Heat Capacities and Derived Thermodynamic Functions of 1-Propanol between 10 K and 350 K and of 1-Pentanol between 85 K and 370 K

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Molar heat capacities of 1-propanol were measured from 10 K to 350 K, and $S_{abs,m}(T)$ and $H_m(T)-H_m(0)$ were calculated. The enthalpy of fusion was found to be (5400 ± 10) J·mol^{-1}; the triple-point temperature was calculated as (148.71 ± 0.02) K. Similar measurements were made on 1-pentanol between 85 K and 370 K; the enthalpy of fusion was found to be (10510 ± 20) J·mol^{-1}; the triple-point temperature was (195.6 ± 0.1) K. The molar heat capacity of the liquid 1-alcohols with a number of carbon atoms n in the linear chain between 3 and 22 can be described by $C_{p,l}(n,T) = \{99.38 + 17.769n + 0.05199n(T/\mathrm{K}) - 0.8742(T/\mathrm{K}) + 1265.2/(T/\mathrm{K}) + 0.0022603(T/\mathrm{K})^2\}$ J·K^{-1}·mol^{-1}, with a standard deviation of 3.1 J·K^{-1}·mol^{-1}. The main deviations occur above 370 K, where the experimental data start to flatten. Plotting the experimental heat capacity data for the 1-alcohols with a carbon number in the chain between 3 and 22 on a mass basis showed that all curves pass through almost the same value around 290 K.

Introduction

In previous publications,[1−3] we reported heat capacities and derived thermodynamic properties of 1-alcohols with carbon number in the chain ranging between 6 and 22. To extend the series, we present in this publication heat capacities of 1-propanol and of 1-pentanol. 1-Propanol was measured between 10 K and 350 K, 1-pentanol between 85 K and 370 K. The heat capacities of the liquid phase of all compounds measured, in total 944 data points, are used to derive a correlation function with the variables T/K and n (number of carbon atoms in the chain). A survey and a critical evaluation and correlation of the heat capacities of the individual 1-alcohols is given in the monograph by Zábranský et al.[4] The complete condensed phases of 1-propanol are reviewed by Wilthoit et al.[5] We compare our results to the adiabatic calorimetry measurements reported by Parks et al.[6] and Counsell et al.[7]

Experimental Section

The compounds were bought from Sigma-Aldrich Chemie; the stated purity of 1-propanol was 99.9 mass % and of 1-pentanol 99.8 mass %. The compounds were used as received; all manipulations were performed in a glovebox under dry nitrogen atmosphere. 1-Propanol and 1-pentanol were measured in CALV (laboratory design indication).[8,9] Below 30 K, the reproducibility of this calorimeter is about 1%, between 30 K and 100 K, it is 0.05 to 0.1%, and above 100 K, it is 0.03%. Oxford Instruments calibrated the thermometer with an uncertainty of 0.001 K using the ITS-90[10] temperature scale. Measurements on *n*-heptane[11,12] and synthetic sapphire[13,14] verified the uncertainty of the heat capacity measurements. No deviations from the recommended values larger than 0.2% were found. When we did find deviations from the literature[7] for 1-propanol in the liquid phase, the measurement of synthetic sapphire was repeated between 300 K and 400 K. No deviation larger than 0.07% was found. Measurements were made in the intermittent mode, using stabilization periods of about 600 s and heat input periods of about 500 s. In the melting range, longer stabilization periods of (1200 to 2000) s were used in order to allow the temperature to stabilize to within about 0.002 K of the extrapolated equilibrium value. Below 30 K, time periods of 100 s were used. For 1-propanol, the data below 10 K were used to calculate the values of S(10 K) and H(10 K)−H(0) using the low-temperature limit of the Debye function, $C_p = \alpha T^3$; the derived thermodynamic properties at higher temperatures were calculated by numerical integration of the interpolated data set. The purity of the compounds was calculated from the melting experiments using the van't Hoff relation

$$(T_{\mathrm{triple}} - T_{\mathrm{eq}}) = \frac{RT^2_{\mathrm{triple}}}{\Delta H_{\mathrm{fus}}}\frac{x}{F}$$

in which T_{triple} is the triple-point temperature, T_{eq} is the experimental equilibrium temperature in the melt at the melted fraction F, x is the impurity in mol, and ΔH_{fus} is the calculated enthalpy of fusion.

1-Propanol. About 7 g was loaded in the calorimeter vessel, after evacuation, 1 kPa of helium gas was admitted before closing the vessel. The calorimeter was cooled in the first run to 84 K, without any crystallization of the compound. In series 1, given with the other experimental data in Table 1, the glass transition took place around 99 K, followed by measurements of the undercooled liquid phase up to 128 K. At that temperature, the first exothermic effect in the stabilization periods started, and in the subsequent measurements, the crystallization took place, which heated the sample close to the melting point of the stable crystalline form. To prepare the stable crystalline form, this measurement was repeated but stopped at 130 K and the calorimeter was left under adiabatic conditions

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10.1021/je0499768 CCC: $27.50
Published on Web 03/23/2004

Table 1. Experimental Molar Heat Capacities of 1-Propanol

T/K	C_p/J·K^{-1}·mol^{-1}	T/K	C_p/J·K^{-1}·mol^{-1}	T/K	C_p/J·K^{-1}·mol^{-1}	T/K	C_p/J·K^{-1}·mol^{-1}	T/K	C_p/J·K^{-1}·mol^{-1}
					Series 1 Glass				
84.71	55.24	104.95	107.62	128.38	105.81	150.40	106.53	172.18	107.94
86.52	56.57	107.92	107.36	131.28	102.65	153.16	106.61	174.85	108.18
89.38	58.64	110.88	107.06	134.34	83.94	155.90	106.79	177.52	108.45
92.19	61.10	113.84	106.76	138.23	33.56	158.64	106.94	180.18	108.71
94.96	66.41	116.78	106.54	143.61	0.83	161.37	107.10	182.83	108.99
97.54	89.12	119.70	106.25	147.64	200.01	164.09	107.28	185.46	109.33
99.83	115.43	122.61	106.26	148.62	5742.22	166.80	107.50		
102.19	108.01	125.50	106.17	148.83	1424.51	169.49	107.71		
					Series 2 Glass				
85.67	55.90	96.51	73.54	107.14	107.45	119.02	106.43	130.95	102.08
86.99	56.91	98.20	99.02	109.12	107.26	121.00	106.19	133.05	90.12
88.93	58.37	99.73	117.97	111.10	107.06	122.99	106.31	135.47	57.95
90.84	59.85	101.34	108.37	113.08	106.86	124.97	106.24		
92.75	61.72	103.19	107.81	115.06	106.68	126.95	106.06		
94.65	64.99	105.17	107.60	117.04	106.55	128.93	105.30		
					Series 3 Crystal				
119.02	63.38	124.90	65.83	130.77	68.26	136.64	70.81	142.50	73.80
120.99	64.04	126.86	66.59	132.73	69.08	138.60	71.71	144.45	75.77
122.95	65.02	128.82	67.41	134.69	69.95	140.55	72.66		
					Series 4				
4.99	0.20	7.72	0.61	11.83	2.23	17.37	5.81	24.15	11.43
5.41	0.22	8.94	0.94	13.50	3.19	19.52	7.46	26.63	13.58
6.36	0.35	10.33	1.49	15.36	4.38	21.78	9.32	29.24	15.59
					Series 5				
5.01	0.17	8.72	0.90	13.48	3.15	19.60	7.53	26.79	13.71
6.14	0.29	10.13	1.44	15.38	4.40	21.90	9.44	29.43	15.75
7.33	0.52	11.74	2.19	17.42	5.83	24.29	11.57		
					Series 6				
32.10	18.09	46.52	28.98	62.13	38.64	78.58	46.95	94.68	53.91
34.44	20.16	49.05	30.75	64.82	40.12	81.38	48.22	97.15	54.90
36.72	21.88	51.61	32.44	67.54	41.54	84.17	49.46	99.58	55.88
39.11	23.50	54.20	34.01	70.28	42.95	86.90	50.65		
41.56	25.36	56.81	35.59	73.03	44.31	89.55	51.79		
44.03	27.19	59.46	37.12	75.80	45.65	92.15	52.87		
					Series 7				
101.41	56.44	130.34	68.07	148.67	33599	158.49	106.55	185.32	109.37
104.32	57.81	133.25	69.29	148.68	52191	161.22	106.79	187.95	109.64
107.19	59.01	136.16	70.53	148.69	88291	163.93	107.01	190.57	109.94
110.07	60.14	139.06	71.90	148.69	89920	166.64	107.32	193.19	110.41
112.95	61.20	141.97	73.60	148.70	73311	169.34	107.61	195.79	110.64
115.84	62.28	144.84	79.58	148.72	18411	172.03	107.88	198.38	110.93
118.73	63.39	147.32	135.10	148.95	1165	174.71	108.22	200.97	111.40
121.63	64.43	148.49	2361	150.39	130.40	177.37	108.49		
124.53	65.69	148.61	12329	153.00	106.26	180.03	108.81		
127.43	66.87	148.65	22423	155.75	106.33	182.68	109.05		
					Series 8				
203.35	111.76	225.84	116.05	248.70	122.27	270.68	130.22	291.66	140.59
205.56	112.13	228.74	116.74	251.50	123.20	273.36	131.39	294.20	141.98
208.15	112.54	231.64	117.43	254.28	123.87	276.02	132.62	296.74	143.51
211.11	113.05	234.52	118.20	257.05	124.80	278.67	133.86	299.25	144.96
214.08	113.58	237.38	118.92	259.81	125.83	281.30	135.13		
217.04	114.16	240.23	119.70	262.55	126.88	283.91	136.42		
219.99	114.78	243.07	120.56	265.28	127.98	286.51	137.76		
222.92	115.39	245.89	121.39	267.99	129.08	289.09	139.17		
					Series 9				
301.34	146.10	312.85	153.53	324.58	162.01	336.31	170.92	348.07	180.10
303.15	147.31	314.81	155.09	326.53	163.40	338.26	172.53	350.04	181.64
305.04	148.46	316.76	156.34	328.49	164.94	340.22	174.06		
306.99	149.78	318.71	157.68	330.44	166.42	342.17	175.45		
308.94	151.07	320.67	159.11	332.40	167.90	344.13	177.04		
310.90	152.22	322.62	160.57	334.35	169.41	346.10	178.10		

overnight. The temperature increased spontaneously to 147.9 K. Setting the adiabatic shield regulation temperature of the inner shield 10 K below the vessel temperature lead to a slow cooling curve in which the remaining liquid crystallized over a period of 24 h. The experimental heat capacity data of the glass state, the undercooled liquid state, the crystalline form, and the stable liquid are shown in Figure 1. The calculated thermodynamic properties $S(T)$ and $H(T)-H(0)$ are given at selected temperatures in Table 2. The enthalpy of fusion and the fits of the heat capacity of the solid and the liquid phase used to calculate this value are given in Table 4 and are compared to literature values.[7]

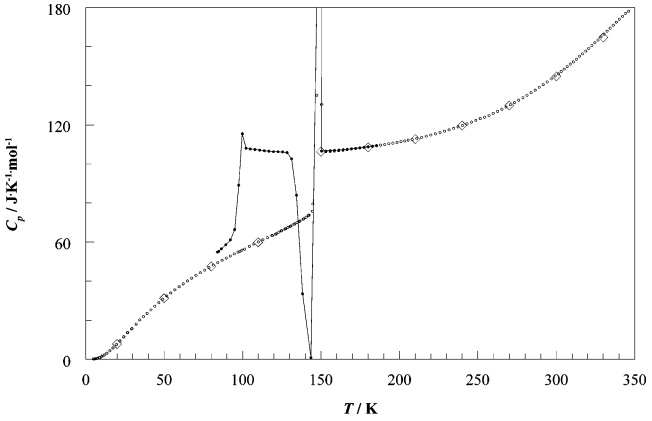

Figure 1. Experimental molar heat capacities of 1-propanol. ●, this work, the glass-liquid transition and crystallization; ○, this work, stable crystalline form and the liquid phase; ◇, ref 7.

Table 2. Thermodynamic Properties at Selected Temperatures for 1-Propanol (Molar Mass = 60.096 g·mol^{-1})

T/K	$C_{p,m}°$/J·K^{-1}·mol^{-1}	$S_{abs,m}°$/J·K^{-1}·mol^{-1}	$\Delta H_m°$/J·mol^{-1}
10	1.39	0.46	3.45
20	7.86	3.20	46.83
30	16.25	8.02	168.7
40	24.17	13.82	372.2
50	31.39	20.01	650.8
60	37.43	26.27	995.6
70	42.81	32.46	1397
80	47.60	38.49	1850
90	51.98	44.35	2348
100	56.02	50.04	2888
110	60.11	55.57	3468
120	63.84	60.96	4088
130	67.93	66.23	4747
140	72.40	71.42	5447
148.72[a]	75.60	75.51	6028
148.72[b]	105.92	111.82	11428
150	106.00	112.73	11564
160	106.68	120.02	12692
170	107.68	126.52	13763
180	108.80	132.70	14845
190	109.87	138.61	15939
200	111.22	144.28	17044
210	112.85	149.75	18165
220	114.79	155.04	19302
230	117.04	160.19	20461
240	119.64	165.23	21644
250	122.70	170.17	22856
260	125.90	175.04	24098
270	129.93	179.87	25377
280	134.50	184.68	26698
290	139.67	189.48	28068
298.15	144.33	193.42	29225
300	145.36	194.31	29493
310	151.69	199.17	30978
320	158.65	204.10	32529
330	166.08	209.09	34152
340	173.77	214.18	35851
350	181.52	219.32	37628

[a] Solid phase. [b] Liquid phase.

The purity of the sample was calculated from the melting experiment and was found to be 99.94 mol %.

1-Pentanol. A controlled cooling curve at −0.047 K·min^{-1}, obtained by setting the temperature regulation of the inner shield and the wire heater 10 K below the vessel temperature, showed an undercooling of the melting point of 10 K. Because of the released heat from the crystallization process, the temperature of the vessel rose to the melting point and the continuation of the cooling curve showed no indication of a metastable crystalline form. The experimental heat capacity data are given in Table 3 and are plotted in Figure 2, together with values from refs 6 and 7. The enthalpy of fusion was measured twice; the mean value measured was (10510 ± 10) J·K^{-1}·mol^{-1}. In Table 4, the melting experiments of 1-propanol and 1-pentanol are given, together with the fits of the molar heat capacities of the solid and liquid phases used in the calculation as a baseline and the literature values. The purity calculated from the fractional melting curve was (99.8 ± 0.05) mol %; the triple-point temperature was (195.6 ± 0.1) K. The error margin in the triple point was quite large, as near the end of the melting process the equilibrium temperatures in the partially melted sample did not follow the trend given by the measurements with $1/F = 10$ and $1/F = 1.5$ but remained constant.

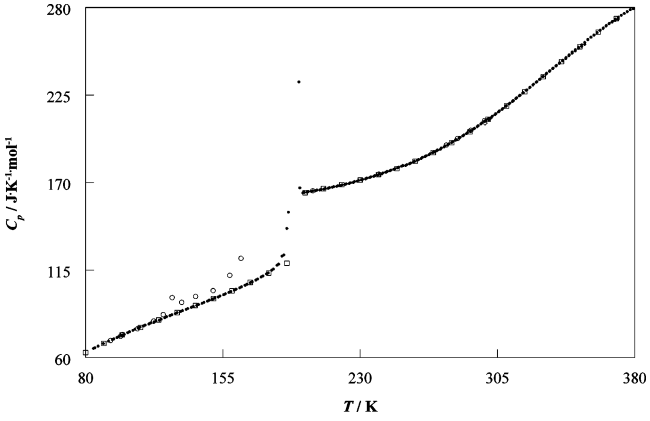

Figure 2. Experimental molar heat capacities of 1-pentanol. ●, this work; ○, ref 6; □, ref 7.

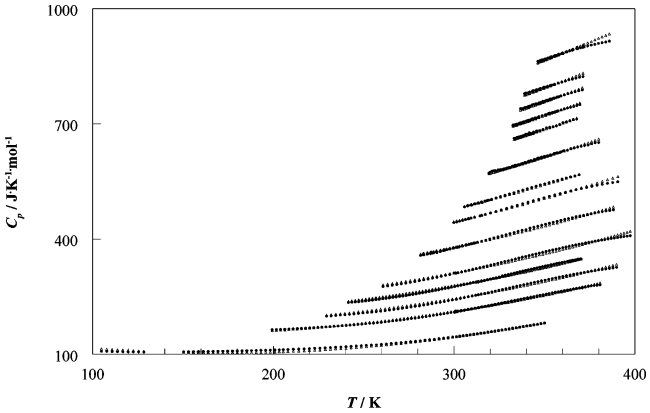

Figure 3. Experimental molar heat capacities of the liquid phase of the 1-alcohols with a number of carbon atoms (n) from 3 to 22. Not measured were the alcohols with $n = 4$, $n = 9$, $n = 11$, $n = 14$, $n = 16$, and $n = 21$. ●, experimental data; △, calculated values.

Comparing with the Literature. Of the two data sets available for 1-pentanol,[6,7] the data of Counsell[7] are the most reliable. The data of Parks[6] are probably measured on a less pure sample. This assumption is based on the premelting visible in their data as given in Figure 2. For 1-propanol, the data of ref 7 do correspond within the error margin up to 300 K. For instance, the differences in S(300 K) and H(300 K)−H(0) are in the order of 0.1% and 0.16% respectively. At 350 K however, our value for the molar heat capacity of 1-propanol is 1.2% higher than the value reported by ref 7. To check our values, we remeasured the heat capacity of synthetic sapphire between 300 K and 400 K; the maximum deviation from the recommended values[14] found was 0.07%. Remarkably however, is that the heat

Table 3. Experimental Molar Heat Capacities of 1-Pentanol

T / K	C_p / J·K^{-1}·mol^{-1}	T / K	C_p / J·K^{-1}·mol^{-1}	T / K	C_p / J·K^{-1}·mol^{-1}	T / K	C_p / J·K^{-1}·mol^{-1}	T / K	C_p / J·K^{-1}·mol^{-1}
					Series 1				
84.35	65.89	141.73	93.48	195.13	4077	215.58	167.46	261.84	184.56
85.06	66.25	144.65	94.77	195.25	7317	217.86	168.06	263.95	185.84
86.86	67.27	147.58	96.12	195.32	11911	220.14	168.68	266.05	186.93
89.74	68.87	150.51	97.45	195.37	17851	222.41	169.28	268.14	188.12
92.58	70.39	153.44	98.80	195.40	26446	224.67	169.98	270.23	189.24
95.42	71.88	156.38	100.20	195.42	37677	226.92	170.74	272.30	190.52
98.27	73.33	159.31	101.61	195.43	62673	229.17	171.45	274.36	191.79
101.12	74.67	162.24	103.05	195.44	182954	231.40	172.08	276.41	193.06
103.99	76.36	165.18	104.56	195.44	901049	233.63	172.91	278.46	194.40
106.86	77.84	168.11	106.11	195.45	124994	235.85	173.67	280.49	195.74
109.74	79.23	171.04	107.72	195.45	77471	238.06	174.45	282.51	197.04
112.62	80.53	173.97	109.43	195.46	49638	240.27	175.24	284.53	198.45
115.51	81.81	176.89	111.30	195.48	42959	242.46	176.08	286.53	199.91
118.41	83.11	179.80	113.33	195.69	1520	244.65	177.02	288.52	201.35
121.31	84.26	182.67	115.64	197.05	166.69	246.83	177.90	290.50	202.81
124.22	85.78	185.50	118.77	199.38	163.90	249.00	178.81	292.48	204.11
127.13	87.05	188.28	124.56	201.72	164.40	251.16	179.81	294.44	205.79
130.04	88.35	190.88	151.47	204.05	164.85	253.31	180.73	296.39	207.42
132.96	89.63	192.93	283.82	206.37	165.31	255.46	181.29	298.34	208.88
135.88	90.90	194.22	594.98	208.68	165.79	257.60	182.33	300.27	210.28
138.80	92.19	194.87	1743	210.99	166.35	259.72	183.42		
					Series 2				
300.30	209.40	316.96	224.55	335.20	241.58	352.67	256.89	369.37	272.76
300.60	209.89	318.82	226.26	336.98	243.24	354.38	259.82	371.01	274.05
301.72	211.03	320.67	228.00	338.75	244.92	356.07	261.38	372.64	275.14
303.67	212.74	322.52	229.67	340.51	246.60	357.76	262.85	374.27	276.38
305.60	214.44	324.36	231.42	342.27	248.02	359.43	264.36	375.89	277.43
307.52	216.02	326.19	233.09	344.02	249.71	361.10	265.85	377.52	278.66
309.43	217.84	328.01	234.81	345.76	251.26	362.77	267.17	379.14	279.32
311.32	219.47	329.82	236.60	347.50	252.83	364.43	268.78	380.76	280.36
313.21	221.03	331.62	238.27	349.23	254.25	366.08	270.13		
315.09	222.83	333.42	239.94	350.95	255.52	367.73	271.33		
					Series 3				
94.72	71.43	152.49	98.21	195.35	14572	221.71	168.88	267.57	187.55
95.39	71.74	155.42	99.58	195.39	21556	223.98	169.49	269.66	188.85
97.19	72.64	158.36	101.02	195.41	31291	226.24	170.19	271.74	190.03
100.10	74.14	161.29	102.48	195.43	45801	228.49	170.97	273.81	190.93
102.99	75.73	164.23	103.98	195.44	63686	230.73	171.69	275.87	192.50
105.87	77.16	167.16	105.55	195.45	75757	232.96	172.37	277.92	193.85
108.76	78.64	170.08	107.17	195.46	52928	235.19	173.18	279.97	195.18
111.65	79.96	173.01	108.87	195.48	46668	237.41	174.00	282.00	196.61
114.54	81.27	175.94	110.70	195.50	24313	239.61	174.80	284.02	197.96
117.45	82.55	178.85	112.70	195.55	7465	241.81	175.57	286.03	199.37
120.35	83.59	181.73	115.01	196.54	233.29	244.00	176.53	288.04	200.78
123.26	85.21	184.57	118.07	198.65	163.65	246.19	177.41	290.03	202.30
126.17	86.52	187.36	123.84	200.99	163.99	248.36	178.37	292.01	203.82
129.09	87.81	190.01	141.18	203.32	164.43	250.53	179.33	293.99	205.24
132.00	89.11	192.07	308.38	205.65	164.91	252.69	180.35	295.95	206.87
134.92	90.35	193.43	448.14	207.96	165.40	254.84	180.78	297.91	208.52
137.85	91.65	194.34	918.4	210.27	165.93	256.98	181.89	299.85	210.01
140.77	92.89	194.82	1984	212.58	166.46	259.12	182.97		
143.70	94.19	195.06	3720	214.87	167.08	261.25	184.11		
146.63	95.55	195.20	6055	217.16	167.65	263.36	185.17		
149.56	96.87	195.29	9526	219.44	168.24	265.47	186.38		
					Series 4				
300.81	210.54	315.46	223.30	331.85	238.73	347.57	253.58	362.67	266.89
301.09	210.46	317.31	224.93	333.63	240.30	349.27	255.13	364.32	268.43
302.20	211.81	319.16	226.53	335.40	241.97	350.97	256.62	365.96	269.86
304.12	213.39	320.99	228.31	337.16	243.65	352.66	258.17	367.59	270.92
306.03	215.06	322.82	229.96	338.92	245.30	354.35	259.96	369.23	271.93
307.94	216.66	324.65	231.73	340.66	246.90	356.02	261.44	370.86	272.95
309.83	218.39	326.46	233.41	342.40	248.57	357.70	262.72		
311.72	219.98	328.27	235.00	344.13	250.30	359.36	264.29		
313.59	221.54	330.07	236.82	345.85	252.05	361.02	265.62		

Table 4. Melting Experiments of 1-Propanol and 1-Pentanol

compound	linear fit solid phase / J·K^{-1}·mol^{-1}	linear fit liquid phase / J·K^{-1}·mol^{-1}	ΔH_{fusion} / J·mol^{-1}	T_{triple} / K	purity (calc) / mol %	ΔH_{fusion} (lit) / J·mol^{-1}
1-propanol	$14.72 + 0.409T$	$96.02 + 0.067T$	5400 ± 10	148.71 ± 0.01	99.94	5372
1-pentanol	$22.15 + 0.499T$	$123.85 + 0.201T$	10521 ± 20	195.6 ± 0.1	99.8	10502
1-pentanol	$22.15 + 0.499T$	$123.85 + 0.201T$	10500 ± 20	195.6 ± 0.1	99.8	

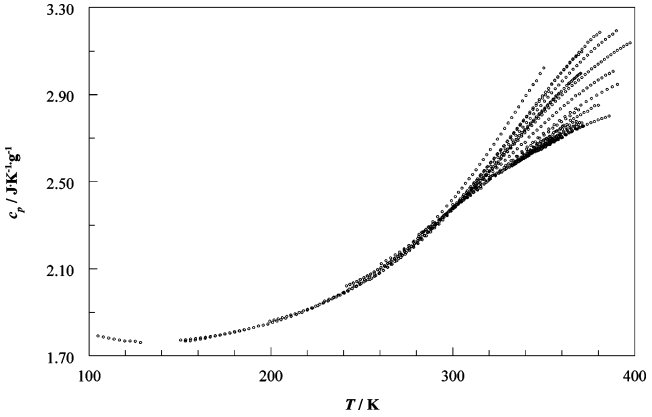

Figure 4. The heat capacities of the 1-alcohols on a mass basis. Above 300 K, the highest values of the heat capacity belongs to $n = 3$; the other values diminish with increasing n.

capacities of 1-pentanol, published in the same article,[7] do not show differences larger than 0.1% with our values.

Correlation of the Liquid Heat Capacities of the 1-Alcohols with Carbon Number in the Chain between 3 and 22. All measured heat capacities of the liquid phase of the 1-alcohols, a total of 944 measurements, were collected in one file, containing temperature (T), carbon number (n), and heat capacity. Using the solver option of the Excel program, the following correlation function was found

$$C_{p,l}(n,T) = \{99.38 + 17.769n + 0.05199n(T/\mathrm{K}) - 0.8742(T/\mathrm{K}) + 1265.2/(T/\mathrm{K}) + 0.0022603(T/\mathrm{K})^2\}\ \mathrm{J{\cdot}K^{-1}{\cdot}mol^{-1}}$$

The mean absolute percentage deviation of the function with the experimental data was 0.86%; the standard deviation was 3.1 J·K^{-1}·mol^{-1}. The experimental data and the calculated values are given in Figure 3. From this figure, it is clear that the calculated function did not follow the curvature of the experimental data above 370 K. Zábranský[15] discussed the peculiar shape of the liquid heat capacities of 1-alcohols; showing a point of inflection, they assumed that there is a relation between the inflection point on the heat capacity curve and the breakdown of hydrogen bonds in the liquid. In Figure 4, the experimental heat capacities of the liquid phase of the 1-alcohols were plotted on a gram basis. This gave a compact representation in which all curves pass through almost the same value around 290 K.

Literature Cited

(1) van Miltenburg, J. C.; Oonk, H. A. J.; Ventola, L. Heat Capacities and Derived Thermodynamic Functions of 1-Octadecanol, 1-Nonadecanol, 1-Eicosanol, and 1-Docosanol Between 10 K and 370 K. *J. Chem. Eng. Data* **2001**, *46*, 90−97.

(2) van Miltenburg, J. C.; van den Berg, G. J. K.; Ramirez, M. Heat Capacities and Derived Thermodynamic Functions of 1-Dodecanol and 1-Tridecanol between 10 K and 370 K and Heat Capacities of 1-Pentadecanol and 1-Heptadecanol between 300 K and 380 K and Correlations for the Heat Capacity and the Entropy of Liquid *n*-Alcohols. *J. Chem. Eng. Data* **2003**, *48*, 36−43.

(3) van Miltenburg, J. C.; Gabrielová, H.; Růžička, K. Heat Capacities and Derived Thermodynamic Functions of 1-Hexanol, 1-Heptanol, 1-Octanol, and 1-Decanol between 5 K and 390 K. *J. Chem. Eng. Data* **2003**, *48*, 1323−1331.

(4) Zábranský, M.; Růžička, V., Jr.; Majer, V.; Domalski, E. S. Heat Capacity of Liquids: Volume II, Critical Review and Recommended Values, *J. Phys. Chem. Ref. Data*, *Monograph 6* **1996**. (b) Zábranský, M.; Růžička, V.; Domalski, E. S. Heat Capacity of Liquids: Critical Review and Recommended Values Supplement I. *J. Phys. Chem. Ref. Data* **2001**, *30*, 1199−1689.

(5) Wilthoit, C.; Chao, J.; Hall, K. R. Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C1 to C4. *J. Phys. Chem. Ref. Data* **1985**, *14*, 1−175.

(6) Parks, S.; Huffman, H. H.; Barmore, M. Thermal Data on Organic Compounds. XI. The Heat Capacities, Entropies, and Free Energies of Ten Compounds Containing Oxygen or Nitrogen. *J. Am. Chem. Soc.* **1933**, *55*, 2733−2740.

(7) Counsell, J. F.; Lees, E. B.; Martin, J. F. Thermodynamic Properties of Organic Compounds. Part XIX. Low-Temperature Heat Capacity and Entropy of Propan-1-ol, 2-Methyl-propan-1-ol, and Pentan-1-ol. *J. Chem. Soc. A* **1968**, *8*, 1819−1823.

(8) van Miltenburg, J. C.; van den Berg, G. J. K.; van Bommel, M. J. Construction of an Adiabatic Calorimeter. Measurement of the Molar Heat Capacity of Synthetic Sapphire and of *n*-Heptane. *J. Chem. Thermodyn.* **1987**, *19*, 1129−1137.

(9) van Miltenburg, J. C.; van Genderen, A. C. G.; van den Berg, G. J. K. Design Improvements in Adiabatic Calorimetry. The Heat Capacity of Cholesterol Between 10 and 425 K. *Thermochim. Acta* **1998**, *319*, 151−162.

(10) Preston-Thomas, H. The International Temperature Scale of 1990 (ITS-90). *Metrologia* **1990**, *27*, 3−10.

(11) Douglas. J. P.; Furukawa, G. T.; McCloskey, R. E.; Ball, A. F. Calorimetric Properties of Normal Heptane from 0 to 520 K. *J. Res. Natl. Inst. Stand. Technol.* **1954**, *53*, 139−153.

(12) McCullough, J. P.; Messerly, J. F. The Chemical Thermodynamic Properties of Hydrocarbons and Related Substances. *Bur. Mines Bull.* **1961**, 596.

(13) National Bureau of Standard, Standard Reference Material 720, Washington D. C., 1982.

(14) Archer, D. G. Thermodynamic Properties of Synthetic Sapphire (α-Al_2O_3). Standard Reference Material 720 and the Effect of Temperature-Scale Differences on Thermodynamic Properties. *J. Phys. Chem. Ref. Data* **1993**, *6*, 1441−1453.

(15) Zábranský, M.; Bureš. M.; Růžička, V., Jr. Types of Curves for the Temperature Dependence of the Heat Capacity of Pure Liquids. *Thermochim. Acta* **1993**, *215*, 25−45.

Received for review January 6, 2004. Accepted February 23, 2004.

JE0499768