiol	478.1	479.2	539.7	596.7	650.4	700.8	748.2	792.7	834.6
5-methyl-3(RS)-hexanethiol	478.1	479.2	539.7	596.7	650.4	700.8	748.2	792.7	834.6
2-methyl-3(RS)-hexanethiol	478.1	479.2	539.7	596.7	650.4	700.8	748.2	792.7	834.6
2-methyl-2-hexanethiol	465.6	466.8	528.0	585.7	640.0	690.9	738.6	783.2	825.2
2(RS)-methyl-1-hexanethiol	488.1	489.2	549.4	606.2	659.6	710.0	757.5	802.3	844.6
4(RS)-methyl-1-hexanethiol	488.1	489.2	549.4	606.2	659.6	710.0	757.5	802.3	844.6
4(RS)-methyl-2(RS)-hexanethiol	483.8	485.0	545.5	602.5	656.2	706.6	753.9	798.4	840.3
4(RS)-methyl-3(RS)-hexanethiol	483.8	485.0	545.5	602.5	656.2	706.6	753.9	798.4	840.3
3(RS)-methyl-3-hexanethiol	471.4	472.6	533.8	591.5	645.8	696.7	744.4	789.0	830.9
3(RS)-methyl-2(RS)-hexanethiol	483.8	485.0	545.5	602.5	656.2	706.6	753.9	798.4	840.3
3(RS)-methyl-1-hexanethiol	488.1	489.2	549.4	606.2	659.6	710.0	757.5	802.3	844.6
4,4-dimethyl-1-pentanethiol	455.5	456.7	517.8	575.6	630.2	681.6	729.8	775.3	818.2
4,4-dimethyl-2(RS)-pentanethiol	451.3	452.4	513.8	572.0	626.8	678.1	726.3	771.4	813.9
2,2-dimethyl-1-pentanethiol	451.3	452.4	513.8	572.0	626.8	678.1	726.3	771.4	813.9
2,2-dimethyl-1-pentanethiol	464.7	465.8	526.9	584.8	639.3	690.7	739.0	784.4	827.3
3,3-dimethyl-1-pentanethiol	464.7	465.8	526.9	584.8	639.3	690.7	739.0	784.4	827.3
3,3-dimethyl-2(RS)-pentanethiol	460.4	461.6	523.0	581.1	635.9	687.3	735.4	780.6	823.0
3(RS),4-dimethyl-1-pentanethiol	476.9	478.0	538.0	594.7	648.3	698.8	746.3	791.2	833.6
3(RS),4-dimethyl-2(RS)-pentanethiol	472.6	473.8	534.0	591.1	644.9	695.4	742.8	787.4	829.4
2(RS),3(RS)-dimethyl-1-pentanethiol	482.6	483.8	543.8	600.5	654.1	704.5	752.1	797.0	839.4
2,3(RS)-dimethyl-2-pentanethiol	460.2	461.3	522.3	580.1	634.5	685.5	733.2	778.0	820.0
2,3(RS)-dimethyl-3-pentanethiol	460.2	461.3	522.3	580.1	634.5	685.5	733.2	778.0	820.0
2(RS),4-dimethyl-1-pentanethiol	476.9	478.0	538.0	594.7	648.3	698.8	746.3	791.2	833.6
2,4-dimethyl-2-pentanethiol	454.4	455.6	516.6	574.3	628.7	679.7	727.5	772.2	814.2
2,4-dimethyl-3-pentanethiol	461.1	462.2	522.5	579.6	633.3	683.8	731.3	775.8	817.8
2(RS)-ethyl-1-pentanethiol	488.1	489.2	549.4	606.2	659.6	710.0	757.5	802.3	844.6
3-ethyl-1-pentanethiol	482.3	483.5	543.7	600.4	653.9	704.3	751.7	796.5	838.8
3-ethyl-2(RS)-pentanethiol	478.1	479.2	539.7	596.7	650.4	700.8	748.2	792.7	834.6
3-ethyl-3-pentanethiol	465.6	466.8	528.0	585.7	640.0	690.9	738.6	783.2	825.2
2-ethyl-2-methyl-1-butanethiol	464.7	465.8	526.9	584.8	639.3	690.7	739.0	784.4	827.3
2(RS)-ethyl-3-methyl-1-butanethiol	476.9	478.0	538.0	594.7	648.3	698.8	746.3	791.2	833.6
2(RS),3,3-trimethyl-1-butanethiol	450.1	451.2	512.1	570.0	624.6	676.1	724.5	770.0	813.0
2,3,3-trimethyl-2-butanethiol	427.6	428.8	490.7	549.5	605.0	657.0	705.6	751.0	793.5
2,2,3-trimethyl-1-butanethiol	453.4	454.6	515.5	573.3	628.0	679.5	727.8	773.4	816.3
C8H18S									
1-octanethiol	533.0	534.3	602.1	665.9	726.0	782.6	836.0	886.3	933.9
2(RS)-octanethiol	528.7	530.0	598.1	662.3	722.6	779.2	832.4	882.4	929.6
3(RS)-octanethiol	528.7	530.0	598.1	662.3	722.6	779.2	832.4	882.4	929.6
4(RS)-octanethiol	528.7	530.0	598.1	662.3	722.6	779.2	832.4	882.4	929.6
2(RS)-methyl-1-heptanethiol	527.5	528.8	596.4	660.3	720.5	777.2	830.6	881.0	928.6
2-methyl-2-heptanethiol	505.0	506.4	575.0	639.8	700.9	758.1	811.7	862.0	909.2
2-methyl-3(RS)-heptanethiol	517.5	518.8	586.7	650.8	711.2	768.0	821.3	871.4	918.6
2-methyl-4(RS)-heptanethiol	517.5	518.8	586.7	650.8	711.2	768.0	821.3	871.4	918.6
6-methyl-3(RS)-heptanethiol	517.5	518.8	586.7	650.8	711.2	768.0	821.3	871.4	918.6
6-methyl-2(RS)-heptanethiol	517.5	518.8	586.7	650.8	711.2	768.0	821.3	871.4	918.6
6-methyl-1-heptanethiol	521.7	523.0	590.7	654.5	714.7	771.4	824.8	875.2	922.9
3(RS)-methyl-1-heptanethiol	527.5	528.8	596.4	660.3	720.5	777.2	830.6	881.0	928.6
3(RS)-methyl-2(RS)-heptanethiol	523.3	524.6	592.5	656.6	717.0	773.7	827.0	877.1	924.4
3(RS)-methyl-3-heptanethiol	510.8	512.1	580.8	645.6	706.6	763.8	817.5	867.7	915.0
3(RS)-methyl-4(RS)-heptanethiol	523.3	524.6	592.5	656.6	717.0	773.7	827.0	877.1	924.4
5(RS)-methyl-3(RS)-heptanethiol	523.3	524.6	592.5	656.6	717.0	773.7	827.0	877.1	924.4
5(RS)-methyl-2(RS)-heptanethiol	523.3	524.6	592.5	656.6	717.0	773.7	827.0	877.1	924.4
5(RS)-methyl-1-heptanethiol	527.5	528.8	596.4	660.3	720.5	777.2	830.6	881.0	928.6

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

T/K	298.15	300	400	500	600	700	800	900	1000
4(RS)-methyl-1-heptanethiol	527.5	528.8	596.4	660.3	720.5	777.2	830.6	881.0	928.6
4(RS)-methyl-2(RS)-heptanethiol	523.3	524.6	592.5	656.6	717.0	773.7	827.0	877.1	924.4
4(RS)-methyl-3(RS)-heptanethiol	523.3	524.6	592.5	656.6	717.0	773.7	827.0	877.1	924.4
4-methyl-4-heptanethiol	505.0	506.4	575.0	639.8	700.9	758.1	811.7	862.0	909.2
2,2-dimethyl-1-hexanethiol	504.1	505.4	573.9	638.9	700.2	757.8	812.1	863.2	911.3
2,2-dimethyl-3(RS)-hexanethiol	490.7	492.0	560.8	626.1	687.6	745.3	799.4	850.2	897.9
5,5-dimethyl-3(RS)-hexanethiol	490.7	492.0	560.8	626.1	687.6	745.3	799.4	850.2	897.9
5,5-dimethyl-2(RS)-hexanethiol	490.7	492.0	560.8	626.1	687.6	745.3	799.4	850.2	897.9
5,5-dimethyl-1-hexanethiol	494.9	496.2	564.8	629.7	691.0	748.7	802.9	854.0	902.2
3,3-dimethyl-1-hexanethiol	504.1	505.4	573.9	638.9	700.2	757.8	812.1	863.2	911.3
3,3-dimethyl-2(RS)-hexanethiol	499.8	501.1	570.0	635.2	696.7	754.4	808.5	859.3	907.1
4,4-dimethyl-3(RS)-hexanethiol	499.8	501.1	570.0	635.2	696.7	754.4	808.5	859.3	907.1
4,4-dimethyl-2(RS)-hexanethiol	499.8	501.1	570.0	635.2	696.7	754.4	808.5	859.3	907.1
4,4-dimethyl-1-hexanethiol	504.1	505.4	573.9	638.9	700.2	757.8	812.1	863.2	911.3
4(RS),5-dimethyl-1-hexanethiol	516.3	517.6	585.0	648.8	709.1	765.9	819.4	869.9	917.7
4(RS),5-dimethyl-2(RS)-hexanethiol	512.0	513.3	581.0	645.2	705.7	762.5	815.9	866.1	913.4
4(RS),5-dimethyl-3(RS)-hexanethiol	512.0	513.3	581.0	645.2	705.7	762.5	815.9	866.1	913.4
2,3-dimethyl-3(RS)-hexanethiol	499.6	500.9	569.3	634.2	695.3	752.6	806.3	856.7	904.0
2,3(RS)-dimethyl-2-hexanethiol	499.6	500.9	569.3	634.2	695.3	752.6	806.3	856.7	904.0
2(RS),3(RS)-dimethyl-1-hexanethiol	522.0	523.3	590.8	654.6	714.9	771.7	825.2	875.7	923.4
3(RS),5-dimethyl-1-hexanethiol	516.3	517.6	585.0	648.8	709.1	765.9	819.4	869.9	917.7
3(RS),5-dimethyl-2(RS)-hexanethiol	512.0	513.3	581.0	645.2	705.7	762.5	815.9	866.1	913.4
3(RS),5-dimethyl-3-hexanethiol	499.6	500.9	569.3	634.2	695.3	752.6	806.3	856.7	904.0
2,4(RS)-dimethyl-3(RS)-hexanethiol	512.0	513.3	581.0	645.2	705.7	762.5	815.9	866.1	913.4
2,4(RS)-dimethyl-2-hexanethiol	499.6	500.9	569.3	634.2	695.3	752.6	806.3	856.7	904.0
2(RS),4(RS)-dimethyl-1-hexanethiol	522.0	523.3	590.8	654.6	714.9	771.7	825.2	875.7	923.4
2(RS),5-dimethyl-1-hexanethiol	516.3	517.6	585.0	648.8	709.1	765.9	819.4	869.9	917.7
2,5-dimethyl-2-hexanethiol	493.8	495.1	563.6	628.4	689.5	746.8	800.6	850.9	898.2
2,5-dimethyl-3(RS)-hexanethiol	506.3	507.6	575.3	639.4	699.9	756.7	810.1	860.3	907.6
3(RS),4(RS)-dimethyl-1-hexanethiol	522.0	523.3	590.8	654.6	714.9	771.7	825.2	875.7	923.4
3(RS),4(RS)-dimethyl-2(RS)-hexanethiol	517.8	519.1	586.8	650.9	711.4	768.3	821.7	871.9	919.2
3(RS),4(RS)-dimethyl-3-hexanethiol	505.3	506.6	575.1	639.9	701.0	758.4	812.1	862.5	909.8
2(RS)-ethyl-1-hexanethiol	527.5	528.8	596.4	660.3	720.5	777.2	830.6	881.0	928.6
3(RS)-ethyl-1-hexanethiol	527.5	528.8	596.4	660.3	720.5	777.2	830.6	881.0	928.6
3(RS)-ethyl-2(RS)-hexanethiol	523.3	524.6	592.5	656.6	717.0	773.7	827.0	877.1	924.4
3-ethyl-3-hexanethiol	505.0	506.4	575.0	639.8	700.9	758.1	811.7	862.0	909.2
4-ethyl-3(RS)-hexanethiol	517.5	518.8	586.7	650.8	711.2	768.0	821.3	871.4	918.6
4-ethyl-2(RS)-hexanethiol	517.5	518.8	586.7	650.8	711.2	768.0	821.3	871.4	918.6
4-ethyl-1-hexanethiol	521.7	523.0	590.7	654.5	714.7	771.4	824.8	875.2	922.9
2(RS)-ethyl-2-methyl-1-pentanethiol	509.8	511.1	579.7	644.6	705.9	763.6	817.8	868.9	917.1
2(RS)-isopropyl-1-pentanethiol	516.3	517.6	585.0	648.8	709.1	765.9	819.4	869.9	917.7
2(RS)-ethyl-4-methyl-1-pentanethiol	516.3	517.6	585.0	648.8	709.1	765.9	819.4	869.9	917.7
3(RS),4,4-trimethyl-1-pentanethiol	489.5	490.8	559.1	624.1	685.4	743.2	797.6	848.7	897.0
3(RS),4,4-trimethyl-2(RS)-pentanethiol	485.2	486.5	555.2	620.4	682.0	739.8	794.0	844.9	892.7
2,2,3(RS)-trimethyl-3-pentanethiol	472.8	474.1	543.5	609.4	671.6	729.9	784.4	835.5	883.3
2,2,3(RS)-trimethyl-1-pentanethiol	498.6	499.9	568.3	633.2	694.6	752.4	806.7	857.9	906.1
2(RS),4,4-trimethyl-1-pentanethiol	489.5	490.8	559.1	624.1	685.4	743.2	797.6	848.7	897.0
2,4,4-trimethyl-2-pentanethiol	467.0	468.3	537.7	603.6	665.8	724.2	778.7	829.7	877.6
2,2,4-trimethyl-3(RS)-pentanethiol	479.5	480.8	549.4	614.7	676.2	734.1	788.3	839.1	887.0
2,2,4-trimethyl-1-pentanethiol	492.8	494.2	562.5	627.4	688.8	746.6	800.9	852.1	900.4
3,3,4-trimethyl-1-pentanethiol	492.8	494.2	562.5	627.4	688.8	746.6	800.9	852.1	900.4
3,3,4-trimethyl-2(RS)-pentanethiol	488.6	489.9	558.5	623.8	685.4	743.2	797.4	848.3	896.1
2,3,3-trimethyl-2-pentanethiol	476.1	477.5	546.8	612.8	675.0	733.3	787.8	838.9	886.7
2(RS),3,3-trimethyl-1-pentanethiol	498.6	499.9	568.3	633.2	694.6	752.4	806.7	857.9	906.1
3-ethyl-3-methyl-1-pentanethiol	504.1	505.4	573.9	638.9	700.2	757.8	812.1	863.2	911.3
3-ethyl-3-methyl-2(RS)-pentanethiol	499.8	501.1	570.0	635.2	696.7	754.4	808.5	859.3	907.1
2(RS)-ethyl-3(RS)-methyl-1-pentanethiol	522.0	523.3	590.8	654.6	714.9	771.7	825.2	875.7	923.4
2(RS),3(RS),4-trimethyl-1-pentanethiol	510.8	512.1	579.3	643.2	703.5	760.5	814.1	864.7	912.4
2,3(RS),4-trimethyl-2-pentanethiol	488.3	489.7	557.9	622.7	683.9	741.4	795.2	845.6	893.0
2,3,4-trimethyl-3-pentanethiol	482.6	483.9	552.1	617.0	678.2	735.6	789.4	839.9	887.3
2-propyl-1-pentanethiol	521.7	523.0	590.7	654.5	714.7	771.4	824.8	875.2	922.9
3(RS)-ethyl-4-methyl-1-pentanethiol	516.3	517.6	585.0	648.8	709.1	765.9	819.4	869.9	917.7
3(RS)-ethyl-4-methyl-2(RS)-pentanethiol	512.0	513.3	581.0	645.2	705.7	762.5	815.9	866.1	913.4
3-ethyl-2-methyl-3-pentanethiol	493.8	495.1	563.6	628.4	689.5	746.8	800.6	850.9	898.2
3-ethyl-2-methyl-2-pentanethiol	493.8	495.1	563.6	628.4	689.5	746.8	800.6	850.9	898.2
3-ethyl-2(RS)-methyl-1-pentanethiol	516.3	517.6	585.0	648.8	709.1	765.9	819.4	869.9	917.7
2(RS)-ethyl-3,3-dimethyl-1-butanethiol	489.5	490.8	559.1	624.1	685.4	743.2	797.6	848.7	897.0
2(RS)-ethyl-2-methyl-3-methyl-1-butanethiol	498.6	499.9	568.3	633.2	694.6	752.4	806.7	857.9	906.1
2,2-diethyl-1-butanethiol	504.1	505.4	573.9	638.9	700.2	757.8	812.1	863.2	911.3
2,2,3,3-tetramethyl-1-butanethiol	466.0	467.4	536.6	602.7	665.2	723.9	778.1	830.9	879.7
2-isopropyl-3-methyl-1-butanethiol	499.3	500.6	567.8	631.6	692.0	748.9	802.6	853.1	900.9

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

T/K	298.15	300	400	500	600	700	800	900	1000
CH4S									
methanethiol	-22.97	-23.05	-29.04	-33.85	-37.87	-41.21	-98.62	-99.70	-100.46
C2H6S									
ethanethiol	-46.11	-46.19	-53.51	-59.37	-64.10	-67.86	-125.56	-126.65	-127.28
C3H8S									
1-propanethiol	-67.86	-67.99	-76.69	-83.68	-89.20	-93.47	-151.34	-152.30	-152.51
2-propanethiol	-76.23	-76.36	-84.89	-91.63	-97.03	-101.21	-159.12	-160.33	-160.92
C4H10S									
1-butanethiol	-88.07	-88.24	-98.24	-106.15	-112.38	-116.98	-174.89	-175.60	-175.31
2(RS)-butanethiol	-96.23	-96.40	-106.29	-114.01	-120.16	-124.99	-183.26	-184.77	-185.52
2-methyl-1-propanethiol	-97.24	-97.40	-107.28	-115.10	-121.29	-126.19	-184.68	-186.44	-187.49
2-methyl-2-propanethiol	-109.50	-109.66	-119.24	-126.65	-132.34	-136.61	-194.43	-195.39	-195.60
C5H12S									
1-pentanethiol	-108.9	-109.1	-120.3	-129.3	-136.4	-141.8	-200.4	-201.8	-202.3
2(RS)-pentanethiol	-118.3	-118.5	-129.6	-138.5	-145.5	-150.9	-209.6	-211.3	-212.1
3-pentanethiol	-118.3	-118.5	-129.6	-138.5	-145.5	-150.9	-209.6	-211.3	-212.1
2(RS)-methyl-1-butanethiol	-114.9	-115.1	-126.4	-135.4	-142.4	-147.7	-206.3	-207.7	-208.0
2-methyl-2-butanethiol	-128.3	-128.5	-139.4	-147.9	-154.5	-159.5	-217.9	-219.4	-220.2
3-methyl-2(RS)-butanethiol	-124.3	-124.5	-135.7	-144.6	-151.5	-156.8	-215.5	-217.1	-217.9
3-methyl-1-butanethiol	-114.9	-115.1	-126.4	-135.4	-142.4	-147.7	-206.3	-207.7	-208.0
2,2-dimethyl-1-propanethiol	-130.2	-130.4	-141.4	-149.9	-156.3	-161.0	-219.0	-219.8	-219.6
C6H14S									
1-hexanethiol	-129.5	-129.7	-142.3	-152.3	-160.2	-166.2	-225.2	-226.9	-227.4
2(RS)-hexanethiol	-139.0	-139.2	-151.6	-161.5	-169.3	-175.3	-234.4	-236.4	-237.3
3(RS)-hexanethiol	-139.0	-139.2	-151.6	-161.5	-169.3	-175.3	-234.4	-236.4	-237.3
2(RS)-methyl-1-pentanethiol	-135.5	-135.7	-148.4	-158.4	-166.3	-172.2	-231.1	-232.8	-233.2
2-methyl-2-pentanethiol	-148.9	-149.1	-161.4	-171.0	-178.4	-184.0	-242.8	-244.5	-245.3
2-methyl-3(RS)-pentanethiol	-145.0	-145.2	-157.7	-167.6	-175.4	-181.3	-240.3	-242.2	-243.0
4-methyl-2(RS)-pentanethiol	-145.0	-145.2	-157.7	-167.6	-175.4	-181.3	-240.3	-242.2	-243.0
4-methyl-1-pentanethiol	-135.5	-135.7	-148.4	-158.4	-166.3	-172.2	-231.1	-232.8	-233.2
3(RS)-methyl-1-pentanethiol	-135.5	-135.7	-148.4	-158.4	-166.3	-172.2	-231.1	-232.8	-233.2
3(RS)-methyl-2(RS)-pentanethiol	-145.0	-145.2	-157.7	-167.6	-175.4	-181.3	-240.3	-242.2	-243.0
3-methyl-3-pentanethiol	-148.9	-149.1	-161.4	-171.0	-178.4	-184.0	-242.8	-244.5	-245.3
2(RS),3-dimethyl-1-butanethiol	-141.5	-141.8	-154.5	-164.5	-172.3	-178.2	-237.0	-238.6	-239.0
2,3-dimethyl-2-butanethiol	-154.9	-155.1	-167.5	-177.1	-184.4	-190.0	-248.7	-250.3	-251.1
2-ethyl-1-butanethiol	-135.5	-135.7	-148.4	-158.4	-166.3	-172.2	-231.1	-232.8	-233.2
2,2-dimethyl-1-butanethiol	-144.2	-144.4	-156.7	-166.2	-173.5	-178.8	-237.1	-238.2	-238.1
3,3-dimethyl-2(RS)-butanethiol	-153.6	-153.9	-166.1	-175.5	-182.6	-187.9	-246.3	-247.6	-247.9
3,3-dimethyl-1-butanethiol	-144.2	-144.4	-156.7	-166.2	-173.5	-178.8	-237.1	-238.2	-238.1
C7H16S									
1-heptanethiol	-150.1	-150.4	-164.2	-175.4	-184.1	-190.7	-250.1	-252.0	-252.6
2(RS)-heptanethiol	-159.6	-159.8	-173.6	-184.6	-193.2	-199.8	-259.3	-261.5	-262.5
3(RS)-heptanethiol	-159.6	-159.8	-173.6	-184.6	-193.2	-199.8	-259.3	-261.5	-262.5
4-heptanethiol	-159.6	-159.8	-173.6	-184.6	-193.2	-199.8	-259.3	-261.5	-262.5
5-methyl-1-hexanethiol	-156.1	-156.4	-170.3	-181.4	-190.1	-196.7	-256.0	-257.9	-258.4
5-methyl-2(RS)-hexanethiol	-165.6	-165.9	-179.7	-190.7	-199.2	-205.7	-265.2	-267.3	-268.2
5-methyl-3(RS)-hexanethiol	-165.6	-165.9	-179.7	-190.7	-199.2	-205.7	-265.2	-267.3	-268.2
2-methyl-3(RS)-hexanethiol	-165.6	-165.9	-179.7	-190.7	-199.2	-205.7	-265.2	-267.3	-268.2
2-methyl-2-hexanethiol	-169.5	-169.8	-183.4	-194.0	-202.2	-208.4	-267.6	-269.6	-270.5
2(RS)-methyl-1-hexanethiol	-156.1	-156.4	-170.3	-181.4	-190.1	-196.7	-256.0	-257.9	-258.4
4(RS)-methyl-1-hexanethiol	-156.1	-156.4	-170.3	-181.4	-190.1	-196.7	-256.0	-257.9	-258.4
4(RS)-methyl-2(RS)-hexanethiol	-165.6	-165.9	-179.7	-190.7	-199.2	-205.7	-265.2	-267.3	-268.2
4(RS)-methyl-3(RS)-hexanethiol	-165.6	-165.9	-179.7	-190.7	-199.2	-205.7	-265.2	-267.3	-268.2
3(RS)-methyl-3-hexanethiol	-169.5	-169.8	-183.4	-194.0	-202.2	-208.4	-267.6	-269.6	-270.5
3(RS)-methyl-2(RS)-hexanethiol	-165.6	-165.9	-179.7	-190.7	-199.2	-205.7	-265.2	-267.3	-268.2
3(RS)-methyl-1-hexanethiol	-156.1	-156.4	-170.3	-181.4	-190.1	-196.7	-256.0	-257.9	-258.4
4,4-dimethyl-1-pentanethiol	-164.8	-165.1	-178.7	-189.3	-197.3	-203.3	-262.0	-263.3	-263.3
4,4-dimethyl-2(RS)-pentanethiol	-174.3	-174.5	-188.0	-198.5	-206.4	-212.3	-271.2	-272.7	-273.1
2,2-dimethyl-1-pentanethiol	-174.3	-174.5	-188.0	-198.5	-206.4	-212.3	-271.2	-272.7	-273.1
2,2-dimethyl-1-pentanethiol	-164.8	-165.1	-178.7	-189.3	-197.3	-203.3	-262.0	-263.3	-263.3
3,3-dimethyl-1-pentanethiol	-164.8	-165.1	-178.7	-189.3	-197.3	-203.3	-262.0	-263.3	-263.3
3,3-dimethyl-2(RS)-pentanethiol	-174.3	-174.5	-188.0	-198.5	-206.4	-212.3	-271.2	-272.7	-273.1
3(RS),4-dimethyl-1-pentanethiol	-162.2	-162.4	-176.4	-187.5	-196.2	-202.6	-261.9	-263.7	-264.1
3(RS),4-dimethyl-2(RS)-pentanethiol	-171.6	-171.9	-185.8	-196.7	-205.3	-211.7	-271.1	-273.1	-274.0
2(RS),3(RS)-dimethyl-1-pentanethiol	-162.2	-162.4	-176.4	-187.5	-196.2	-202.6	-261.9	-263.7	-264.1
2,3(RS)-dimethyl-2-pentanethiol	-175.6	-175.8	-189.5	-200.1	-208.3	-214.4	-273.5	-275.4	-276.3
2,3(RS)-dimethyl-3-pentanethiol	-175.6	-175.8	-189.5	-200.1	-208.3	-214.4	-273.5	-275.4	-276.3
2(RS),4-dimethyl-1-pentanethiol	-162.2	-162.4	-176.4	-187.5	-196.2	-202.6	-261.9	-263.7	-264.1
2,4-dimethyl-2-pentanethiol	-175.6	-175.8	-189.5	-200.1	-208.3	-214.4	-273.5	-275.4	-276.3
2,4-dimethyl-3-pentanethiol	-171.6	-171.9	-185.8	-196.7	-205.3	-211.7	-271.1	-273.1	-274.0
2(RS)-ethyl-1-pentanethiol	-156.1	-156.4	-170.3	-181.4	-190.1	-196.7	-256.0	-257.9	-258.4
3-ethyl-1-pentanethiol	-156.1	-156.4	-170.3	-181.4	-190.1	-196.7	-256.0	-257.9	-258.4
3-ethyl-2(RS)-pentanethiol	-165.6	-165.9	-179.7	-190.7	-199.2	-205.7	-265.2	-267.3	-268.2
3-ethyl-3-pentanethiol	-169.5	-169.8	-183.4	-194.0	-202.2	-208.4	-267.6	-269.6	-270.5
2-ethyl-2-methyl-1-butanethiol	-164.8	-165.1	-178.7	-189.3	-197.3	-203.3	-262.0	-263.3	-263.3
2(RS)-ethyl-3-methyl-1-butanethiol	-162.2	-162.4	-176.4	-187.5	-196.2	-202.6	-261.9	-263.7	-264.1
2(RS),3,3-trimethyl-1-butanethiol	-167.5	-167.7	-181.4	-192.0	-200.0	-205.9	-264.5	-265.7	-265.7
2,3,3-trimethyl-2-butanethiol	-180.9	-181.1	-194.4	-204.6	-212.2	-217.7	-276.2	-277.5	-277.8
2,2,3-trimethyl-1-butanethiol	-167.5	-167.7	-181.4	-192.0	-200.0	-205.9	-264.5	-265.7	-265.7
C8H18S									
1-octanethiol	-170.7	-171.0	-186.2	-198.4	-207.9	-215.1	-275.0	-277.1	-277.8
2(RS)-octanethiol	-180.2	-180.5	-195.6	-207.6	-217.0	-224.2	-284.2	-286.6	-287.6
3(RS)-octanethiol	-180.2	-180.5	-195.6	-207.6	-217.0	-224.2	-284.2	-286.6	-287.6
4(RS)-octanethiol	-180.2	-180.5	-195.6	-207.6	-217.0	-224.2	-284.2	-286.6	-287.6
2(RS)-methyl-1-heptanethiol	-176.8	-177.1	-192.3	-204.5	-214.0	-221.1	-280.9	-282.9	-283.5
2-methyl-2-heptanethiol	-190.2	-190.4	-205.3	-217.1	-226.1	-232.9	-292.5	-294.7	-295.7
2-methyl-3(RS)-heptanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
2-methyl-4(RS)-heptanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
6-methyl-3(RS)-heptanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
6-methyl-2(RS)-heptanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
6-methyl-1-heptanethiol	-176.8	-177.1	-192.3	-204.5	-214.0	-221.1	-280.9	-282.9	-283.5
3(RS)-methyl-1-heptanethiol	-176.8	-177.1	-192.3	-204.5	-214.0	-221.1	-280.9	-282.9	-283.5
3(RS)-methyl-2(RS)-heptanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
3(RS)-methyl-3-heptanethiol	-190.2	-190.4	-205.3	-217.1	-226.1	-232.9	-292.5	-294.7	-295.7
3(RS)-methyl-4(RS)-heptanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
5(RS)-methyl-3(RS)-heptanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
5(RS)-methyl-2(RS)-heptanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
5(RS)-methyl-1-heptanethiol	-176.8	-177.1	-192.3	-204.5	-214.0	-221.1	-280.9	-282.9	-283.5

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

T/K	298.15	300	400	500	600	700	800	900	1000
4(RS)-methyl-1-heptanethiol	-176.8	-177.1	-192.3	-204.5	-214.0	-221.1	-280.9	-282.9	-283.5
4(RS)-methyl-2(RS)-heptanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
4(RS)-methyl-3(RS)-heptanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
4-methyl-4-heptanethiol	-190.2	-190.4	-205.3	-217.1	-226.1	-232.9	-292.5	-294.7	-295.7
2,2-dimethyl-1-hexanethiol	-185.4	-185.7	-200.6	-212.3	-221.2	-227.7	-286.8	-288.4	-288.5
2,2-dimethyl-3(RS)-hexanethiol	-194.9	-195.2	-210.0	-221.5	-230.3	-236.8	-296.0	-297.8	-298.3
5,5-dimethyl-3(RS)-hexanethiol	-194.9	-195.2	-210.0	-221.5	-230.3	-236.8	-296.0	-297.8	-298.3
5,5-dimethyl-2(RS)-hexanethiol	-194.9	-195.2	-210.0	-221.5	-230.3	-236.8	-296.0	-297.8	-298.3
5,5-dimethyl-1-hexanethiol	-185.4	-185.7	-200.6	-212.3	-221.2	-227.7	-286.8	-288.4	-288.5
3,3-dimethyl-1-hexanethiol	-185.4	-185.7	-200.6	-212.3	-221.2	-227.7	-286.8	-288.4	-288.5
3,3-dimethyl-2(RS)-hexanethiol	-194.9	-195.2	-210.0	-221.5	-230.3	-236.8	-296.0	-297.8	-298.3
4,4-dimethyl-3(RS)-hexanethiol	-194.9	-195.2	-210.0	-221.5	-230.3	-236.8	-296.0	-297.8	-298.3
4,4-dimethyl-2(RS)-hexanethiol	-194.9	-195.2	-210.0	-221.5	-230.3	-236.8	-296.0	-297.8	-298.3
4,4-dimethyl-1-hexanethiol	-185.4	-185.7	-200.6	-212.3	-221.2	-227.7	-286.8	-288.4	-288.5
4(RS),5-dimethyl-1-hexanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
4(RS),5-dimethyl-2(RS)-hexanethiol	-192.3	-192.5	-207.8	-219.8	-229.1	-236.2	-296.0	-298.2	-299.2
4(RS),5-dimethyl-3(RS)-hexanethiol	-192.3	-192.5	-207.8	-219.8	-229.1	-236.2	-296.0	-298.2	-299.2
2,3-dimethyl-3(RS)-hexanethiol	-196.2	-196.5	-211.4	-223.2	-232.1	-238.9	-298.4	-300.5	-301.5
2,3(RS)-dimethyl-2-hexanethiol	-196.2	-196.5	-211.4	-223.2	-232.1	-238.9	-298.4	-300.5	-301.5
2(RS),3(RS)-dimethyl-1-hexanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
3(RS),5-dimethyl-1-hexanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
3(RS),5-dimethyl-2(RS)-hexanethiol	-192.3	-192.5	-207.8	-219.8	-229.1	-236.2	-296.0	-298.2	-299.2
3(RS),5-dimethyl-3-hexanethiol	-196.2	-196.5	-211.4	-223.2	-232.1	-238.9	-298.4	-300.5	-301.5
2,4(RS)-dimethyl-3(RS)-hexanethiol	-192.3	-192.5	-207.8	-219.8	-229.1	-236.2	-296.0	-298.2	-299.2
2,4(RS)-dimethyl-2-hexanethiol	-196.2	-196.5	-211.4	-223.2	-232.1	-238.9	-298.4	-300.5	-301.5
2(RS),4(RS)-dimethyl-1-hexanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
2(RS),5-dimethyl-1-hexanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
2,5-dimethyl-2-hexanethiol	-196.2	-196.5	-211.4	-223.2	-232.1	-238.9	-298.4	-300.5	-301.5
2,5-dimethyl-3(RS)-hexanethiol	-192.3	-192.5	-207.8	-219.8	-229.1	-236.2	-296.0	-298.2	-299.2
3(RS),4(RS)-dimethyl-1-hexanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
3(RS),4(RS)-dimethyl-2(RS)-hexanethiol	-192.3	-192.5	-207.8	-219.8	-229.1	-236.2	-296.0	-298.2	-299.2
3(RS),4(RS)-dimethyl-3-hexanethiol	-196.2	-196.5	-211.4	-223.2	-232.1	-238.9	-298.4	-300.5	-301.5
2(RS)-ethyl-1-hexanethiol	-176.8	-177.1	-192.3	-204.5	-214.0	-221.1	-280.9	-282.9	-283.5
3(RS)-ethyl-1-hexanethiol	-176.8	-177.1	-192.3	-204.5	-214.0	-221.1	-280.9	-282.9	-283.5
3(RS)-ethyl-2(RS)-hexanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
3-ethyl-3-hexanethiol	-190.2	-190.4	-205.3	-217.1	-226.1	-232.9	-292.5	-294.7	-295.7
4-ethyl-3(RS)-hexanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
4-ethyl-2(RS)-hexanethiol	-186.2	-186.5	-201.7	-213.7	-223.1	-230.2	-290.1	-292.4	-293.4
4-ethyl-1-hexanethiol	-176.8	-177.1	-192.3	-204.5	-214.0	-221.1	-280.9	-282.9	-283.5
2(RS)-ethyl-2-methyl-1-pentanethiol	-185.4	-185.7	-200.6	-212.3	-221.2	-227.7	-286.8	-288.4	-288.5
2(RS)-isopropyl-1-pentanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
2(RS)-ethyl-4-methyl-1-pentanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
3(RS),4,4-trimethyl-1-pentanethiol	-188.1	-188.4	-203.4	-215.1	-223.9	-230.3	-289.4	-290.8	-290.9
3(RS),4,4-trimethyl-2(RS)-pentanethiol	-197.6	-197.8	-212.7	-224.3	-233.0	-239.4	-298.6	-300.3	-300.7
2,2,3(RS)-trimethyl-3-pentanethiol	-201.5	-201.8	-216.4	-227.6	-236.0	-242.1	-301.0	-302.6	-303.0
2,2,3(RS)-trimethyl-1-pentanethiol	-188.1	-188.4	-203.4	-215.1	-223.9	-230.3	-289.4	-290.8	-290.9
2(RS),4,4-trimethyl-1-pentanethiol	-188.1	-188.4	-203.4	-215.1	-223.9	-230.3	-289.4	-290.8	-290.9
2,4,4-trimethyl-2-pentanethiol	-201.5	-201.8	-216.4	-227.6	-236.0	-242.1	-301.0	-302.6	-303.0
2,2,4-trimethyl-3(RS)-pentanethiol	-197.6	-197.8	-212.7	-224.3	-233.0	-239.4	-298.6	-300.3	-300.7
2,2,4-trimethyl-1-pentanethiol	-188.1	-188.4	-203.4	-215.1	-223.9	-230.3	-289.4	-290.8	-290.9
3,3,4-trimethyl-1-pentanethiol	-188.1	-188.4	-203.4	-215.1	-223.9	-230.3	-289.4	-290.8	-290.9
3,3,4-trimethyl-2(RS)-pentanethiol	-197.6	-197.8	-212.7	-224.3	-233.0	-239.4	-298.6	-300.3	-300.7
2,3,3-trimethyl-2-pentanethiol	-201.5	-201.8	-216.4	-227.6	-236.0	-242.1	-301.0	-302.6	-303.0
2(RS),3,3-trimethyl-1-pentanethiol	-188.1	-188.4	-203.4	-215.1	-223.9	-230.3	-289.4	-290.8	-290.9
3-ethyl-3-methyl-1-pentanethiol	-185.4	-185.7	-200.6	-212.3	-221.2	-227.7	-286.8	-288.4	-288.5
3-ethyl-3-methyl-2(RS)-pentanethiol	-194.9	-195.2	-210.0	-221.5	-230.3	-236.8	-296.0	-297.8	-298.3
2(RS)-ethyl-3(RS)-methyl-1-pentanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
2(RS),3(RS),4-trimethyl-1-pentanethiol	-185.5	-185.8	-201.2	-213.3	-222.7	-229.7	-289.3	-291.3	-291.7
2,3(RS),4-trimethyl-2-pentanethiol	-198.9	-199.1	-214.2	-225.9	-234.8	-241.5	-301.0	-303.0	-303.9
2,3,4-trimethyl-3-pentanethiol	-198.9	-199.1	-214.2	-225.9	-234.8	-241.5	-301.0	-303.0	-303.9
2-propyl-1-pentanethiol	-176.8	-177.1	-192.3	-204.5	-214.0	-221.1	-280.9	-282.9	-283.5
3(RS)-ethyl-4-methyl-1-pentanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
3(RS)-ethyl-4-methyl-2(RS)-pentanethiol	-192.3	-192.5	-207.8	-219.8	-229.1	-236.2	-296.0	-298.2	-299.2
3-ethyl-2-methyl-3-pentanethiol	-196.2	-196.5	-211.4	-223.2	-232.1	-238.9	-298.4	-300.5	-301.5
3-ethyl-2-methyl-2-pentanethiol	-196.2	-196.5	-211.4	-223.2	-232.1	-238.9	-298.4	-300.5	-301.5
3-ethyl-2(RS)-methyl-1-pentanethiol	-182.8	-183.1	-198.4	-210.6	-220.0	-227.1	-286.8	-288.8	-289.3
2(RS)-ethyl-3,3-dimethyl-1-butanethiol	-188.1	-188.4	-203.4	-215.1	-223.9	-230.3	-289.4	-290.8	-290.9
2(RS)-ethyl-2-methyl-3-methyl-1-butanethiol	-188.1	-188.4	-203.4	-215.1	-223.9	-230.3	-289.4	-290.8	-290.9
2,2-diethyl-1-butanethiol	-185.4	-185.7	-200.6	-212.3	-221.2	-227.7	-286.8	-288.4	-288.5
2,2,3,3-tetramethyl-1-butanethiol	-193.4	-193.7	-208.4	-219.5	-227.8	-233.6	-292.0	-292.9	-292.4
2-isopropyl-3-methyl-1-butanethiol	-185.5	-185.8	-201.2	-213.3	-222.7	-229.7	-289.3	-291.3	-291.7

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

T/K	298.15	300	400	500	600	700	800	900	1000
CH4S									
methanethiol	-9.90	-9.83	-4.78	1.86	9.39	17.62	20.94	35.93	51.09
C2H6S									
ethanethiol	-4.60	-4.33	10.45	27.10	44.86	63.46	77.10	102.52	128.03
C3H8S									
1-propanethiol	2.30	2.73	27.37	54.17	82.29	111.32	135.48	171.42	207.44
2-propanethiol	-2.46	-2.01	23.81	51.78	80.94	111.08	136.33	173.33	210.45
C4H10S									
1-butanethiol	11.18	11.78	46.37	83.47	121.97	161.51	196.24	242.67	289.14
2(RS)-butanethiol	5.56	6.17	41.59	79.43	118.73	159.07	194.60	241.86	289.35
2-methyl-1-propanethiol	5.70	6.32	42.15	80.39	120.11	160.83	196.82	244.56	292.58
2-methyl-2-propanethiol	.85	1.52	39.77	80.39	122.35	165.26	203.31	253.08	302.95
C5H12S									
1-pentanethiol	19.3	20.1	64.7	112.0	160.9	211.0	256.4	313.6	370.9
2(RS)-pentanethiol	11.1	11.9	56.9	104.6	153.9	204.3	250.1	307.6	365.3
3-pentanethiol	12.9	13.7	59.2	107.5	157.4	208.4	254.7	312.8	371.1
2(RS)-methyl-1-butanethiol	14.9	15.7	60.9	108.7	158.3	208.9	254.8	312.5	370.3
2-methyl-2-butanethiol	8.2	9.1	56.4	106.4	157.9	210.5	258.3	317.9	377.6
3-methyl-2(RS)-butanethiol	8.5	9.3	55.4	104.2	154.7	206.2	253.1	311.7	370.5
3-methyl-1-butanethiol	16.7	17.5	63.2	111.6	161.7	212.9	259.4	317.7	376.1
2,2-dimethyl-1-propanethiol	9.3	10.1	58.5	109.5	162.0	215.5	264.3	324.7	385.2
C6H14S									
1-hexanethiol	27.6	28.6	83.1	140.6	200.0	260.6	316.6	384.4	452.3
2(RS)-hexanethiol	19.4	20.4	75.3	133.2	192.9	253.9	310.2	378.4	446.8
3(RS)-hexanethiol	19.4	20.4	75.3	133.2	192.9	253.9	310.2	378.4	446.8
2(RS)-methyl-1-pentanethiol	23.2	24.2	79.2	137.3	197.3	258.4	315.0	383.3	451.8
2-methyl-2-pentanethiol	16.5	17.6	74.8	135.0	196.9	260.0	318.5	388.7	459.1
2-methyl-3(RS)-pentanethiol	16.8	17.8	73.8	132.8	193.7	255.8	313.2	382.5	452.0
4-methyl-2(RS)-pentanethiol	16.8	17.8	73.8	132.8	193.7	255.8	313.2	382.5	452.0
4-methyl-1-pentanethiol	24.9	25.9	81.6	140.2	200.7	262.5	319.6	388.5	457.6
3(RS)-methyl-1-pentanethiol	23.2	24.2	79.2	137.3	197.3	258.4	315.0	383.3	451.8
3(RS)-methyl-2(RS)-pentanethiol	15.0	16.0	71.5	129.9	190.2	251.7	308.6	377.3	446.2
3-methyl-3-pentanethiol	16.5	17.6	74.8	135.0	196.9	260.0	318.5	388.7	459.1
2(RS),3-dimethyl-1-butanethiol	20.6	21.6	77.7	137.0	198.0	260.3	318.0	387.4	457.0
2,3-dimethyl-2-butanethiol	13.9	14.9	73.3	134.6	197.7	261.9	321.5	392.8	464.3
2-ethyl-1-butanethiol	24.9	25.9	81.6	140.2	200.7	262.5	319.6	388.5	457.6
2,2-dimethyl-1-butanethiol	21.6	22.6	79.9	140.2	202.2	265.4	323.8	394.0	464.2
3,3-dimethyl-2(RS)-butanethiol	16.1	17.1	75.8	137.4	200.7	265.1	324.8	396.2	467.7
3,3-dimethyl-1-butanethiol	24.3	25.3	83.6	144.8	207.7	271.8	331.1	402.2	473.3
C7H16S									
1-heptanethiol	35.9	37.1	101.5	169.2	239.0	310.1	376.7	455.2	533.8
2(RS)-heptanethiol	27.7	28.9	93.7	161.8	232.0	303.4	370.4	449.2	528.2
3(RS)-heptanethiol	27.7	28.9	93.7	161.8	232.0	303.4	370.4	449.2	528.2
4-heptanethiol	29.4	30.6	96.0	164.7	235.4	307.5	375.0	454.4	534.0
5-methyl-1-hexanethiol	33.2	34.4	99.9	168.8	239.8	312.0	379.8	459.3	539.0
5-methyl-2(RS)-hexanethiol	25.1	26.2	92.2	161.4	232.7	305.3	373.4	453.3	533.4
5-methyl-3(RS)-hexanethiol	25.1	26.2	92.2	161.4	232.7	305.3	373.4	453.3	533.4
2-methyl-3(RS)-hexanethiol	25.1	26.2	92.2	161.4	232.7	305.3	373.4	453.3	533.4
2-methyl-2-hexanethiol	24.8	26.0	93.2	163.6	235.9	309.6	378.6	459.5	540.5
2(RS)-methyl-1-hexanethiol	31.5	32.7	97.6	166.0	236.3	308.0	375.1	454.1	533.3
4(RS)-methyl-1-hexanethiol	31.5	32.7	97.6	166.0	236.3	308.0	375.1	454.1	533.3
4(RS)-methyl-2(RS)-hexanethiol	23.3	24.5	89.9	158.6	229.3	301.3	368.8	448.1	527.7
4(RS)-methyl-3(RS)-hexanethiol	23.3	24.5	89.9	158.6	229.3	301.3	368.8	448.1	527.7
3(RS)-methyl-3-hexanethiol	23.1	24.3	90.9	160.7	232.5	305.5	374.0	454.3	534.8
3(RS)-methyl-2(RS)-hexanethiol	23.3	24.5	89.9	158.6	229.3	301.3	368.8	448.1	527.7
3(RS)-methyl-1-hexanethiol	31.5	32.7	97.6	166.0	236.3	308.0	375.1	454.1	533.3
4,4-dimethyl-1-pentanethiol	32.6	33.8	102.0	173.4	246.7	321.3	391.3	473.0	554.8
4,4-dimethyl-2(RS)-pentanethiol	24.4	25.6	94.2	166.0	239.7	314.6	384.9	467.0	549.2
2,2-dimethyl-1-pentanethiol	24.4	25.6	94.2	166.0	239.7	314.6	384.9	467.0	549.2
2,2-dimethyl-1-pentanethiol	29.8	31.1	98.3	168.8	241.2	314.9	384.0	464.7	545.6
3,3-dimethyl-1-pentanethiol	29.8	31.1	98.3	168.8	241.2	314.9	384.0	464.7	545.6
3,3-dimethyl-2(RS)-pentanethiol	21.7	22.9	90.5	161.4	234.2	308.2	377.6	458.8	540.1
3(RS),4-dimethyl-1-pentanethiol	28.8	30.0	96.1	165.6	237.1	309.9	378.2	458.2	538.5
3(RS),4-dimethyl-2(RS)-pentanethiol	20.7	21.8	88.4	158.2	230.0	303.2	371.8	452.3	532.9
2(RS),3(RS)-dimethyl-1-pentanethiol	27.1	28.3	93.8	162.7	233.6	305.8	373.5	453.0	532.7
2,3(RS)-dimethyl-2-pentanethiol	20.4	21.6	89.4	160.3	233.2	307.4	377.0	458.4	540.0
2,3(RS)-dimethyl-3-pentanethiol	20.4	21.6	89.4	160.3	233.2	307.4	377.0	458.4	540.0
2(RS),4-dimethyl-1-pentanethiol	28.8	30.0	96.1	165.6	237.1	309.9	378.2	458.2	538.5
2,4-dimethyl-2-pentanethiol	22.2	23.4	91.7	163.2	236.7	311.5	381.6	463.6	545.7
2,4-dimethyl-3-pentanethiol	24.1	25.3	93.0	163.9	236.9	311.3	381.0	462.6	544.4
2(RS)-ethyl-1-pentanethiol	31.5	32.7	97.6	166.0	236.3	308.0	375.1	454.1	533.3
3-ethyl-1-pentanethiol	33.2	34.4	99.9	168.8	239.8	312.0	379.8	459.3	539.0
3-ethyl-2(RS)-pentanethiol	25.1	26.2	92.2	161.4	232.7	305.3	373.4	453.3	533.4
3-ethyl-3-pentanethiol	24.8	26.0	93.2	163.6	235.9	309.6	378.6	459.5	540.5
2-ethyl-2-methyl-1-butanethiol	29.8	31.1	98.3	168.8	241.2	314.9	384.0	464.7	545.6
2(RS)-ethyl-3-methyl-1-butanethiol	28.8	30.0	96.1	165.6	237.1	309.9	378.2	458.2	538.5
2(RS),3,3-trimethyl-1-butanethiol	31.5	32.8	101.5	173.6	247.4	322.6	393.0	475.2	557.6
2,3,3-trimethyl-2-butanethiol	24.8	26.1	97.0	171.1	247.0	324.1	396.5	480.6	564.9
2,2,3-trimethyl-1-butanethiol	30.5	31.7	100.1	171.8	245.4	320.2	390.3	472.2	554.2
C8H18S									
1-octanethiol	44.2	45.5	119.9	197.8	278.0	359.7	436.9	526.0	615.2
2(RS)-octanethiol	36.0	37.4	112.1	190.4	271.0	353.0	430.6	520.0	609.7
3(RS)-octanethiol	36.0	37.4	112.1	190.4	271.0	353.0	430.6	520.0	609.7
4(RS)-octanethiol	36.0	37.4	112.1	190.4	271.0	353.0	430.6	520.0	609.7
2(RS)-methyl-1-heptanethiol	39.8	41.2	116.0	194.6	275.3	357.5	435.3	524.9	614.7
2-methyl-2-heptanethiol	33.1	34.5	111.6	192.2	275.0	359.1	438.8	530.3	622.0
2-methyl-3(RS)-heptanethiol	33.3	34.7	110.6	190.1	271.7	354.9	433.6	524.1	614.9
2-methyl-4(RS)-heptanethiol	33.3	34.7	110.6	190.1	271.7	354.9	433.6	524.1	614.9
6-methyl-3(RS)-heptanethiol	33.3	34.7	110.6	190.1	271.7	354.9	433.6	524.1	614.9
6-methyl-2(RS)-heptanethiol	33.3	34.7	110.6	190.1	271.7	354.9	433.6	524.1	614.9
6-methyl-1-heptanethiol	41.5	42.9	118.3	197.4	278.8	361.6	439.9	530.1	620.5
3(RS)-methyl-1-heptanethiol	39.8	41.2	116.0	194.6	275.3	357.5	435.3	524.9	614.7
3(RS)-methyl-2(RS)-heptanethiol	31.6	33.0	108.3	187.2	268.3	350.8	429.0	518.9	609.1
3(RS)-methyl-3-heptanethiol	31.4	32.8	109.3	189.3	271.5	355.1	434.2	525.1	616.2
2(RS)-methyl-4(RS)-heptanethiol	31.6	33.0	108.3	187.2	268.3	350.8	429.0	518.9	609.1
5(RS)-methyl-3(RS)-heptanethiol	31.6	33.0	108.3	187.2	268.3	350.8	429.0	518.9	609.1
5(RS)-methyl-2(RS)-heptanethiol	31.6	33.0	108.3	187.2	268.3	350.8	429.0	518.9	609.1
5(RS)-methyl-1-heptanethiol	39.8	41.2	116.0	194.6	275.3	357.5	435.3	524.9	614.7

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

T/K	298.15	300	400	500	600	700	800	900	1000
4(RS)-methyl-1-heptanethiol	39.8	41.2	116.0	194.6	275.3	357.5	435.3	524.9	614.7
4(RS)-methyl-2(RS)-heptanethiol	31.6	33.0	108.3	187.2	268.3	350.8	429.0	518.9	609.1
4(RS)-methyl-3(RS)-heptanethiol	31.6	33.0	108.3	187.2	268.3	350.8	429.0	518.9	609.1
4-methyl-4-heptanethiol	33.1	34.5	111.6	192.2	275.0	359.1	438.8	530.3	622.0
2,2-dimethyl-1-hexanethiol	38.1	39.5	116.7	197.4	280.3	364.5	444.1	535.5	627.1
2,2-dimethyl-3(RS)-hexanethiol	32.7	34.1	112.6	194.6	278.7	364.2	445.1	537.8	630.7
5,5-dimethyl-3(RS)-hexanethiol	32.7	34.1	112.6	194.6	278.7	364.2	445.1	537.8	630.7
5,5-dimethyl-2(RS)-hexanethiol	32.7	34.1	112.6	194.6	278.7	364.2	445.1	537.8	630.7
5,5-dimethyl-1-hexanethiol	40.9	42.3	120.4	202.0	285.8	370.9	451.4	543.8	636.2
3,3-dimethyl-1-hexanethiol	38.1	39.5	116.7	197.4	280.3	364.5	444.1	535.5	627.1
3,3-dimethyl-2(RS)-hexanethiol	30.0	31.3	108.9	190.0	273.2	357.8	437.8	529.6	621.5
4,4-dimethyl-3(RS)-hexanethiol	30.0	31.3	108.9	190.0	273.2	357.8	437.8	529.6	621.5
4,4-dimethyl-2(RS)-hexanethiol	30.0	31.3	108.9	190.0	273.2	357.8	437.8	529.6	621.5
4,4-dimethyl-1-hexanethiol	38.1	39.5	116.7	197.4	280.3	364.5	444.1	535.5	627.1
4(RS),5-dimethyl-1-hexanethiol	37.1	38.5	114.5	194.2	276.1	359.4	438.3	529.0	619.9
4(RS),5-dimethyl-2(RS)-hexanethiol	29.0	30.3	106.7	186.8	269.0	352.7	432.0	523.0	614.3
4(RS),5-dimethyl-3(RS)-hexanethiol	29.0	30.3	106.7	186.8	269.0	352.7	432.0	523.0	614.3
2,3-dimethyl-3(RS)-hexanethiol	28.7	30.1	107.8	188.9	272.3	357.0	437.2	529.2	621.4
2,3(RS)-dimethyl-2-hexanethiol	28.7	30.1	107.8	188.9	272.3	357.0	437.2	529.2	621.4
2(RS),3(RS)-dimethyl-1-hexanethiol	35.4	36.8	112.2	191.3	272.6	355.4	433.7	523.8	614.2
3(RS),5-dimethyl-1-hexanethiol	37.1	38.5	114.5	194.2	276.1	359.4	438.3	529.0	619.9
3(RS),5-dimethyl-2(RS)-hexanethiol	29.0	30.3	106.7	186.8	269.0	352.7	432.0	523.0	614.3
3(RS),5-dimethyl-3-hexanethiol	28.7	30.1	107.8	188.9	272.3	357.0	437.2	529.2	621.4
2,4(RS)-dimethyl-3(RS)-hexanethiol	29.0	30.3	106.7	186.8	269.0	352.7	432.0	523.0	614.3
2,4(RS)-dimethyl-2-hexanethiol	28.7	30.1	107.8	188.9	272.3	357.0	437.2	529.2	621.4
2(RS),4(RS)-dimethyl-1-hexanethiol	35.4	36.8	112.2	191.3	272.6	355.4	433.7	523.8	614.2
2(RS),5-dimethyl-1-hexanethiol	37.1	38.5	114.5	194.2	276.1	359.4	438.3	529.0	619.9
2,5-dimethyl-2-hexanethiol	30.5	31.9	110.1	191.8	275.7	361.0	441.8	534.4	627.2
2,5-dimethyl-3(RS)-hexanethiol	30.7	32.0	109.1	189.7	272.5	356.8	436.6	528.2	620.1
3(RS),4(RS)-dimethyl-1-hexanethiol	35.4	36.8	112.2	191.3	272.6	355.4	433.7	523.8	614.2
3(RS),4(RS)-dimethyl-2(RS)-hexanethiol	27.2	28.6	104.4	183.9	265.6	348.7	427.4	517.9	608.6
3(RS),4(RS)-dimethyl-3-hexanethiol	27.0	28.4	105.5	186.1	268.8	352.9	432.6	524.0	615.7
2(RS)-ethyl-1-hexanethiol	39.8	41.2	116.0	194.6	275.3	357.5	435.3	524.9	614.7
3(RS)-ethyl-1-hexanethiol	39.8	41.2	116.0	194.6	275.3	357.5	435.3	524.9	614.7
3(RS)-ethyl-2(RS)-hexanethiol	31.6	33.0	108.3	187.2	268.3	350.8	429.0	518.9	609.1
3-ethyl-3-hexanethiol	33.1	34.5	111.6	192.2	275.0	359.1	438.8	530.3	622.0
4-ethyl-3(RS)-hexanethiol	33.3	34.7	110.6	190.1	271.7	354.9	433.6	524.1	614.9
4-ethyl-2(RS)-hexanethiol	33.3	34.7	110.6	190.1	271.7	354.9	433.6	524.1	614.9
4-ethyl-1-hexanethiol	41.5	42.9	118.3	197.4	278.8	361.6	439.9	530.1	620.5
2(RS)-ethyl-2-methyl-1-pentanethiol	36.4	37.8	114.4	194.5	276.8	360.4	439.5	530.4	621.3
2(RS)-isopropyl-1-pentanethiol	37.1	38.5	114.5	194.2	276.1	359.4	438.3	529.0	619.9
2(RS)-ethyl-4-methyl-1-pentanethiol	37.1	38.5	114.5	194.2	276.1	359.4	438.3	529.0	619.9
3(RS),4,4-trimethyl-1-pentanethiol	39.8	41.2	119.9	202.1	286.4	372.1	453.2	546.0	639.0
3(RS),4,4-trimethyl-2(RS)-pentanethiol	31.6	33.0	112.1	194.7	279.4	365.4	446.8	540.1	633.5
2,2,3(RS)-trimethyl-3-pentanethiol	31.4	32.8	113.1	196.8	282.6	369.6	452.0	546.2	640.5
2,2,3(RS)-trimethyl-1-pentanethiol	37.1	38.5	116.2	197.5	280.9	365.7	445.9	537.8	629.9
2(RS),4,4-trimethyl-1-pentanethiol	39.8	41.2	119.9	202.1	286.4	372.1	453.2	546.0	639.0
2,4,4-trimethyl-2-pentanethiol	33.1	34.6	115.4	199.7	286.0	373.6	456.6	551.4	646.3
2,2,4-trimethyl-3(RS)-pentanethiol	33.3	34.8	114.4	197.6	282.8	369.4	451.4	545.3	639.2
2,2,4-trimethyl-1-pentanethiol	38.8	40.2	118.5	200.4	284.4	369.7	450.5	543.0	635.7
3,3,4-trimethyl-1-pentanethiol	38.8	40.2	118.5	200.4	284.4	369.7	450.5	543.0	635.7
3,3,4-trimethyl-2(RS)-pentanethiol	30.6	32.0	110.8	193.0	277.3	363.0	444.1	537.0	630.1
2,3,3-trimethyl-2-pentanethiol	30.4	31.8	111.8	195.2	280.6	367.2	449.3	543.2	637.2
2(RS),3,3-trimethyl-1-pentanethiol	37.1	38.5	116.2	197.5	280.9	365.7	445.9	537.8	629.9
3-ethyl-3-methyl-1-pentanethiol	38.1	39.5	116.7	197.4	280.3	364.5	444.1	535.5	627.1
3-ethyl-3-methyl-2(RS)-pentanethiol	30.0	31.3	108.9	190.0	273.2	357.8	437.8	529.6	621.5
2(RS)-ethyl-3(RS)-methyl-1-pentanethiol	35.4	36.8	112.2	191.3	272.6	355.4	433.7	523.8	614.2
2(RS),3(RS),4-trimethyl-1-pentanethiol	36.1	37.5	114.0	194.3	276.7	360.6	440.1	531.3	622.7
2,3(RS),4-trimethyl-2-pentanethiol	29.4	30.8	109.6	191.9	276.4	362.2	443.5	536.7	630.0
2,3,4-trimethyl-3-pentanethiol	31.1	32.5	111.9	194.8	279.8	366.2	448.1	541.9	635.8
2-propyl-1-pentanethiol	41.5	42.9	118.3	197.4	278.8	361.6	439.9	530.1	620.5
3(RS)-ethyl-4-methyl-1-pentanethiol	37.1	38.5	114.5	194.2	276.1	359.4	438.3	529.0	619.9
3(RS)-ethyl-4-methyl-2(RS)-pentanethiol	29.0	30.3	106.7	186.8	269.0	352.7	432.0	523.0	614.3
3-ethyl-2-methyl-3-pentanethiol	30.5	31.9	110.1	191.8	275.7	361.0	441.8	534.4	627.2
3-ethyl-2-methyl-2-pentanethiol	30.5	31.9	110.1	191.8	275.7	361.0	441.8	534.4	627.2
3-ethyl-2(RS)-methyl-1-pentanethiol	37.1	38.5	114.5	194.2	276.1	359.4	438.3	529.0	619.9
2(RS)-ethyl-3,3-dimethyl-1-butanethiol	39.8	41.2	119.9	202.1	286.4	372.1	453.2	546.0	639.0
2(RS)-ethyl-2-methyl-3-methyl-1-butanethiol	37.1	38.5	116.2	197.5	280.9	365.7	445.9	537.8	629.9
2,2-diethyl-1-butanethiol	38.1	39.5	116.7	197.4	280.3	364.5	444.1	535.5	627.1
2,2,3,3-tetramethyl-1-butanethiol	41.5	42.9	123.9	208.3	294.7	382.3	465.3	560.0	654.8
2-isopropyl-3-methyl-1-butanethiol	39.5	40.9	118.6	200.0	283.7	368.7	449.3	541.7	634.3

Table 14. Log K for the formation of a thiol isomer group from an alkene isomer group and hydrogen sulfide (reaction 7)

T/K	C2H6S	C3H8S	C4H10S	C5H12S	C6H14S	C7H16S	C8H18S
298.15	6.910	5.655	4.248	3.646	3.188	3.611	3.577
300.00	6.834	5.579	4.181	3.584	3.126	3.550	3.516
400.00	3.433	2.330	1.202	.865	.471	.832	.795
500.00	1.392	.413	-.507	-.724	-1.073	-.770	-.809
600.00	.031	-.840	-1.609	-1.764	-2.087	-1.821	-1.860
700.00	-.940	-1.722	-2.377	-2.494	-2.796	-2.561	-2.600
800.00	-1.660	-2.369	-2.943	-3.039	-3.323	-3.106	-3.144
900.00	-2.216	-2.864	-3.367	-3.449	-3.718	-3.523	-3.559
1000.00	-2.658	-3.253	-3.705	-3.776	-4.031	-3.853	-3.887

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

$$C_nH_{2n}\,(\text{alkene isomer group}) + H_2S = C_nH_{2n+2}\,(\text{alkanethiol isomer group}), \quad (7)$$

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 carbon number is much greater at low temperatures than high temperatures. The values of $\Delta_f G°(I)$ for the alkene isomer groups are from Alberty and Gehrig,[4] and the values of $\Delta_f G°$ for $H_2S(g)$ are from Stull and Prophet.[17]

8. Nomenclature

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

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

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

$\Delta_f G°(I)$ = 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}

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

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

$\Delta_f H°(I)$ = 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

9. Acknowledgments

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