

Supporting Information

Tomáš Katriňák, Lubomír Hnědkovský and Ivan Cibulka: Partial Molar Volumes and Partial Molar Isentropic Compressions of Three Polyhydric Alcohols Derived from Propane at Infinite Dilution in Water at Temperatures $T = (278 \text{ to } 318) \text{ K}$ and Atmospheric Pressure.

Experimental standard molar volumes obtained in this work were combined with data measured in the ranges from $(298.15 \text{ to } 573.15) \text{ K}$ and $(0.1 \text{ to } 30) \text{ MPa}^1$ and the entire set was smoothed using a polynomial function

$$V_{m,2}^0/(\text{cm}^3 \cdot \text{mol}^{-1}) = \sum_{i=1}^{N_T} \sum_{j=1}^3 a_{ij} (T/\text{K})^{(i-1)} (p/\text{MPa})^{(j-1)} \quad (\text{S1})$$

The adjustable parameters a_{ij} were evaluated using the weighted least squares procedure by minimizing the objective function

$$\phi(\{a_{ij}\}) = \sum_{k=1}^N \left\{ \frac{\left((V_{m,2}^{0(\text{exp})})_k - \sum_{i=1}^{N_T} \sum_{j=1}^3 a_{ij} T_k^{(i-1)} p_k^{(j-1)} \right)^2}{\sigma(V_{m,2}^{0(\text{exp})})_k} \right\} \quad (\text{S2})$$

Estimated experimental uncertainties were used for the weights $1/\left[\sigma(V_{m,2}^{0(\text{exp})})_k\right]^2$. The summation in eq S2 is performed over all experimental data points N measured for a particular solute. Since measurements at three pressures were performed for each isotherm (except for $T < 298 \text{ K}$) the resulting fits are interpolations in pressure (isotherms are fitted with the second order polynomials in pressure) while the maximum order of the polynomial with respect to temperature, N_T , was chosen according to the significance of respective parameters. A random distribution of deviations between experimental values and those calculated from eq S1 was adopted as a criterion. Values of parameters along with standard deviations and weighted standard deviations of the fits are presented in Table S1. Extrapolations using a polynomial function are not reliable and therefore the calculations of standard molar volumes and derived quantities from the fits for $T < 298 \text{ K}$ are not recommended for pressures other than 0.1 MPa .

Table S1. Parameters a_{ij} of Eq S1. Temperature Range of All Fits is from (278.15 to 573.15) K, for the Pressure Range see the text.

		Propane-1,2-diol(aq)	Propane-1,3-diol(aq)	Propane-1,2,3-triol(aq)
i	j	a_{ij}	a_{ij}	a_{ij}
1	1	$5.9703704 \cdot 10^2$	$3.1215198 \cdot 10^2$	$-1.4598238 \cdot 10^3$
1	2	98.350981	91.730057	-63.531470
1	3	-3.9226540	-3.6593408	$7.8873705 \cdot 10^{-2}$
2	1	-8.5178884	-3.5886996	23.404901
2	2	-1.3782357	-1.3224136	0.83201855
2	3	$5.6549600 \cdot 10^{-2}$	$5.3404500 \cdot 10^{-2}$	$1.4548479 \cdot 10^{-3}$
3	1	$5.6855927 \cdot 10^{-2}$	$2.2342015 \cdot 10^{-2}$	-0.14919017
3	2	$7.9247577 \cdot 10^{-3}$	$7.8610916 \cdot 10^{-3}$	$-4.3494163 \cdot 10^{-3}$
3	3	$-3.3565712 \cdot 10^{-4}$	$-3.2158663 \cdot 10^{-4}$	$-2.6070143 \cdot 10^{-5}$
4	1	$-2.0152316 \cdot 10^{-4}$	$-7.5143983 \cdot 10^{-5}$	$5.0579796 \cdot 10^{-4}$
4	2	$-2.3895419 \cdot 10^{-5}$	$-2.4657565 \cdot 10^{-5}$	$1.1449503 \cdot 10^{-5}$
4	3	$1.0498082 \cdot 10^{-6}$	$1.0227966 \cdot 10^{-6}$	$1.4307950 \cdot 10^{-7}$
5	1	$4.0077539 \cdot 10^{-7}$	$1.4441358 \cdot 10^{-7}$	$-9.5981146 \cdot 10^{-7}$
5	2	$3.9766161 \cdot 10^{-8}$	$4.3023514 \cdot 10^{-8}$	$-1.5561906 \cdot 10^{-8}$
5	3	$-1.8243383 \cdot 10^{-9}$	$-1.8121481 \cdot 10^{-9}$	$-3.6888412 \cdot 10^{-10}$
6	1	$-4.2292063 \cdot 10^{-10}$	$-1.4914672 \cdot 10^{-10}$	$9.6643119 \cdot 10^{-10}$
6	2	$-3.4528476 \cdot 10^{-11}$	$-3.9574327 \cdot 10^{-11}$	$9.6692650 \cdot 10^{-12}$
6	3	$1.6696546 \cdot 10^{-12}$	$1.6958801 \cdot 10^{-12}$	$4.6109576 \cdot 10^{-13}$
7	1	$1.8536367 \cdot 10^{-13}$	$6.4787942 \cdot 10^{-14}$	$-4.0326592 \cdot 10^{-13}$
7	2	$1.2159292 \cdot 10^{-14}$	$1.4976397 \cdot 10^{-14}$	$-1.6575051 \cdot 10^{-15}$
7	3	$-6.2839720 \cdot 10^{-16}$	$-6.5485771 \cdot 10^{-16}$	$-2.2575327 \cdot 10^{-16}$
Standard deviation/ ($\text{cm}^3 \cdot \text{mol}^{-1}$)		0.03	0.03	0.07
Weighted standard deviation		1.07	1.19	1.76
Total number of experimental data points		39	39	41