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Ideal Gas Thermodynamic Properties of Simple Alkanols[1]

J. Chao[2] and K. R. Hall[3]

The ideal gas thermodynamic properties [C_p^0, $S^0(T) - S^0(0)$ and $H^0(T) - H^0(0)$] of methanol (CH_3OH), ethanol (C_2H_5OH), 1-propanol ($CH_3CH_2CH_2OH$), and 2-propanol [$(CH_3)_2CHOH$] over the temperature range 0 to 1500 K at 1.01325-bar (1-atm) pressure are calculated by the statistical mechanical method, employing the recent molecular and spectroscopic constants. The internal rotational contributions to the thermodynamic properties caused by the presence of $-CH_3$, $-C_2H_5$, and $-OH$ rotors in these molecules are evaluated using an internal rotational partition function formed by the summation of internal rotational energy levels for each rotor. In the calculation of the thermodynamic properties of ethanol (g) and 1-propanol (g), we adopted a molecular model that the vapor of each compound contains an equilibrium mixture of trans and gauche isomers. The existence of such isomers was observed spectroscopically in recent years. Our calculated results, such as C_p^0 and $S^0(T) - S^0(0)$, agree with available experimental values.

KEY WORDS: ethanol; internal rotation; methanol; 1-propanol; 2-propanol; thermodynamic properties.

1. INTRODUCTION

The ideal gas thermodynamic properties of methanol, ethanol, 1-propanol, and 2-propanol have been evaluated using the statistical mechanical method, based upon a rigid-rotor harmonic-oscillator molecular model. The calculated heat capacity, C_p^0, and entropy, $S^0(T) - S^0(0)$, are compared with experimental values. Because of the presence of associated molecules in the alkanol vapors [1, 2], a special equation of state has been

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[2] Thermodynamics Research Center, Texas Engineering Experimental Station, Texas A&M University, College Station, Texas 77843, U.S.A.

[3] Texas Engineering Experimental Station, Texas A & M University, College Station, Texas 77843, U.S.A.

employed [2–7] for extrapolating the measured properties to zero-pressure values. Kretschmer and Wiebe [3] used the equation of state proposed by Weltner and Pitzer [2] and Barrow [4] to fit their vapor density and heat capacity measurements with good agreement. Strömsöe et al. [7] found an empirical heat capacity equation for the homologous series of associating alkanol vapors.

Many ways exist to derive an appropriate equation of state for extrapolating the measured alkanol C_p to zero-pressure $C^0_\mathrm{p}(T)$ and for evaluating the nonideal behavior of the real gas. However, the reliability and applicability of such new equations need extensive investigation for acceptance.

2. METHOD OF CALCULATION

The input data required for each compound are the molecular weight (m), product of three principal moments of inertia ($I_\mathrm{a} I_\mathrm{b} I_\mathrm{c}$), fundamental vibrational frequencies (v_i, $i = 3n - 6$, where n is the number of atoms in the given compound molecule), and internal rotational constants. The values of I_a, I_b, and I_c usually result from the rotational constants A, B, and C obtained from microwave spectroscopy; otherwise, they are calculated from the molecular structural parameters, i.e., bond distances, angles, and dihedral angles of the given molecule.

To evaluate the internal rotational contributions to the thermodynamic properties of these alkanols, we employ an internal rotational partition function formed by the summation of internal rotational energy levels for each rotor. Methanol has one rotor, namely, $-OH$. Ethanol has two rotors, $-OH$ and $-CH_3$. There are three rotors in each propanol molecule, i.e., $-CH_3$, $-C_2H_5$, $-OH$ for 1-propanol and $-CH_3$, $-CH_3$, $-OH$ for 2-propanol. The internal rotational constants required to generate the internal rotational energy levels for each rotor are the reduced moment of inertia (I_r) or internal rotational constant (F) and the potential barrier height (V_n) of an appropriate internal rotation potential function, $V(\phi)$. The V_n may also be derived from the known torsional frequency of the rotor. The method of generating the internal rotational energy levels has been described [8–10].

A molecular model of an equilibrium mixture of trans and gauche isomers was employed for calculating the ideal gas thermodynamic properties of ethanol and 1-propanol. In addition to the thermodynamic properties of trans and gauche species, the enthalpy of isomerization was also needed for computing the compositions of the equilibrium mixture of the alkanol vapors at selected temperatures [11].

The recent physical constants [12] and the 1984 atomic weights [13], C = 12.011, H = 1.00794, and O = 15.9994, are employed in all calculations. The ideal gas thermodynamic properties, $C_p^0(T)$, $S^0(T) - S^0(0)$, and enthalpy $[H^0(T) - H^0(0)]$ are calculated in the temperature range from 0 to 1500 K at 1.001325 bar (1 atm) and appear in SI units for the four simple alkanols.

3. SOURCES OF DATA

3.1. Methanol

The molecular structure of methanol was investigated with X-ray diffraction [14–16], electron diffraction [17, 18], and microwave spectroscopy [19–28]. Lees and Baker [25] studied extensively the internal rotation in methanol and its deuterated analogs and determined the moments of inertia. We adopted their results to obtain $I_a I_b I_c = 7.9048 \times 10^{-117} \mathrm{g}^3 \cdot \mathrm{cm}^6$ for computing the rotational contributions. Falk and Whalley [29] reviewed the vibrational assignments for methanol vapor before 1961. Shimanouchi [30] critically reviewed the spectroscopic studies on this compound and assigned a complete set of fundamental vibrational frequencies for $CH_3OH(g)$. His recommended values, except the torsional frequency (ν_{12}), were selected for calculating the vibrational contributions to the thermodynamic properties of methanol.

Investigation of internal rotation in CH_3OH molecules has been the subject of numerous microwave and infrared studies [19–21, 23–25, 31–33]. Kwan and Dennison [33] employed a perturbation term for the potential function of the OH asymmetric rotor in the CH_3OH molecule. From a nonlinear least-squares fit to the observed microwave and infrared data, they derived $V_3 = 4.44 \mathrm{kJ \cdot mol^{-1}}$ and $V_6 = -0.006 \mathrm{kJ \cdot mol^{-1}}$ for the potential function $V(\phi) = \frac{1}{2} V_3 (1 - \cos 3\phi) + \frac{1}{2} V_6 (1 - \cos 6\phi)$ for OH rotor in $CH_3OH(g)$, where ϕ is the angle of internal rotation. This potential function was adopted to generate 84 internal rotation energy levels (0–50,000 cm^{-1}) for calculating the internal rotational contributions to the thermodynamical properties of $CH_3OH(g)$. The reduced moment, $I_r = 0.9933 \times 10^{-40} \mathrm{g \cdot cm^2}$, was evaluated based upon the molecular structure reported by Lees and Baker [25]. The selected molecular and spectroscopic constants are listed in Tables I and II.

3.2. Ethanol

Michielsen-Effinger [44] established the existence of two stable rotational isomers, trans and gauche, in ethanol vapor, from microwave spectroscopy. Consequently, we adopted a molecular model that ethanol

Table I. Molecular Weight, Product of Moments of Inertia, and Vibrational Assignments for Simple Alkanols[a]

Compound name	MW	$I_a I_b I_c \times 10^{117}$ ($g^3 \cdot cm^6$)	Fundamental vibrational wave numbers (cm^{-1})
Methanol	32.0420	7.89719	3681, 3000, 2844, 1477, 1455, 1345, 1060, 1033, 2960, 1477, 1165
Ethanol (T–G)	46.0688	218.459 (T) 233.455 (G)	3639, 2985, 2939, 2900, 1460, 1430, 1395, 1320, 1245, 1055, 1026, 883, 422, 2887, 2887, 1460, 1270, 1117, 801 (T) 3675, 2985, 2939, 2900, 1460, 1430, 1395, 1320, 1245, 1055, 1026, 887, 596, 2887, 2887, 1460, 1270, 1070, 801 (G)
1-Propanol (T–G)	60.0956	1660.0 (T) 1855.1 (G)	3680, 2940(7), 1478, 1463, 1450(2), 1393, 1381, 890, 860, 730, 463, 300 (T) 3705, 2971, 2970, 2941, 2924, 2911, 2903, 2877, 1465, 1462, 1461, 1459, 1394, 1388, 1330, 1255, 1227, 1180, 1075, 1056, 1003, 917, 880, 862, 600, 524, 300 (G)
2-Propanol	60.0956	1831.0	3650, 2940(6), 2875, 1475(2), 1460(2), 1387, 1367, 1340, 1256(2), 1153, 1130, 1072, 955(2), 940, 818, 488, 427, 373

[a] T, trans isomer; G, gauche isomer; T–G, mixture of trans and gauche isomers.

vapor contained an equilibrium mixture of trans and gauche isomers. To evaluate the thermodynamic properties of this equilibrium mixture of rotational isomers, the thermodynamic properties of each isomer were first calculated.

The moments of inertia of the trans isomer in the ground vibrational state are reported by Takano et al. [45] and Lovas [46] from microwave spectra of this species. Their results are in reasonable agreement. The values reported by Lovas [46] are adopted to obtain $I_a I_b I_c$. The fundamental vibrational frequencies, listed in Table I, come from During et al. [43], Barnes and Hallam [47], and Green [48]. Lovas [46] reports $F = 192.273$ GHz and $V_3 = 13.95\ \mathrm{kJ \cdot mol^{-1}}$ for the CH_3 rotor in trans-C_2H_5OH. Employing these F and V_3 together with the potential function $V = \frac{1}{2}V_3(1 - \cos 3\phi)$, we have generated 96 internal rotational energy levels (0–1500 cm^{-1}) for computing the CH_3 internal rotational contributions to the thermodynamic properties of the trans isomer. The calculated torsional frequency 244 cm^{-1} agrees with the observed values 253 cm^{-1} [43] and 243 cm^{-1} [47]. From $F = 21.07\ cm^{-1}$ and $V_3 = 2.12\ \mathrm{kJ \cdot mol^{-1}}$ for the OH

Table II. Internal Rotational Constants for Simple Alkanols[a]

Compound	σ	ν_{tor} (cm^{-1})	$I_r \times 10^{40}$ ($\text{g} \cdot \text{cm}^2$)	F (cm^{-1})	V_n ($\text{kJ} \cdot \text{mol}^{-1}$)
$CH_3{-}OH$	3	298	0.993	28.19	4.465 (V_3), −0.0062 (V_6)
$CH_3{-}CH_2{-}OH$					
Trans					
CH_3 rotor	3	244.1	4.365	6.414	13.95 (V_3)
OH rotor	3	205.2	1.329	21.07	2.117 (V_3)
Gauche					
CH_3 rotor	3	261.9	4.363	6.416	15.92 (V_3)
OH rotor	3	248.5	1.337	20.94	0.682 (V_1), 0.096 (V_2), 4.725 (V_3)
$CH_3{-}CH_2{-}CH_2{-}OH$					
Trans					
CH_3 rotor	3	214.2	4.591	6.097	11.42 (V_3)
OH rotor	3	226.5	1.321	21.34	3.347 (V_3)
C_2H_5 rotor	3	112.4	14.93	1.875	9.666 (V_3)
Gauche					
CH_3 rotor	3	214.5	4.850	5.711	12.001 (V_3)
OH rotor	3	224	1.330	21.05	3.347 (V_3)
C_2H_5	3	130.6	4.863	5.756	4.84 (V_3)
$(CH_3)_2CH{-}OH$					
CH_3 rotor	3	251.4	5.036	5.559	16.74 (V_3)
OH rotor	3	209.6	1.281	21.853	0.364(V_1), -1.031(V_2), 4.801(V_3)

[a] σ, symmetry number of the rotor; ν_{tor}, torsional frequency; I_r, reduced moment of inertia of the rotor; F, internal rotational constant of the rotor; V_n, potential barrier height in the potential function $= V(\phi) = \frac{1}{2}V_1(1 - \cos\phi) + \frac{1}{2}V_2(1 - \cos 2\phi) + \frac{1}{2}V_3(1 - \cos 3\phi) + \frac{1}{2}V_6(1 - \cos 6\phi)$, where ϕ = angle of internal rotation.

rotor in the trans molecule, we have generated 48 internal rotation energy levels for calculating the OH rotor internal rotational contributions. The F value is calculated from molecular structural parameters [49] and the $V_3(-\text{OH})$ is obtained from [43]. The calculated torsional frequency, $\nu_{\text{tor}}(0 \rightarrow 1) = 205\ \text{cm}^{-1}$, agrees reasonably well with the observations, $209\ \text{cm}^{-1}$ [52], $201\ \text{cm}^{-1}$ [47], and $199\ \text{cm}^{-1}$ [50]. Tables I and II contain the selected values.

For evaluation of the thermodynamic properties of gauche isomer, we adopt the $I_a I_b I_c$, $V_3(\text{CH}_3)$, and $V(\text{OH})$ determined by Kakar and Quade [51] from microwave spectroscopy. The internal rotation potential function of the OH rotor is $V(\text{OH}) = \frac{1}{2}V_1(1 - \cos\phi) + \frac{1}{2}V_2(1 - \cos 2\phi) + \frac{1}{2}V_3(1 - \cos 3\phi)$, where $V_1 = 0.682\ \text{kJ} \cdot \text{mol}^{-1}$, $V_2 = 0.096\ \text{kJ} \cdot \text{mol}^{-1}$, and $V_3 = 4.725\ \text{kJ} \cdot \text{mol}^{-1}$. From the above barrier heights and the calculated F

values for CH_3 and OH rotors in the gauche-C_2H_5OH molecule, we generate 96 and 54 energy levels for CH_3 and OH internal rotations, respectively, to evaluate their respective internal rotational contributions. The F values are calculated using the molecular structural parameters of the trans isomer [49] with a dihedral angle of 70° for the OH rotor. The calculated torsion frequencies, $\nu_{\text{tor}}(CH_3) = 261.9\ \text{cm}^{-1}$ and $\nu_{\text{tor}}(OH) = 248.5\ \text{cm}^{-1}$, agree with the reported values of $253.3\ \text{cm}^{-1}$ [43] and $234\ \text{cm}^{-1}$ [52], respectively. The fundamental vibrational frequencies come from During et al. [43].

The enthalpy of isomerization $(\Delta_i H^0)$ for the reaction: trans-$C_2H_5OH(g) = $ gauche-$C_2H_5OH(g)$ was reported as $493\ \text{J} \cdot \text{mol}^{-1}$ by Kakar and Quade [51]. This $\Delta_i H^0(\text{OK})$ was used together with the calculated thermodynamic properties of the trans and gauche isomers for evaluating the ideal gas thermodynamic properties of ethanol.

3.3. 1-Propanol

1-Propanol (*n*-propyl alcohol) has two rotational isomers, trans and gauche [53]. Recent work [54] has established that the gauche isomer is more stable by $1.213\ \text{kJ} \cdot \text{mol}^{-1}$. For the gauche isomer, the $I_a I_b I_c$ comes from Abdurahmanov et al. [55]. The fundamental vibrational frequencies are reported by Fukushima and Zwolinski [56]. $V_3(CH_3)$ and $V_3(OH)$ come from Refs. 57 and 58, respectively. $V_3(C_2H_5)$ is estimated. The value of I_r and F for the CH_3, OH, and C_2H_5 rotors are calculated employing the molecular structural parameters determined from electron diffraction for 1-propanol (g) by Aziz and Rogowski [59].

The $I_a I_b I_c$ for trans-1-propanol (g) is based upon the three principal moments of inertial obtained from microwave spectroscopy by Abdurahmanov et al. [55]. From the reported infrared and Raman spectra, Mathews and McKetta [58] assign the fundamental vibrational frequencies for the trans isomer. Dreizler and Scappini [54] have reported $V_3(CH_3)$. We obtained the $V_3(OH)$ and $V_3(C_2H_5)$ from the work of Mathews and McKetta [58]. The values of I_r and F, listed in Table II, are calculated using the molecular structural parameters of Aziz and Rogowski [59]. The value $\Delta_i H^0 = 1.213\ \text{kJ} \cdot \text{mol}^{-1}$ [54] for the reaction gauche isomer (g) = trans isomer (g) is employed for evaluating the equilibrium compositions of the isomeric mixture at selected temperatures. We incorporate the calculated equilibrium compositions with the evaluated thermodynamic properties of the gauche and trans isomers to calculate the thermodynamic properties of 1-propanol (g).

3.4. 2-Propanol

The $I_aI_bI_c$ is derived from the rotational constants determined by Kondo and Hirota [60]. The vibrational frequencies, $V_3(CH_3)$, and $F(CH_3)$ are those reported by Green [61]. The $F(OH)$ and $V(OH)$ for the OH rotor come from Inagaki et al. [52]. From the torsional transitions of the far-infrared spectra of isopropyl alcohol and its deuterated species, Inagaki and his co-workers obtain a potential function for the OH rotor:

Table III. Ideal Gas Thermodynamic Properties of Methanol and Ethanol

	Methanol			Ethanol		
T (K)	C_p^0 $(J\cdot K^{-1}\cdot mol^{-1})$	$S^0(T)-S^0(0)$ $(J\cdot K^{-1}\cdot mol^{-1})$	$H^0(T)-H^0(0)$ $(kJ\cdot mol^{-1})$	C_p^0 $(J\cdot K^{-1}\cdot mol^{-1})$	$S^0(T)-S^0(0)$ $(J\cdot K^{-1}\cdot mol^{-1})$	$H^0(T)-H^0(0)$ $(kJ\cdot mol^{-1})$
50	33.997	172.15	1736.7	37.533	199.20	1956.6
100	36.902	196.59	3508.8	41.614	226.21	3916.8
150	38.591	211.92	5402.1	46.437	244.01	6120.6
200	39.677	223.17	7358.0	51.432	258.03	8563.5
250	41.416	232.19	9381.3	57.638	270.15	11285.
300	44.156	239.97	11517.	64.994	281.30	14347.
350	47.676	247.03	13810.	72.914	291.91	17793.
400	51.618	253.66	16291.	80.842	302.17	21638.
450	55.684	259.97	18974.	88.421	312.13	25872.
500	59.690	266.05	21859.	95.491	321.82	30472.
550	63.537	271.92	24940.	102.01	331.23	35412.
600	67.186	277.60	28209.	108.02	340.36	40665.
650	70.626	283.12	31655.	113.54	349.23	46205.
700	73.861	288.47	35268.	118.65	357.84	52012.
750	76.900	293.67	39038.	123.38	366.19	58064.
800	79.755	298.73	42955.	127.78	374.29	64345.
850	82.436	303.64	47011.	131.88	382.16	70837.
900	84.954	308.43	51196.	135.70	389.81	77528.
950	87.319	313.08	55504.	139.26	397.24	84402.
1000	89.538	317.62	59926.	142.58	404.47	91449.
1050	91.621	322.04	64455.	145.69	411.50	98657.
1100	93.574	326.35	69085.	148.60	418.35	106020.
1150	95.406	330.55	73810.	151.31	425.01	113510.
1200	97.123	334.65	78624.	153.85	431.51	121140.
1250	98.733	338.64	83521.	156.22	437.84	128900.
1300	100.24	342.54	88496.	158.44	444.01	136760.
1350	101.66	346.35	93544.	160.51	450.03	144740.
1400	102.98	350.08	98660.	162.45	455.90	152810.
1450	104.23	353.71	103841.	164.27	461.63	160980.
1500	105.40	357.27	109082.	165.97	467.23	169240.

$V = \frac{1}{2}V_1(1-\cos\phi) + \frac{1}{2}V_2(1-\cos 2\phi) + \frac{1}{2}V_3(1-\cos 3\phi)$, where $V_1 = 0.364\ \mathrm{kJ \cdot mol^{-1}}$, $V_2 = -1.031\ \mathrm{kJ \cdot mol^{-1}}$, and $V_3 = 4.801\ \mathrm{kJ \cdot mol^{-1}}$. We use the above V and F values for generating internal rotational energy levels for use in the internal rotation partition functions to evaluate the internal rotational contributions to the thermodynamic properties of 2-propanol (g).

Table IV. Ideal Gas Thermodynamic Properties of 1-Propanol and 2-Propanol

	1-Propanol			2-Propanol		
T (K)	C_p^0	$S^0(T)-S^0(0)$	$H^0(T)-H^0(0)$	C_p^0	$S^0(T)-S^0(0)$	$H^0(T)-H^0(0)$
	$(\mathrm{J \cdot K^{-1} \cdot mol^{-1}})$		$(\mathrm{kJ \cdot mol^{-1}})$	$(\mathrm{J \cdot K^{-1} \cdot mol^{-1}})$		$(\mathrm{kJ \cdot mol^{-1}})$
50	40.206	218.18	1802.3	35.316	211.55	1781.1
100	53.543	250.48	4171.0	46.040	238.88	3784.1
150	61.784	273.85	7066.3	57.979	259.88	6393.7
200	69.129	292.61	10336.	68.283	277.99	9553.2
250	77.659	308.93	14000.	78.668	294.33	13224.
300	87.456	323.94	18124.	89.740	309.64	17432.
350	97.897	338.20	22756.	101.09	324.33	22203.
400	108.35	351.96	27914.	112.15	338.56	27536.
450	118.40	365.31	33585.	122.49	352.37	33406.
500	127.84	378.27	29743.	131.96	365.77	39771.
550	136.62	390.88	46358.	140.54	378.76	46587.
600	144.75	403.12	53395.	148.30	391.33	53811.
650	152.28	415.00	60823.	155.34	403.48	61405.
700	159.27	426.55	68614.	161.75	415.23	69334.
750	165.77	437.76	76742.	167.63	426.59	77571.
800	171.83	448.66	85184.	173.04	437.59	86090.
850	177.48	459.24	93918.	178.04	448.23	94868.
900	182.75	469.54	102930.	182.67	458.54	103890.
950	187.67	479.55	112190.	186.97	468.53	113130.
1000	192.26	489.30	121690.	190.97	478.22	122580.
1050	196.55	498.78	131410.	194.69	487.63	132220.
1100	200.56	508.02	141340.	198.16	496.77	142040.
1150	204.30	517.02	151460.	201.40	505.65	152030.
1200	207.80	525.79	161760.	204.41	514.29	162180.
1250	211.07	534.34	172240.	207.23	522.69	172470.
1300	214.12	542.68	182870.	209.85	530.87	182900.
1350	216.97	550.81	193640.	212.31	538.84	193460.
1400	219.63	558.75	204560.	214.60	546.60	204130.
1450	222.12	566.50	215610.	216.74	554.17	214910.
1500	224.45	574.07	226770.	218.75	561.55	225800.

4. RESULTS AND DISCUSSION

Employing the selected molecular and spectroscopic constants, presented in Table I and II, we evaluate the ideal gas thermodynamic properties for methanol, ethanol, 1-propanol, and 2-propanol, respectively. The calculated results appear in Tables III and IV. Table V summarizes the reported potential barrier heights for CH_3 and OH rotors in ethanol molecule. The inconsistencies among the results probably result from the use of different molecular and spectroscopic constants for evaluating the barrier heights for the C_2H_5OH molecule by various investigators.

Table VI presents a comparison of our statistically calculated C_p^0 and $S^0(T) - S^0(O)$ with experimental values. Small discrepancies exist between our calculated results and those of the previous works reported in the literature. The thermodynamic properties of methanol (g) are reported by Ivash et al. [62], Chen et al. [63], and Green [64]. Green also has evaluated the thermodynamic properties for 1-propanol [64] and 2-propanol [65]. Thermodynamic properties of 1-propanol are also reported by Mathews and McKetta [58]. Our results are obtained using more recent data and are better values.

Table V. Reported Potential Barrier Heights for $-CH_3$ and $-OH$ Rotors in Ethanol Molecule

$V_3(-CH_3)$ ($kJ \cdot mol^{-1}$)	$V(-OH)$ ($kJ \cdot mol^{-1}$)	Investigator(s) (year)	Reference No.
12.55	41.84	Schumann and Aston (1938)	34
7.53–12.55	10.04–18.41	Aston et al. (1943)	35
8.37–16.74	7.53–20.08	Halford (1949)	36
12.55	4.18	Halford (1950)	37
12.55–16.74		Ito (1952)	38
13.81	3.35	Barrow (1952)	4
12.55		Imanov and Kadzhar (1963)	39
3.35		Michielsen-Effinger (1964)	40
14.10		Imanov and Kadzhar (1967)	41
13.89		Culot (1972)	42
14.85[a]		During et al. (1975)	43
15.15[b]		During et al. (1975)	43
13.95[a]	2.117[a]	Selected in this work	
15.92[b]	5.407[b,c]	Selected in this work	

[a] For trans isomer.
[b] For gauche isomer.
[c] See text for details.

Table VI. Comparison of Calculated C_p^0 and $S^0(T)-S^0(0)$ with Experimental Values

T	$C_p^0(\mathrm{J \cdot K^{-1} \cdot mol^{-1}})$		T	$S^0(T)-S^0(0)(\mathrm{J \cdot K^{-1} \cdot mol^{-1}})$	
(K)	Exptl.	Calc.	(K)	Exptl.	Calc.
	Methanol[a]			Methanol[a]	
358.8	48.20	48.28	313.1	241.99	241.99
401.2	52.34	51.71	327.9	244.20	244.08
420.2	53.22	53.26	337.8	245.84	245.46
442.6	55.90	55.10	323.2	243.58	243.41
499.0	59.58	59.62	363.2	249.02	248.93
556.0	63.60	63.97	383.2	251.44	251.57
585.4	66.57	66.15			
	Ethanol[b]			Ethanol[c]	
200	51.38	51.42	298.2	281.82	281.01
280	62.09	61.97	351.5	292.61	292.28
350	73.05	72.93	403.2	304.29	302.91
370	76.02	76.11			
425	84.06	84.68			
476	91.21	92.17			
	1-Propanol[d]			1-Propanol[e]	
371.2	102.26	102.34	298.2	323.20	323.51
391.2	106.44	106.52			
411.2	110.42	110.62			
431.2	114.35	114.68			
451.2	118.62	118.62			
	2-Propanol[f]			2-Propanol[f]	
358.7	103.05	103.05	298.2	310.14	309.20
373.2	106.28	106.27	324.6	317.42	316.94
398.2	111.63	111.75	339.2	321.69	321.21
423.2	117.03	117.03	355.4	326.59	325.89
448.2	122.09	122.13			
473.2	127.03	126.99			

[a] Experimental values reported in Ref. 63.

[b] From Refs. 48 and 66.

[c] Evaluate from low-temperature measurements with an uncertainly of ±1.67 $\mathrm{J \cdot K^{-1} \cdot mol^{-1}}$.

[d] From Ref. 58.

[e] Evaluated from low-temperature measurements.

[f] From Ref. 65.

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