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Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols

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Molar enthalpies of vaporization of a series of six 1,3-alkanediols were obtained from the temperature dependence of the vapor pressure measured by the transpiration method. A large number of the primary experimental results on temperature dependences of vapor pressures have been collected from the literature and have been evaluated in order to derive vaporization enthalpies at the reference temperature 298.15 K. The experimental enthalpies of vaporization were checked for internal consistency. New experimental results together with those selected from the literature have been recommended for thermochemical calculations.

Introduction

Alcoholic OH groups have a strong tendency to associate with one another due to intermolecular hydrogen bonding. It has been also well-established that 1,3-alkanediols show conformers stabilized by intramolecular hydrogen bonding in solutions. Thus, competition between intra- and inter-molecular types of H-bonding is typical for 1,3-alkanediols in solutions or in the bulk liquid phase. Molar enthalpy of vaporization is defined as the enthalpy required to transfer 1 mol of a compound from the liquid to the gaseous phase. In the bulk liquid phase, alkanediols are present in a form where OH groups are involved partly into the inter-molecular H-bonds and partly into the intra-molecular H-bonds. A pattern of evaporation of intra- and inter-hydrogen-bonded species is different (see Figure 1). In order to remove 1 mol of a 1,3-alkanediol from the liquid to the gaseous phase it is necessary to disconnect (i) the van der Waals' interactions among molecules and (ii) inter-molecular H-bonds. Additionally, because the 1,3-alkanediol exists in intra-hydrogen-bonded form, an enthalpic contribution for its formation should be also taken into account. Thus, the molar enthalpy of vaporization includes all these three contributions. The scheme of a vaporization process is presented in the Figure 1. Assuming that x is the mole ratio of the intra-molecular H-bonded species and $(1 - x)$ is the mole ratio of the inter-molecular H-bonded species, a rough measure of the intra-molecular H-bonding strength could be obtained with help of the homomorph alkanols as we have described it earlier.[24,36] In order to get insight into the energetics of H-bonding, we have collected data on vaporization enthalpies and vapor pressures of 1,3-alkanediols available in the literature (see Table 1).

Enthalpies of vaporization $\Delta_l^g H_m$ can be measured directly using calorimetry or derived from vapor pressure temperature dependence. As can be seen, vapor pressure data of the 1,3-alkanediols have been measured mostly by ebulliometry at elevated temperatures close to the boiling point. It has been pointed out in our previous study of vapor pressures of 1,2-alkanediols[22] that there are a lot of complications in adjusting ebulliometric results to the reference temperature $T = 298.15$ K. Hence, vapor pressure measurements at the ambient temperatures (possibly close to 298.15 K) are desirable in order to obtain enthalpies of vaporization possibly less affected due to temperature adjustment. In this work, we extend our studies of diols with vapor pressure measurements of the six alkanediols (see Figure 2) by using the transpiration method.[23,24] This method offers two advantages. The first advantage is the opportunity to withdraw moisture in preliminary experiments by flushing the sample with dry nitrogen, and the resulting constant sample vapor pressure indicates that all moisture has been removed. The second arises from being able to measure the vapor pressures near ambient temperatures in order to reduce possible uncertainties in adjustment of the derived vaporization enthalpy to the reference temperature $T = 298.15$ K. For these reasons, we decided to determine the vapor pressures of 1,3-alkanediols using the transpiration method.

Experimental Section

Materials. Samples of diols were commercially available from Aldrich and Fluka and were further purified by fractional distillation with a spinning-band column under reduced pressure. The degree of purity was determined using a Hewlett-Packard gas chromatograph 5890 series II equipped with a flame ionization detector and a Hewlett-Packard 3390A integrator. The carrier gas (nitrogen) flow was 7.2 $\mathrm{dm^3 \cdot h^{-1}}$. A capillary column HP-5 (stationary phase crosslinked 5% PH ME silicone) was used with a column length of 30 m, an inside diameter of 0.32 mm, and a film thickness of 0.25 μm. The standard temperature program of the GC was $T = 323$ K for 180 s followed by a heating rate of 10 $\mathrm{K \cdot min^{-1}}$ to $T = 523$ K. No impurities (greater than 0.02 mass %) could be detected in the samples used for the vapor pressure measurements.

Vapor Pressure Measurements on 1,3-Alkanediols Using the Transpiration Method. Vapor pressures were determined using the method of transpiration in a saturated nitrogen stream,[23,24] and enthalpies of vaporization of 1,3-alkanediols were obtained applying the Clausius−Clapeyron equation. About 0.5 g of the sample was mixed with glass beads and placed in a thermostatted U-shaped tube (saturator) having a length of 20 cm and a diameter of 0.5 cm. The temperature in the measuring cell with saturator was kept constant within ± 0.1 K. The temperature inside the cell was measured by a platinum resistance thermometer PT-100 (Burster) with an accuracy of ± 0.1 K. Glass beads with diameter of 1 mm provide a surface that was sufficient for the vapor−liquid equilibration. At constant temperature, a nitrogen stream was

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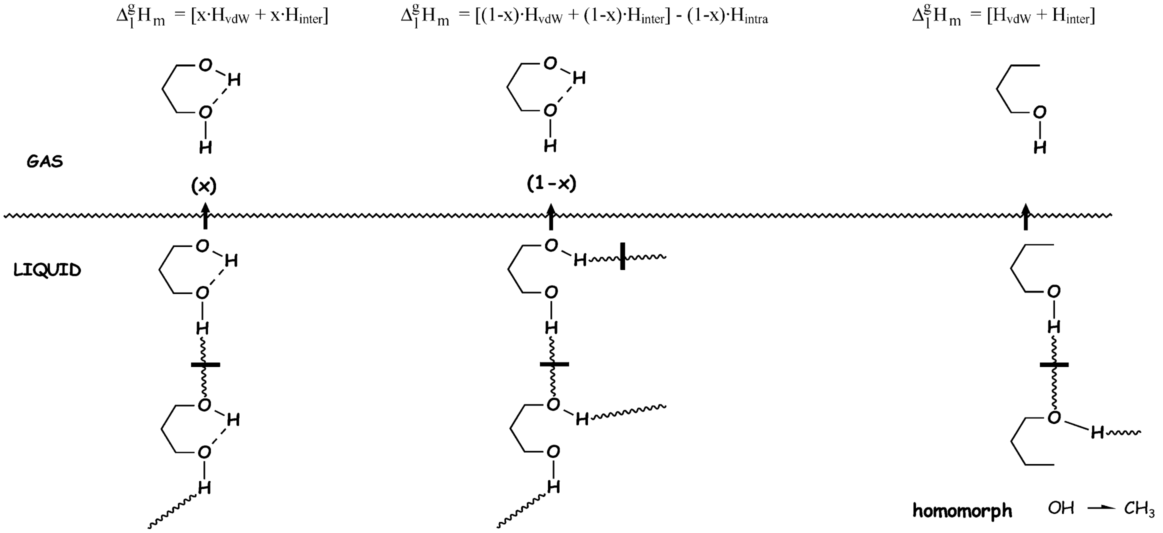

Figure 1. Competition of the inter- and intra-hydrogen bonding in alkanediols, where x is the mole ratio of intra-H-bonded molecules in the liquid, H_{vdW} is the contribution into the vaporization enthalpy due to the van der Waals' interactions among molecules; H_{intra} is the contribution into the vaporization enthalpy due to intra-molecular hydrogen bonding; H_{inter} is the contribution into the vaporization enthalpy due to inter-molecular hydrogen bonding.

passed through the U-tube, and the transported material was collected in a cold trap. The flow rate of the nitrogen stream was measured using a soap bubble flowmeter and optimized in order to reach the saturation equilibrium of the transporting gas at each temperature under study. The mass of compound collected within a certain time interval was determined by using a gas chromatograph equipped with autosampler. Uncertainty of the sample amount determined by GC analysis was assessed to be within (1 to 3) %. Assuming that Dalton's law of partial pressures applied to the nitrogen stream saturated with the substance i of interest is valid, values of p_i^{sat} were calculated as follows:

$$p_i^{sat} = m_i R T_a / V M_i; \quad V = V_{N2} + V_i; \quad (V_{N2} \gg V_i) \qquad (1)$$

where $R = 8.314472\ J \cdot K^{-1} \cdot mol^{-1}$; m_i is the mass of transported compound, M_i is the molar mass of the compound, and V_i is its volume contribution to the gaseous phase. V_{N2} is the volume of transporting gas, and T_a is the temperature of the soap bubble meter. The volume of transporting gas V_{N2} was determined from the flow rate and time measurements. Data of p_i^{sat} have been obtained as a function of temperature and were fitted using following equation:[24]

$$R \ln p_i^{sat} = a + \frac{b}{T} + \Delta_l^g C_p \ln\left(\frac{T}{T_0}\right) \qquad (2)$$

where a and b are adjustable parameters and $\Delta_l^g C_p$ is the difference of the molar heat capacities of the gaseous and the liquid phases, respectively. T_0 appearing in eq 2 is an arbitrarily chosen reference temperature (which has been chosen to be 298.15 K). Consequently, from eq 2 the expression for the vaporization enthalpy at temperature T is derived:

$$\Delta_l^g H_m (T) = -b + \Delta_l^g C_p\, T \qquad (3)$$

Values of $\Delta_l^g C_p$ have been calculated according to a procedure developed by Chickos and Acree.[18] Experimental results and parameters a and b are listed in Table 2. We have checked experimental and calculation procedures with measurements of vapor pressures of n-alcohols.[24] It turned out that vapor pressures derived from the transpiration method were reliable within (1 to 3) % and that their accuracy was governed by reproducibility of the GC analysis. In order to assess the uncertainty of the vaporization enthalpy, the experimental data were approximated with the linear equation $\ln(p_i^{sat}) = f(T^{-1})$ using the method of least-squares. The uncertainty in the enthalpy of vaporization was assumed to be identical with the average deviation of experimental $\ln(p_i^{sat})$ values from this linear correlation.

Results and Discussion

Temperature dependencies of vapor pressures of 1,3-alkanediols have been reported (see Table 1). To avoid discrepancies arising from the use of different algorithms to adjust values of vaporization enthalpies to $T = 298.15$ K, all available experimental vapor pressures were treated using eqs 2 and 3. $\Delta_l^g H_m$ (298.15 K) was calculated for the sake of comparison with results from this work. The collection of the available experimental results and derived $\Delta_l^g H_m$ (298.15 K) values for 1,3-alkanediols is presented in Table 1. The widely used comprehensive compilations by Stephenson and Malanowski[7] and Stull[9] contain vapor pressure data for some alkanediols over a wide range of temperatures. The origin of the data presented there is unclear and not traceable, methods of measurements are unknown, as well as are errors of measurements and purities of compounds. In spite of this fact, we also treated the results from Stephenson and Malanowski[7] and Stull[9] using eqs 2 and 3 and calculated $\Delta_l^g H_m$ (298.15 K) for the sake of comparison with other results. However, the agreement or disagreement with other data in each case should be questionable.

Vapor pressure data of the 1,3-propanediol available from the literature have been measured mostly by using ebulliometry at elevated temperatures close to the boiling point, thus direct comparison with the results from this work measured by transpiration at ambient temperatures was hardly possible (see Figure 3). However, the enthalpy of vaporization of 1,3-propanediol $\Delta_l^g H_m$ (298.15 K) = (70.5 ± 0.2) $kJ \cdot mol^{-1}$ derived in this work (see Table 1) agrees within ± 1.5 $kJ \cdot mol^{-1}$ with most of available results presented in Table 1.

Available vapor pressure data for the 1,3-butanediol are very consistent (Figure 4). Our results seem to be the first

Table 1. Compilation of Data on Enthalpies of Vaporization $\Delta_l^g H_m$ (298.15 K) of 1,3-Alkanediols[a]

	technique[b]	T range	$-\Delta C_p$ (C_p^l)[c]	$\Delta_l^g H_m$[d] (diol)	ref	$\Delta_l^g H_m$[f] (alkanol)	Δ[g]
		K	$J \cdot mol^{-1} \cdot K^{-1}$	$kJ \cdot mol^{-1}$		$kJ \cdot mol^{-1}$	$kJ \cdot mol^{-1}$
1	2	3	4	5	6	7	8
1,3-propanediol **(1)**	E	383−433	56.4	69.4 ± 2.0	1		
	E	373−488	(176.4)[20]	65.2	2		
	NA	332.5−487.3		63.1	9		
	C	298.15		72.4 ± 0.3	3		
	E	367.3−489.0		71.4	4		
	E	401.7−488.1		70.1 ± 0.3	5		
	E	314−460		66.5	6		
	NA	332−488		68.9	7		
	E	413.4−458.4		70.6 ± 0.5	8		
	LRTF	480−716		69.1 ± 0.2	10		
	T	293.5−342.3		**70.5 ± 0.2**	this work	52.4	18.1
± 1,3-butanediol **(2)**	E	373−423	65.7	66.4 ± 2.0	1		
	NA	340.7−449.7	(212.0)[11]	56.7	9		
	E	363.0−481.5		71.6	4		
	E	395.6−481.5		69.8 ± 1.2	5		
		362−483		71.6	7		
	E	365.0−518.3		70.0 ± 0.8	11		
	C	298.15		72.8 ± 0.6	12		
	T	288.3−332.3		**72.6 ± 0.3**	this work	54.2	18.4
(*R*)-1,3-butanediol **(3)**	C	298.15		72.3 ± 0.7	12	54.2	18.1
2,4-pentanediol **(4)**	T	297.2−347.3	76.3 (252.7)	**72.5 ± 0.3**	this work	57.3	15.2
3,5-octanediol **(5)**	NA	375−518	100.9 (347.2)	77.7	7	63.0	14.7
2-Me-2,4-pentanediol **(6)**	NA	373−473	83.1	68.4	7		
	E	369.9−547.2	(278.9)	68.6 ± 0.4	13		
	T	285.2−329.4		**68.9 ± 0.4**	this work	58.5	10.4
2,2-diMe-1,3-propanediol (cr I)	C	318.6	37.2	76.3 ± 3.8	14		
	T	314.3−347.2	(243.3)[19]	**76.8 ± 0.3**	this work		
2,2-diMe-1,3- propanediol (cr II)	C	311.3	26.8	87.9 ± 4.4	14		
	T	283.9−311.3	(173.9)[19]	**87.3 ± 0.4**	this work		
2,2-diMe-1,3-propanediol(liq) **(7)**				**75.7**[e]		56.1	19.6
2-Me-1,3- propanediol **(8)**	LRTF	488−708	69.5	71.3 ± 0.5	10		
	T	297.3−375.5	(226.7)	**73.6 ± 0.2**	this work	54.1	19.5
3-Me-1,3-butanediol **(9)**	E	346−475	76.4	71.8 ± 0.3	15		
	E	346.7−468.3	(253.2)	68.2	7	54.8	13.4
2-Me-1,3-butanediol **(10)**	NA	399−561	76.3 (252.7)	72.6	7	54.2	18.4
3-Me-2,4- pentanediol (11)	E	368.4−424.5	90.1 (305.7)	72.5	4	59.5	13.0
2-Et-1,3-hexanediol **(12)**	TEA	331−413	101.2 (348.4)	79.5	16		
2,2,4-triMe-1,3-pentanediol **(13)**	NA	413−502	99.6	74.0	7		
	E	395.9−489.4	(342.4)[17]	**75.3 ± 0.5**	17		
2,2-diEt−1,3-propanediol **(14)**	T	343−380	93.2 (317.6)	**80.2 ± 0.2**	41	66.0	14.2
2-Et-2-Bu-1,3-propanediol **(15)**	E	424.5−522.8	112.6 (381.4)[17]	**86.3 ± 1.2**	17		
2-Et-2-Bu-1,3-butanediol **(16)**	NA	338−500	116.0 (405.3)	77.2	7		

[a] Values in bold are recommended for the thermochemical calculations. [b] Techniques: E = ebulliometry; T = transpiration; C = calorimetry; LRTF = low residence time flow method; TEA = thermal evolution analysis. NA = not applicable. [c] Values of $\Delta_l^g C_p$ have been estimated from the isobaric molar heat capacity of the liquid diols, C_p^l, according to procedure developed by Chickos and Acree.[18] [d] Vapor pressures available in the literature were treated using eqs 2 and 3 in order to evaluate enthalpy of vaporization at 298.15 K in the same way as our own results in Table 2. [e] Value of vaporization enthalpy was calculated using enthalpy of sublimation $\Delta_{cr}^g H_m$ of cr II phase and the sum of phase transitions between 298 K and the fusion temperature (observed in the ref 31), which has been adjusted to the reference temperature 298.15 K: ($\Delta_{cr}^l H_m + \Delta H_{trs}$) = 11.6 kJ·mol⁻¹ according a procedure developed by Chickos and Acree.[33] [f] Alkanols used for comparison with the 1,3-alaknediols (**1** to **11**) and **14** were as follows: 1-butanol; 2-pentanol; 2-pentanol; 4-methyl-2-pentanol; 6-methyl-4-octanol; 2,4-dimethyl-2-pentanol; 2,2-dimethyl-1-butanol; 2-methyl-1-butanol; 2-methyl-2-pentanol; 3-methyl-2-pentanol; 3,4-dimethyl-2-pentanol; and 2,2-diethyl-1-butanol. [g] Δ is the difference between columns 5 and 7, which was supposed to be a rough measure for the strength of the hydrogen bonding in 1,3-alkanediols.

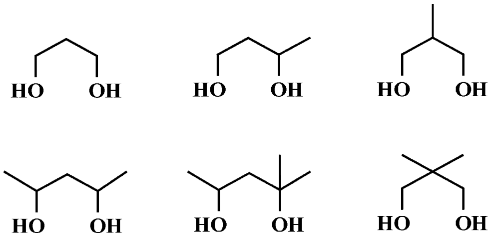

Figure 2. Structure of 1,3-alkanediols studied in this work: 1,3-propanediol; 1,3-butanediol; 2-methyl-1,3-propanediol; 2,4-pentanediol; 2-methyl-2,4-pentanediol; and 2,2-dimethyl-1,3-propanediol.

vapor pressure measurements for 1,3-butanediol at ambient temperatures. Also enthalpies of vaporization derived from ebulliometric and transpiration techniques are in a close agreement (see Table 1). The molar enthalpy of vaporization of 1,3-butanediol $\Delta_l^g H_m$ (298.15 K) = (72.6 ± 0.3) $kJ \cdot mol^{-1}$ obtained in this work (see Table 1) agrees excellently with the calorimetric result measured direct at the reference temperature by Ermelinda Eusebio et al.:[12] $\Delta_l^g H_m$ (298.15 K) = (72.8 ± 0.6) $kJ \cdot mol^{-1}$.

2,2-Dimethyl-1,3-propanediol (or neopentylglycol) is solid at room temperature with the monoclinic (cr, II) crystal structure.[25] At 314 K, 2,2-dimethyl-1,3-propanediol transforms into a plastic crystal phase (cr, I), the structure of which is cubic and remains in this phase until the melting process at (403.0 ± 0.5) K.[25] This compound has been discussed[25−32] as a potential latent heat storage material because of it unusually high (see Table 3) transitional enthalpies. Font and Muntasell[14] reported

Table 2. Vapor Pressures p and Enthalpy of Vaporization $\Delta_l^g H_m$, Obtained by the Transpiration Method

T	m	$V(N_2)$	p	$p_{exp} - p_{calc}$	$\Delta_l^g H_m$	T	m	$V(N_2)$	p	$p_{exp} - p_{calc}$	$\Delta_l^g H_m$
K[a]	mg[b]	dm^3 [c]	Pa[d]	Pa	kJ·mol^{-1}	K[a]	mg[b]	dm^3 [c]	Pa[d]	Pa	kJ·mol^{-1}
1,3-Propanediol $\Delta_l^g H_m$ (298.15 K) = (70.45 ± 0.24) kJ·mol^{-1}											
$\ln(p/\mathrm{Pa}) = \frac{301.4}{R} - \frac{87267.8}{R(T/\mathrm{K})} - \frac{56.4}{R}\ln\left(\frac{T/\mathrm{K}}{298.15}\right)$											
293.5	2.11	37.05	1.86	0.05	70.71	324.3	2.41	2.84	27.64	0.17	68.98
303.2	1.39	10.12	4.47	−0.09	70.17	327.3	2.29	2.09	35.58	0.86	68.81
309.3	0.94	3.87	7.88	0.00	69.82	330.3	2.07	1.54	43.72	0.05	68.64
312.2	1.88	6.15	9.97	−0.18	69.66	333.5	2.04	1.19	55.56	0.07	68.46
315.3	2.22	5.43	13.29	0.09	69.48	336.4	1.93	0.920	68.42	−0.22	68.29
318.4	2.32	4.56	16.59	−0.49	69.31	339.4	2.07	0.798	84.64	−0.51	68.13
321.3	2.32	3.49	21.68	0.05	69.15	342.3	1.93	0.598	105.3	0.86	67.96
1,3-Butanediol $\Delta_l^g H_m$ (298.15 K) = (72.56 ± 0.29) kJ·mol^{-1}											
$\ln(p/\mathrm{Pa}) = \frac{320.2}{R} - \frac{92150.4}{R(T/\mathrm{K})} - \frac{65.7}{R}\ln\left(\frac{T/\mathrm{K}}{298.15}\right)$											
288.3	2.61	51.85	1.39	−0.01	73.21	317.3	2.45	3.08	21.82	−0.27	71.30
290.3	3.17	51.97	1.68	−0.05	73.08	320.3	2.63	2.54	28.52	0.08	71.11
292.9	0.28	3.26	2.35	0.08	72.91	323.3	2.73	2.05	36.64	0.22	70.91
303.5	1.58	6.68	6.51	0.10	72.21	326.3	2.92	1.74	46.18	−0.22	70.71
308.3	1.69	4.66	9.94	−0.06	71.90	329.3	2.87	1.35	58.55	−0.27	70.52
311.3	1.95	4.12	13.01	−0.09	71.70	332.3	2.94	1.09	74.27	0.08	70.32
314.3	2.11	3.37	17.23	0.17	71.50						
2,4-Pentanediol $\Delta_l^g H_m$ (298.15 K) = (72.53 ± 0.30) kJ·mol^{-1}											
$\ln(p/\mathrm{Pa}) = \frac{333.3}{R} - \frac{95281.9}{R(T/\mathrm{K})} - \frac{76.3}{R}\ln\left(\frac{T/\mathrm{K}}{298.15}\right)$											
297.2	1.11	5.51	4.80	0.08	72.61	324.4	3.08	1.33	55.07	1.43	70.53
300.2	1.02	3.75	6.45	0.12	72.38	327.5	3.10	1.05	70.24	1.55	70.30
303.2	1.04	2.92	8.50	0.07	72.15	330.5	3.34	0.910	87.35	0.55	70.07
306.2	1.40	2.99	11.10	−0.05	71.92	333.4	4.20	0.910	109.6	1.3	69.85
309.2	1.74	2.85	14.53	−0.14	71.69	336.5	4.05	0.700	137.6	1.0	69.61
312.2	1.97	2.47	18.92	−0.25	71.46	339.2	3.88	0.560	164.8	−1.6	69.40
315.3	2.11	2.10	23.90	−1.22	71.23	344.4	6.06	0.595	241.9	0.8	69.01
318.4	2.52	1.92	31.19	−1.52	70.99	347.3	5.18	0.420	292.9	−1.9	68.79
321.4	2.79	1.62	40.95	−1.05	70.76						
2-Me-2,4-Pentanediol $\Delta_l^g H_m$ (298.15 K) = (68.88 ± 0.39) kJ·mol^{-1}											
$\ln(p/\mathrm{Pa}) = \frac{332.6}{R} - \frac{93653.4}{R(T/\mathrm{K})} - \frac{83.1}{R}\ln\left(\frac{T/\mathrm{K}}{298.15}\right)$											
285.2	0.61	5.08	2.50	−0.08	69.96	309.4	1.42	1.16	25.65	0.56	67.95
287.9	0.53	3.31	3.33	−0.07	69.73	312.5	1.82	1.16	32.74	0.15	67.69
291.2	0.85	3.74	4.74	0.02	69.46	315.2	1.97	1.00	40.92	0.20	67.46
294.2	0.92	2.97	6.48	0.15	69.21	318.2	10.60	4.24	52.08	0.18	67.22
297.2	1.08	2.62	8.58	0.17	68.96	321.2	11.02	3.54	64.75	−1.01	66.97
300.2	1.06	1.93	11.47	0.36	68.71	323.3	2.72	0.732	77.52	0.13	66.79
303.2	1.08	1.73	14.71	0.12	68.46	326.3	2.62	0.578	94.48	−2.74	66.54
306.5	1.51	1.58	19.97	0.44	68.19	329.4	3.21	0.539	123.9	1.5	66.28
2,2-diMe-1,3-Propanediol (cr, II) $\Delta_{cr}^g H_m$ (298.15 K) = (87.32 ± 0.27) kJ·mol^{-1}											
$\ln(p/\mathrm{Pa}) = \frac{324.1}{R} - \frac{95312.2}{R(T/\mathrm{K})} - \frac{26.8}{R}\ln\left(\frac{T/\mathrm{K}}{298.15}\right)$											
283.9	0.589	48.10	0.29	0.00	87.70	301.7	1.20	10.96	2.61	2.61	87.23
288.5	0.83	37.94	0.52	0.52	87.58	304.7	1.56	10.07	3.67	3.67	87.15
291.2	0.94	30.11	0.74	0.74	87.51	307.9	1.01	4.51	5.35	5.35	87.06
295.2	1.00	20.02	1.19	1.19	87.40	309.4	0.90	3.47	6.15	6.15	87.02
298.4	0.99	13.53	1.74	1.74	87.32	311.3	1.16	3.75	7.35	7.35	86.97
2,2-diMe-1,3-Propanediol (cr, I) $\Delta_{cr}^g H_m$ (298.15 K) = (76.85 ± 0.28) kJ·mol^{-1}											
$\ln(p/\mathrm{Pa}) = \frac{301.0}{R} - \frac{87937.0}{R(T/\mathrm{K})} - \frac{37.2}{R}\ln\left(\frac{T/\mathrm{K}}{298.15}\right)$											
314.3	0.97	2.17	10.57	−0.16	76.25	332.3	1.87	0.859	51.53	−0.24	75.58
317.3	1.12	1.87	14.16	0.03	76.14	335.3	2.15	0.758	67.21	1.09	75.47
320.2	1.42	1.82	18.49	0.14	76.03	338.2	2.16	0.606	84.42	1.04	75.36
323.4	1.51	1.46	24.47	0.14	75.91	341.2	2.14	0.480	105.6	0.08	75.25
326.4	1.41	1.06	31.47	−0.08	75.80	344.2	1.96	0.354	131.4	−1.5	75.13
329.4	1.51	0.884	40.56	−0.12	75.69	347.2	1.76	0.253	165.4	−1.4	75.02

Table 2. (Continued)

T	m	$V(N_2)$	p	$p_{exp} - p_{calc}$	$\Delta_l^g H_m$	T	m	$V(N_2)$	p	$p_{exp} - p_{calc}$	$\Delta_l^g H_m$
K[a]	mg[b]	dm^3 [c]	Pa[d]	Pa	kJ·mol^{-1}	K[a]	mg[b]	dm^3 [c]	Pa[d]	Pa	kJ·mol^{-1}
2-Me-1,3-Propanediol $\Delta_l^g H_m$ (298.15 K) = (73.63 ± 0.18) kJ·mol^{-1}											
$\ln(p/\mathrm{Pa}) = \frac{323.0}{R} - \frac{94350.8}{R(T/\mathrm{K})} - \frac{69.5}{R}\ln\left(\frac{T/\mathrm{K}}{298.15}\right)$											
297.3	1.58	21.28	2.04	0.02	73.69	326.6	2.32	2.24	28.17	−0.09	71.66
300.4	1.72	16.45	2.85	0.11	73.48	328.5	1.11	0.924	32.59	−0.32	71.52
303.4	1.59	12.02	3.64	−0.03	73.27	328.6	2.94	2.35	33.96	0.78	71.52
306.4	1.62	9.05	4.90	0.03	73.06	331.4	2.01	1.33	41.15	−0.23	71.32
309.4	2.07	8.52	6.61	0.17	72.85	333.4	1.59	0.931	46.90	−1.43	71.18
312.4	1.75	5.68	8.41	−0.04	72.64	336.3	2.02	0.924	59.31	−0.97	70.98
312.5	1.91	6.02	8.61	0.09	72.64	338.6	1.86	0.691	72.62	1.00	70.82
314.5	1.72	4.73	9.96	−0.22	72.50	341.4	2.88	0.901	86.56	−1.45	70.63
316.4	2.51	5.66	12.05	0.03	72.36	342.6	1.16	0.333	94.48	−1.55	70.54
318.5	1.94	3.74	14.10	−0.30	72.22	343.5	2.75	0.693	106.8	4.3	70.48
319.5	1.77	3.13	15.51	−0.17	72.15	347.6	2.11	0.416	137.9	0.9	70.20
321.4	2.44	3.61	18.42	0.00	72.02	349.3	1.82	0.311	158.9	4.7	70.08
322.5	2.20	2.99	19.84	−0.35	71.94	352.5	2.28	0.322	192.1	0.2	69.86
323.5	0.74	0.924	21.69	−0.25	71.87	355.4	2.75	0.311	240.7	7.6	69.65
323.6	1.90	2.35	22.02	−0.10	71.86	357.5	3.03	0.311	264.3	−3.4	69.51
326.4	2.10	2.12	26.89	−0.92	71.67						

[a] Temperature of saturation. [b] Mass of transferred sample, condensed at $T = 243$ K. [c] Volume of nitrogen, used to transfer mass m of the sample. [d] Vapor pressure at temperature T, calculated from m and the residual vapor pressure at $T = 243$ K.

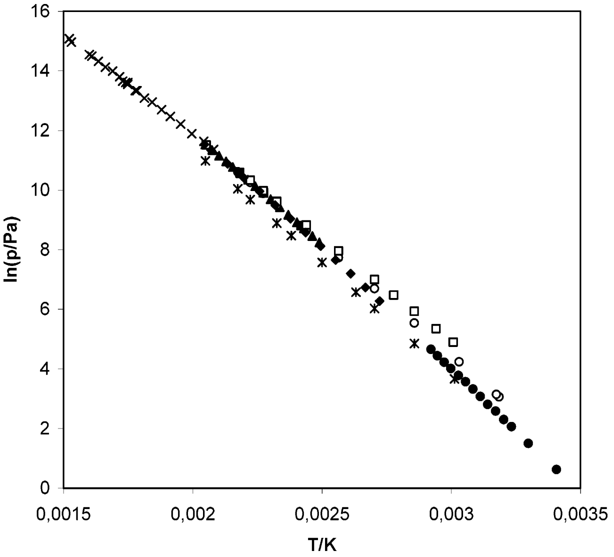

Figure 3. Plot of vapor pressure against reciprocal temperature for 1,3-propanediol: ▲, ref 5; □, ref 9; ×, ref 10; ○, ref 6; ■, ref 8; ∗, ref 7; ◆, ref 4; ●, this work.

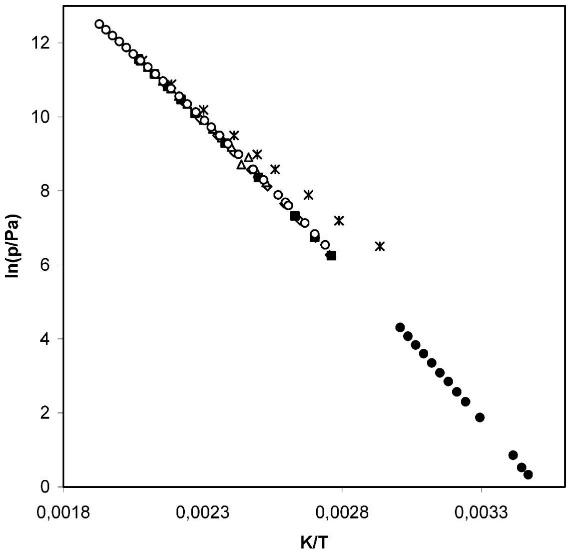

Figure 4. Plot of vapor pressure against reciprocal temperature for 1,3-butanediol: Δ, ref 5; ∗, ref 9; ○, ref 11; ■, ref 7; ◆, ref 4; ●, this work.

the simultaneous measurements of vapor pressure and sublimation enthalpies, $\Delta_{cr}^{g}H_m$, using the Knudsen effusion method combined with a calorimetric device. But vapor pressures were studied only at 313.3 K (crystalline phase) and 318.6 K (plastic phase). In this work, we have performed extended vapor pressure measurements of 2,2-dimethyl-1,3-propanediol for both cr, I and cr, II modifications, and its appropriate enthalpies of sublimation have been obtained (see Tables 1 and 2). As can bee seen from Table 1, our results are in excellent agreement with those from calorimetry;[14] however, our results for $\Delta_{cr}^{g}H_m$ are substantially more accurate. An additional probe of consistency of our experimental data on sublimation enthalpies of 2,2-dimethyl-1,3-propanediol (see Table 1) provides a comparison of the difference $\Delta_{cr}^{g}H_m$ (cr, II) − $\Delta_{cr}^{g}H_m$ (cr, II) = {(87.3 − 76.8) = (10.5 ± 0.5)} kJ·mol^{-1} (referred to 298.15 K) with the experimental enthalpy of phase transition, ΔH_{trs}(315.2 K) = (12.8 ± 0.2) kJ·mol^{-1}, measured by DSC.[31] Because of the comparison is valid at T = 298.15 K, the experimental enthalpy of phase transition of 2,2-dimethyl-1,3-propanediol had to be adjusted to the reference temperature. The adjustment was calculated from the equation suggested for the fusion enthalpy:[33]

$$\{\Delta_{cr}^{l}H_m\,(T_{fus}/\mathrm{K}) - \Delta_{cr}^{l}H_m\,(298.15\ \mathrm{K})\}/(\mathrm{J\cdot mol^{-1}}) = \{(0.75 + 0.15C_p^{cr}/\mathrm{J\cdot mol^{-1}\cdot K^{-1}})[(T_{fus}/\mathrm{K}) - 298.15]\} - \{(10.58 + 0.26C_p^{l}/\mathrm{J\cdot mol^{-1}\cdot K^{-1}})[(T_{fus}/\mathrm{K}) - 298.15]\} \quad (4)$$

where temperature of the phase transition was taken instead of T_{fus}, C_p^{cr} was taken from ref 19, and C_p^{l} was calculated according well-established procedures.[18,33] With this adjustment (the uncertainty of the correlation was not taken into account), the enthalpy of phase transition at T = 298.15 K, ΔH_{trs}315.2 K) = (11.6 ± 0.2) kJ·mol^{-1}, was calculated. Thus, the enthalpy

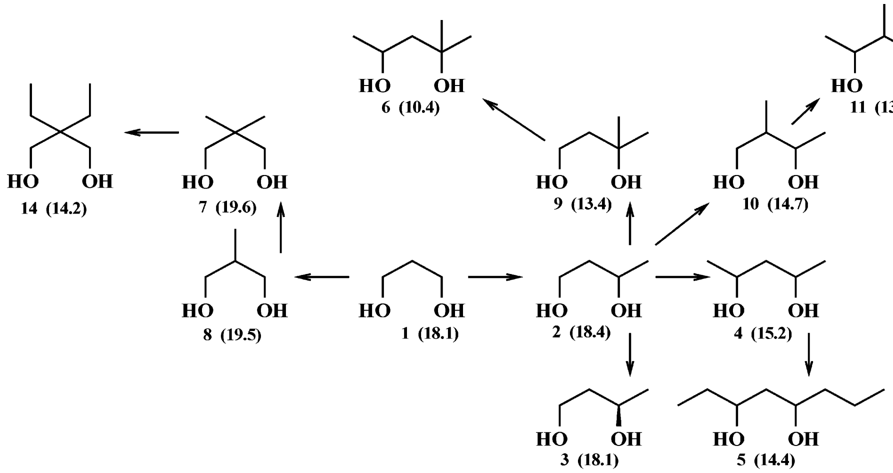

Figure 5. Strength of the hydrogen bonding in the 1,3-alkanediols, derived from differences between vaporization enthalpy of a 1,3-alkanediol and an alkanol (differences are presented in parentheses).

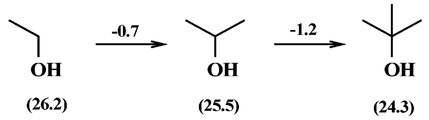

Figure 6. Strength of the inter-molecular hydrogen bonding in alkanols, derived from differences between vaporization enthalpy of an alkanol[40] and an alkane[40] (differences are presented in parentheses).

Table 3. Enthalpy of Phase Transition, ΔH_{trs}, and Enthalpy of Fusion $\Delta_{cr}^{l}H_m$ of the 2,2-Dimethyl-1,3-propanediol

ΔH_{trs} kJ·mol^{-1}	T_{trs} K	$\Delta_{cr}^{l}H_m$ kJ·mol^{-1}	T_{fus} K	ref
13.64	314	4.71	398	26
13.8	315.2	4.6	403.2	27
12.5	310.1	4.59	402.3	28
12.41	314.8	4.44	403.3	29
14.1	313.2	4.0	398.2	25
12.78	314.6			14
12.8	315.2	4.3	402.5	30
12.43[a]	314.4	4.34[a]	402.8	31
12.52	314.5			32
12.5	314.5			19

[a] Results selected for calculations (see text).

of phase transition calculated from the difference of $\Delta_{cr}^{g}H_m$ (for crystalline and plastic phase) measured in this work differs from those measured by calorimetry (and adjusted to $T = 298.15$ K) only by 1.1 kJ·mol^{-1}. Hence, our results for sublimation enthalpies of 2,2-dimethyl-1,3-propanediol have been shown to be consistent. It should be also mentioned that the enthalpy of phase transition selected for the calculations above is in close agreement with other values available from the literature[25−32] (see Table 3).

The comprehensive compilation of the experimental results available for 1,3-alkanediols is presented in Table 1. The successful comparison of our vaporization enthalpies derived from the transpiration techniques with those measured by other methods has allowed recommending the values $\Delta_l^g H_m$ (298.15 K) for compounds studied in this work (Figure 2) as reliable. However, the internal consistency of the whole data set presented in the Table 1 remains questionable.

The correlation of enthalpies of vaporization with the number of C-atoms in the series of homologues is a valuable test to check the internal consistency of the experimental results. Vaporization enthalpies $\Delta_l^g H_m$ appear to be a linear function of the number of carbon atoms of the aliphatic esters[34] and aliphatic nitriles.[35] However, this method is not applicable for the set of 1,3-alkanediols **1** to **16** (as listed in Table 1) due to essentially different types of branching of the alkane chain in each species. Hence, another way to check consistency of the 1,3-alkanediols **1** to **16** is required. In our recent paper enthalpies of vaporization of ethanolamines at 298.15 K were compared with those of their homomorphs (alkylamines).[36] These species are able to form inter- and intra-molecular hydrogen bonding (HB) in solutions and in the gaseous phase similar to alkanediols. In this work we extend a concept of homomorph compounds[24,37] toward 1,3-alkanediols (**1** to **16** in Table 1) in order to assess consistency of their vaporization enthalpies.

The existence of intra-HB in 1,3-alkanediols in the gaseous and in the solutions is well-documented by spectroscopic measurements. This finding is valid for the case of very diluted solutions where inter-HB is absent, and the only observed hydrogen bonds are the intramolecular ones. In pure alkanediols, exact quantification hydrogen of bonding is difficult because of presence of both inter- and intra-molecular bonding simultaneously. Nevertheless, a strength of the overall hydrogen bonding in 1,3-alkanediols in the pure bulk liquid phase can be assessed with help of experimental vaporization enthalpies and a conception of homomorph compounds.[24,36,37] Similar calculations have been performed recently[24] for the comparison of enthalpies of vaporization of *n*-alkanols and those of alkanes. Indeed, for alkanes only non-associating intermolecular van der Waals' interactions determine the values of their enthalpies of vaporization. Enthalpies of vaporization of alkanes that are obtained by replacing the OH group by a CH_3 group (R-CH_3) will essentially represent the non-associative contribution of the alcohol (R-OH) to its enthalpy of vaporization. The difference of the enthalpies of vaporization between alkanols (ROH) and its homomorph (RCH_3) presents a crude measure for contribution to the enthalpy of vaporization due to self-association of alcohols. A remarkable constancy of differences in enthalpies of vaporization at 298.15 K of (24 to 25) kJ·mol^{-1} was observed, indicating that the contribution to $\Delta_l^g H_m^\circ$ of alcohols due to inter-HB is nearly independent of the chain length.[24]

Following this pattern, experimental data on the enthalpies of vaporization of 1,3-alkanediols at 298.15 K (Table 1) were compared with those $\Delta_l^g H_m$ (298.15 K) values of their homomorphs. There are two possible homomorphs, CH_3-R-CH_3 and ROH, that could be suggested for 1,3-alkanediols. In the case of the alkane CH_3-R-CH_3, the overall level of hydrogen bonding could be assessed. For instance, for 1,3-propandiol, the difference $\Delta_l^g H_m$ (298.15 K, 1,3-propandiol) − $\Delta_l^g H_m$ (298.15 K, pentane) = 44.3 kJ·mol^{-1} is distinctly smaller than that value that is expected from alkanols[24] to be 2 × 25 = 50 kJ·mol^{-1} (see above). The reason for this discrepancy is apparently due to the fact that intra-HB is weaker than inter-HB. A crude measure for contribution to the enthalpy of vaporization due to intra-HB could be assessed with the help of ROH (alkanol) as the homomorph (see Figure 1).

For 1,3-propandiol, the difference $\Delta_l^g H_m$ (298.15 K, 1,3-propandiol) − $\Delta_l^g H_m$ (298.15 K, 1-butanol) = 18.1 kJ·mol^{-1} is again smaller than 25 kJ·mol^{-1}, which is expected from alkanols;[24] however, the ratio between intra-HB and inter-HB in 1,3-propandiol in the bulk liquid phase remains not defined. Nevertheless, the concept of ROH as the homomorph is useful for establishing consistency of the alkanediols **1** to **16** listed in the Table 1. Starting with the 1,3-propandiol (**1**), other alkanediols are arranged in Figure 5 in the sequence of branching of the alkane chain in the 1,3-propandiol itself. It is already well-established for alkanols that branching of the alkane chain reduces the association, and evaporation of the branched species is easier in comparison with a linear one (see Figure 5). The same trend has been observed for alkanediols **1** to **14** presented in Figure 5. The experimental vaporization enthalpies of the appropriate branched alkanols (homomorphs) have been reported recently[38,39] and are listed in the Table 1 (column 7). The differences of the enthalpies of vaporization between 1,3-alkanediols and alkanols are presented in Table 1 (column 8) and Figure 4. These differences could be interpreted as a rough measure for the strength of the intra-HB in 1,3-alkanediols. Indeed, it is apparent from Figure 1 that summation of the three contributions into vaporization enthalpy provides the following result:

$$\Delta_l^g H_m \text{ (1,3-alakanediol)} - \Delta_l^g H_m \text{ (alkanol)} = (1 - x) \times \mathrm{H}_{\text{intra}}$$

where x is the mole ratio of the intra-molecular H-bonded species in the bulk liquid phase.

According to Figure 5, it is evident, that alkyl substitution of the 2-position of the 1,3-propanediol does not impact intra-HB in the species **7**, **8**, and **14** and the strength of intra-HB remains constant at the level of (18 to 19) kJ·mol^{-1} because branching take place afar from the OH-groups in diols. What happens with the strength of intra-HB by the consequent alkyl substitution of hydrogens in position 1 and 3 of 1,3-propanediol, namely, in close proximity to the OH-group. It is apparent to expect that spatial crowding of the OH-group should disturb formation of any kind of hydrogen bonding (like in alkanols, see Figure 5). This trend can be seen in Figure 4: strengths of H-bond in 1,3-alkanediols **4**, **5**, **9**, **10**, and **11** are of (4 to 5) kJ·mol^{-1} lower in comparison to 1,3-propanediol. It is apparent that the most crowded diol **6** possess the weakest intra-HB of 10.4 kJ·mol^{-1}. Methyl substitution of hydrogen in position 1 of 1,3-propanediol has hardly any impact on intra-HB in 1,3-butanediols **2** and **3**, in accord with the very small effect on association between ethanol and 2-propanol (see Figure 6).

In spite of the fact that differences of enthalpies of vaporization discussed here present only a crude measure of the strength of the intra-molecular hydrogen bond in 1,3-alkanediols, these differences have fulfilled an expectation (within combined experimental uncertainties of about 1 kJ·mol^{-1}) concerning trends in the alteration of intra-HB strength with the degree of branching of the alkane chain, which have been observed for species presented in Figure 5. These observations have proven the consistency of the experimental results involved in the interpretation in Figure 5. Hence, the set of 1,3-alkanediols from Figure 5 could be recommended for further thermochemical calculations. Several species, namely, **12**, **13**, **15**, and **16** have been excluded from this interpretation because of lack of experimental vaporization enthalpies of their homomorphs. However, due to the high quality of the experimental measurements, the results for **13** and **15** belong to the recommended values.

This investigation was undertaken to establish a consistent set of vapor pressures and vaporization enthalpies of 1,3-alkanediols in the temperature range close to ambient temperatures. A large number of the primary experimental results on vapor pressures at various temperatures and treated them in a consistent manner in order to derive vaporization enthalpies at the reference temperature 298.15 K. Results from this compilation together with the critical surveys reported in our recent studies[21,22] have encouraged the re-evaluation of the Benson-type increments for calculation of thermochemical properties of the aliphatic diols,[41] similar to what has been done for aliphatic alcohols recently.[39]

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