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Please cite this article as: I. Cibulka, L. Hnědkovský, Partial molar volumes of organic solutes in water. XXIV. Selected alkane-α,ω-diols at temperatures T = 298 K to 573 K and pressures up to 30 MPa, *J. Chem. Thermodynamics* (2013), doi: http://dx.doi.org/10.1016/j.jct.2013.05.004

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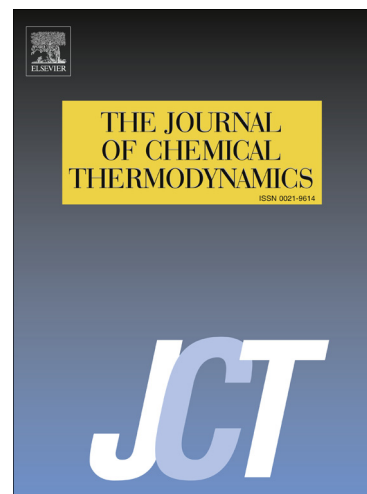
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ABSTRACT

Density data for dilute aqueous solutions of three alkane-α,ω-diols (pentane-1,5-diol, octane-1,8-diol, nonane-1,9-diol) are presented together with standard molar volumes (partial molar volumes at infinite dilution) calculated from the experimental data. The measurements were performed at temperatures from T = 298 K up to T = 573 K. Experimental pressures were slightly above the saturation vapour pressure of water, and (15 and 30) MPa. The data were obtained using a high-temperature high-pressure flow vibrating-tube densimeter. Measured standard molar volumes were combined with data previously published for other members of the homologous series and discussed. Experimental standard molar volumes were correlated as a function of temperature and pressure using an empirical polynomial function. Dependences of standard molar volumes on temperature and pressure were analyzed. Contributions of the methylene group to the standard molar volume were also evaluated and discussed.

Short title: I. Cibulka, $V_{\mathrm{m},2}^{\mathrm{o}}$ of selected alkane-α,ω-diols (aq)

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KEYWORDS: density; partial molar volume; aqueous alkane-α,ω-diols; high temperature; high pressure.

1. Introduction

This paper, as a part of our series of the systematic experimental studies of partial molar volumes of organic solutes at infinite dilution in water (standard molar volumes), is focussed on the homologous series of alkane-α,ω-diols. In our previous papers, the experimental results for standard molar volumes within the ranges of temperature from (298 to 573) K and pressure up to 30 MPa are presented for ethane-1,2-diol [1], propane-1,3-diol [1], butane-1,4-diol [2], and hexane-1,6-diol [3]. Recently data obtained for ethane-1,2-diol [4], propane-1,3-diol [5], butane-1,4-diol [6], pentane-1,5-diol [4], hexane-1,6-diol [4], octane-1,8-diol [4], and nonane-1,9-diol [4] measured by a commercial vibrating-tube densimeter (DSA 5000, Anton Paar) extend the experimental temperature range down to 278 K. Data presented here for aqueous pentane-1,5-diol, octane-1,8-diol, and nonane-1,9-diol complete the information on standard molar volumes over the temperature range from 278 K to 573 K and pressures up to 30 MPa of the homologous series of alkane-α,ω-diols, $HO-(CH_2)_n-OH$, for n from 2 through 9 except for $n = 7$.

2. Experimental

Specifications of the organic solutes are given in table 1. The samples were used without further treatment. Molalities of the prepared solutions of pentane-1,5-diol were corrected with respect to the water content. Distilled and de-mineralized (Millipore RQ) water was used as both a solvent and a

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calibration fluid for the densimeter.

Details concerning the experimental technique and methodology can be found in the previous papers [7,8], here a brief summary only is given. The high-pressure high-temperature densimeter [7] working in the automated flow regime [8] with a high-pressure pump adjusted to the flow rate of 0.6 cm^3·min^{-1} was used for the measurements. Repeated calibrations of the densimeter were performed at each experimental temperature and pressure using water and nitrogen whose densities were taken from the literature [9,10]. Either the thermostatted back-pressure regulator [8] or a gas cylinder of volume about 40 dm^3 (used for measurements at 0.5 MPa) were connected to the end of the pressure line. The maximum systematic error of the measured density differences $\Delta\rho = \rho - \rho_1$ resulting from the densimeter calibration was about 0.2 per cent and the reproducibility of the measurements was within $\pm3\times10^{-3}$ kg·m^{-3} in most cases. The temperature of the densimeter cell was measured using a calibrated (ITS 90) platinum resistance thermometer (BURNS Engineering), with a resistance $R_0 = 100$ Ω at $T = 273.15$ K, connected to a multimeter in a four-lead configuration. The resolution of the temperature measurements was 0.1 mK. Temperature stability of the cell during one experiment (measurement of one sample) was within 1 mK. The total uncertainty of the temperature measurements was estimated to be about ±20 mK at $T = 298$ K and 0.1 K at 573 K. Pressure was measured using a secondary standard gauge (DIGIQUARTZ-740-6K, Paroscientific Inc.) with an accuracy of ±0.1 per cent or $\pm1\times10^{-2}$ MPa, whichever is greater. The pressure stability was within $\pm1\times10^{-2}$ MPa at lower pressures and $\pm3\times10^{-2}$ MPa at $p = 30$ MPa.

The solutions were prepared by mass using a Precisa 40SM-200A balance (resolution = 10^{-2} mg, uncertainty = ±0.1 mg) to determine the mass of the solute and A&D Instruments GF-3000-EC

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balance (resolution = 10 mg, estimated uncertainty = ±2x10⁻² per cent, maximum load 3.1 kg) to determine the total mass of a solution. Mass of each prepared solution was about 1 kg. "Stop-flow" experiments [11,12] revealed that the solutes were stable up to the highest experimental temperature.

3. Results

3.1. Direct experimental data

The values of the density differences $\Delta\rho = \rho - \rho_1$ where ρ and ρ_1 are the densities of the solution and water, respectively, measured at each experimental temperature and pressure, and the molalities of organic solutes m_2 are available in the Supplementary material (tables S1 through S3; 585 data points in the range of molality from (0.10 to 0.52) mol·kg⁻¹ for aqueous pentane-1,5-diol, 460 data points in the range of molality from (0.04 to 0.12) mol·kg⁻¹ for aqueous octane-1,8-diol; and 467 data points in the range of molality from (0.02 to 0.04) mol·kg⁻¹ for aqueous nonane-1,9-diol, totally 1512 data points). Usually five (pentane-1,5-diol) and four (octane-1,8-diol, nonane-1,9-diol) solutions covering the above concentration ranges were measured for each pair of temperature and pressure. Each solution was usually measured three times during the automated run.

   The experimental results obtained for each pair of temperature and pressure were fitted with the equation

$$\Delta\rho \,/\, m_2 \,=\, (\rho - \rho_1) \,/\, m_2 \,=\, a + bm_2 + cm_2^2 \qquad , \tag{1}$$

where a, b, and c are adjustable coefficients. The values of the coefficients were obtained using a least squares method with unit weights and are recorded in table 2. The dependence of

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$\Delta\rho/m_2$ on m_2 at constant temperature and pressure was found to be either a quadratic or a linear (c = 0) function of m_2 in the concentration ranges of measurements. Due to very limited solubility of nonane-1,9-diol in water no concentration dependence was evaluated (b = c = 0) and thus the parameter a is equal to the arithmetic mean of the experimental values of $\Delta\rho/m_2$.

3.2. Partial molar volumes

The partial molar volume at infinite dilution ($m_2 \rightarrow$ 0) of a solute $V_{m,2}^0$ (standard molar volume) is obtained from equation (1) as [7]

$$V_{m,2}^0 = \left\{ M_2 - (a \: / \: \rho_1) \right\} \: / \: \rho_1 \: , \tag{2}$$

where a is the adjustable coefficient of the fitting function (1) and M_2 is the molar mass of the solute.

Standard molar volumes calculated from the experimental data and their estimated uncertainties are presented in table 2. The uncertainties in $V_{m,2}^0$ given in table 2 include random error estimates, that originate from the scatter associated with equation (1), as well as errors estimated from uncertainties in composition, calibration constant, and in the uncertainty of the measured differences between density of nitrogen-saturated and degassed water [12].

In order to provide a tool for smoothing and interpolation of data the polynomial function of temperature and pressure

$$V_{m,2}^0 \: / \: (\text{cm}^3 \cdot \text{mol}^{-1}) = \sum_{i=1}^{N_T} \sum_{j=1}^{3} a_{ij} \left(T/\text{K} - 298.15 \right)^{(i-1)} \left(p/\text{MPa} - 0.1 \right)^{(j-1)} \tag{3}$$

where a_{ij} are adjustable parameters was fitted to the experimental surface $V_{m,2}^{o}(T, p)$ of each solute obtained as a combination of present experimental data (table 2) with those reported in the previous paper [4]. The fits were also performed for other members of the homologous series (ethane-1,2-diol, propane-1,3-diol, butane-1,4-diol, hexane-1,6-diol) using published data [1-6]. The detailed description of the fitting procedure and the values of adjustable parameters are presented in Supplementary material (tables S4 and S5).

Standard molar volumes measured in this work at T = (298 and 318) K and p = 0.5 MPa are compared in table 3 with the data at atmospheric pressure taken from the literature. As it is illustrated by the values given in parentheses in table 3 the effect of pressure is moderate in this temperature range thus the comparison is well justified. Obviously, the agreement within experimental uncertainties is observed for our recent data obtained by the DSA 5000 device [4]. With the exceptions of values reported by Wurzburger *et al.* [13] and Edward *et al.* [14] the other deviations can be regarded as being either within or close to the experimental uncertainties.

Data at elevated pressures were found for aqueous pentane-1,5-diol [15, 22] and are compared with our values in table 4. Hakin and Høiland [15] reported the standard molar volumes of aqueous butane-1,4-diol, pentane-1,5-diol, and hexane-1,6-diol at T = 298.15 K and at pressures p = (0.1, 20, 40, 60, 80, and 120) MPa. Their value for pentane-1,5-diol at p = 20 MPa differs from that of ours by 0.21 cm^3·mol^{-1}. The same deviation is, however, observed at atmospheric pressure (see table 3). The agreement at T = 298.15 K and p = 20 MPa for other two solutes is better; butane-1,4-diol: 88.09 cm^3·mol^{-1} [15], 88.16 cm^3·mol^{-1} (function (3)); hexane-1,6-diol: 120.19 cm^3·mol^{-1} [15], 120.26 cm^3·mol^{-1}(function (3)). It may be concluded that the

agreement between our data and those reported by Hakin and Høiland [15] is very satisfactory, our values are, however, systematically higher. The agreement of our smoothed values with experimental data obtained for aqueous pentane-1,5-diol by Schulte *et al.* [22] is within the experimental uncertainties except for the highest temperature 521 K.

4. Discussion

Experimental standard molar volumes at low pressures are plotted against temperature in figure 1. Similar plots can be drawn for the isobar *p* = 30 MPa. In this work the isobars *p* = 15 MPa were measured for the entire experimental temperature range while our older data reported for aqueous ethane-1,2-diol [1], propane-1,3-diol [1], butane-1,4-diol [2], and hexane-1,6-diol [3] in the middle pressure range for T > 473 K were obtained for pressure gradually increasing from (15 to 20) MPa and therefore the experimental isobar p = 15 MPa could be drawn for a limited temperature range only. As can be seen from figure 1, the experimental values follow smooth curves with the slopes increasing with increasing molecular size. The distances between neighbouring curves correspond to the contribution of the methylene group $V_{\mathrm{m}}^0\left(-\mathrm{CH}_2-\right)$ (two contributions $V_{\mathrm{m}}^0\left(-\mathrm{CH}_2-\right)$ for curves for *n* = 6 and 8). Since the measurements for various solutes were not performed for exactly identical pairs of temperature and pressure, the smoothed standard molar volumes were calculated from function (3) (see above and Supplementary material) at selected values of temperature and pressure. In the following considerations smoothed values of $V_{\mathrm{m,2}}^0$ calculated from function (3) for pressure 0.1 MPa up to 373.15 K and for saturation pressure of water at T > 373.15 K (named "saturation pressure" set) were used. The contributions of the methylene group were evaluated as

$$V_m^0\left(-CH_2-\right) \;=\; V_{m,2}^0\left[HO-\left(CH_2\right)_{n+1}-OH\right] \;-\; V_{m,2}^0\left[HO-\left(CH_2\right)_n-OH\right] \textbf{ or}$$

$$V_m^0\left(-CH_2-\right) \;=\; \left\{V_{m,2}^0\left[HO-\left(CH_2\right)_8-OH\right] \;-\; V_{m,2}^0\left[HO-\left(CH_2\right)_6-OH\right]\right\}/2 \textbf{ for } \textbf{\textit{n}} \textbf{ = 6. The}$$

contributions calculated for saturation pressure are shown as functions of *n* in figure 2. It can be seen that the contribution of the methylene group is dependent on *n* and the extent of this dependence is affected by temperature. The values for *n* = 2 are evidently influenced by the close vicinity of the two hydroxyl groups. If they are omitted then one can see that sufficiently *n*-independent contributions are observed in the temperature range approximately from (298 to 373) K. The values of the contribution $V_m^0\left(-CH_2-\right)$ obtained from the first-order group contribution approach applied to aliphatic alcohols, ethers, and ketones [23] are shown as the horizontal dotted lines in figure 2 for a comparison. Since only structural contributions related to the close vicinity of the functional groups (-C(OH)-C(OH)-), -O-C-O-, -CO-C-CO-) were included in the procedure [23] the contributions $V_m^0\left(-CH_2-\right)$ are averages over all solutes and consequently independent of the molecular structure. Apparently the average values [23] are close to the averages of the present data for n ≥ 3. A coincidence can be observed for *T* = 323 K where the present contributions are nearly independent of *n* and their average value over *n* from 3 to 8 (16.58 cm^3·mol^{-1}) is identical with that resulting from the group contribution approach [23] (16.55 cm^3·mol^{-1}).

A question may arise whether the present behaviour of the contribution of the methylene group shown in figure 2 is caused by the presence of the second hydroxyl group. Unfortunately the isothermal dependencies of $V_m^0\left(-CH_2-\right)$ on *n* cannot be analyzed for aliphatic solutes with one hydroxyl group, i.e., for alkane-1-ols, H-(CH$_2$)$_n$-OH, due to the lack of sufficient data at higher

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temperatures for n > 4. The plots analogical to figure 2 obtained using data for methanol [24], ethanol [24], propane-1-ol [24], and butane-1-ol [25] in the range from (298 to 573) K, i.e. values of $V_m^0\left(-CH_2-\right) = V_{m,2}^0\left[H-\left(CH_2\right)_{n+1}-OH\right] - V_{m,2}^0\left[H-\left(CH_2\right)_n-OH\right]$ for *n* = 1, 2, and 3, do not show anything except the indication that the contributions calculated from standard molar volumes of two first members of the homologous series (*n* = 1) do not fit, as can be expected for the first member of the homologous series, the dependence for higher member pairs (*n* = 2 and 3). Tentative evaluation of the contribution $V_m^0\left(-CH_2-\right)$ for a wider range of *n* from selected data [26] of standard molar volumes at *T* = 298.15 K and atmospheric pressure of alkane-1-ols for *n* from 1 to 7 showed *n*-independent contribution for *n* ≥ 2. The average value of the contribution calculated from the values $V_m^0\left(-CH_2-\right) = V_{m,2}^0\left[H-\left(CH_2\right)_{n+1}-OH\right] - V_{m,2}^0\left[H-\left(CH_2\right)_n-OH\right]$ for n = 2, 3, 4, 6 (the value for *n* = 5 was found to be significantly lower than the other ones and was excluded) is 15.90 cm^3·mol^{-1} which is close to the values 16.07 cm^3·mol^{-1} [23] and 15.80 cm^3·mol^{-1} [26]. Since the temperature *T* = 298.15 K is in the region of moderate dependency of $V_m^0\left(-CH_2-\right)$ on *n* (figure 2) it is not possible to decide whether the effect illustrated in figure 2 is caused by the presence of the second hydroxyl group or not. On the other hand, within the group contribution method employing experimental data for 425 aqueous non-ionic solutes at *T* = 298.15 K and atmospheric pressure Cabani *et al.* [26] have proposed the structural contribution for bifunctional solutes $Y_1-C_n-Y_2$ which reflects the effect of the number of carbon atoms *n* separating the two functional groups (Y_1, Y_2). This structural contribution decreases with increasing *n* which is in accord with our observations (line for *T* = 298.15 K in figure 2). An opposite trend should be introduced for high temperatures, as follows from figure 2.

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Temperature dependence of the standard molar volume is strongly affected by the hydrophilic character of the solute, i.e., by the ratio between the hydrophilic (hydroxyl groups) and the hydrophobic (hydrocarbon chain) parts of the solute molecule. Decrease of $\left(\partial V_{m,2}^0 / \partial T\right)_p$ with increasing temperature at low temperatures [5, 27-30] and even negative $\left(\partial V_{m,2}^0 / \partial T\right)_p$ at high temperatures [1, 3, 5, 30] were observed for highly hydrophilic solutes. The temperature dependences of the analog of the isobaric thermal expansivity, $\alpha_{p,2}^0 = \left(1 / V_{m,2}^0\right)\left(\partial V_{m,2}^0 / \partial T\right)_p$ (named shortly isobaric expansivity in the following text), on temperature evaluated from function (3) for saturation pressure of water are depicted in figure 3. The present data agree with our previous observations, i.e., the curve of the most hydrophilic solute (ethane-1,2-diol) exhibits a decrease of $\alpha_{p,2}^0$ at the low temperature region and smaller slope at high temperatures compared to less hydrophilic higher alkane-α,ω-diols. Figure 4 shows the plots of $\alpha_{p,2}^0$ against the number of methylene groups *n* for several selected temperatures. In accordance with figure 3 the anomalous behaviour of ethane-1,2-diol is seen at low temperatures. Evidently $\alpha_{p,2}^0$ of alkane-α,ω-diols depends on the length of the hydrocarbon chain *n*, and the effect is more pronounced as temperature increases. Three isotherms calculated for alkane-1-ols from methanol (*n* = 1) through butane-1-ol (*n* = 4) using the fits presented in [23] are plotted in figure 4 for a comparison. The value for butane-1-ol at *T* = 573.15 K is rather suspicious; analysis showed that while values of $\alpha_{p,2}^0$ for all four alkane-1-ols at each temperature in the range *T* = (320 to 550) K are within ±0.2 kK^{-1} interval, larger deviations of $\alpha_{p,2}^0$ for butane-1-ol from values for other three alkane-1-ols (up to ±0.5 kK^{-1}) are observed for

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temperatures T < 320 K and T > 550 K. It is likely that these discrepancies issue from experimental data rather than from true behaviour of aqueous butane-1-ol. Thus it might be concluded that the isobaric expansivity of aqueous alkane-1-ols (at least for $n \leq 4$) is nearly independent of n while that of aqueous alkane-α,ω-diols is affected by the length of the hydrocarbon chain. The presence of the second hydroxyl group leads to significantly smaller expansivities compared to monohydric alkane-1-ols with the same hydrocarbon frame.

Figure 5 shows the plots of the derivative $\left(\partial c_{p,m,2}^0 / \partial p\right)_T$ related to the second derivative of standard molar volume with respect to temperature, $\left(\partial c_{p,m,2}^0 / \partial p\right)_T = - T \left(\partial^2 V_{m,2}^0 / \partial T^2\right)_p$. The derivatives $\left(\partial^2 V_{m,2}^0 / \partial T^2\right)_p$ were evaluated from function (3) for saturation pressure of water. Again we can see the characteristic dependence on the hydrophilic/hydrophobic ratio as observed for other classes of the solutes, i.e., positive $\left(\partial c_{p,m,2}^0 / \partial p\right)_T$ (a concave shape of $V_{m,2}^0 (T)$) at low and high temperatures for highly hydrophilic solutes [5, 27-30], becoming more and more negative (a convex shape of $V_{m,2}^0 (T)$) when the ratio between hydrophilic and hydrophobic parts of the solute molecule decreases. As can be seen in figure 5 the values for ethane-1,2-diol is the highest (even positive at low temperatures) and $\left(\partial c_{p,m,2}^0 / \partial p\right)_T$ obviously drops down to negative values with increasing number of methylene groups n which is particularly obvious at higher temperatures. The plots also show a monotonous dependence of $\left(\partial c_{p,m,2}^0 / \partial p\right)_T$ on n (at least at elevated temperatures) and thus confirm a reasonable description of the $V_m^0 (T)$ dependence by function (3) without any substantial ill-behaviour issuing from the polynomial character of the fits.

Plots of the analog to the isothermal compressibility,

$\kappa_{T,2}^0 = -\left(1/V_{m,2}^0\right)\left(\partial V_{m,2}^0 / \partial p\right)_T$, **(named shortly isothermal compressibility in the following text) evaluated from function (3) at saturation pressure of water as functions of temperature are shown in figure 6. Contrary to the isobaric expansivity $\alpha_{p,2}^0$ (figure 3) all curves are of a similar shape. No exceptional course is observed for ethane-1,2-diol compared to some highly hydrophilic solutes for which the values of $\kappa_{T,2}^0$ may reach even negative values at high temperatures (propane-1,2,3-triol [1], 2,2-bis(hydroxymethyl)-1,3-propanediol [3], pentane,1,2,3,4,5-pentaol [3]). Isothermal dependences of $\kappa_{T,2}^0$ on *n* are monotonously increasing (one should take into account that the roughly estimated uncertainties might be around 0.3 GPa^{-1}; higher for higher *n*) as can be seen for selected temperatures in figure 7, analogical to figure 4. It was observed for the series of aqueous isomeric alkanols from methanol to butanol [25] (except for 2-methylpropane-2-ol) that values of the isothermal compressibility of these alcohols at each temperature along the saturation line of water or along an isobar are close to each other, deviations from the polynomial fits $\kappa_{T,2}^0\left(T\right)$ were found to be within about ±0.5 GPa^{-1}. Besides that values of the isothermal compressibility of aqueous alkanols are significantly higher than those of aqueous alkane-α,ω-diols as it is indicated by the isotherms *T* = (473, 523, and 573) K calculated from the fits presented in [23] and shown in figure 7 for a comparison. Obviously, the effect of the second hydroxyl group on the isothermal compressibility is significant and naturally decreases with increasing *n*. Similarity of figures 4 and 7 is obvious.**

5. Conclusions

  New experimental data for three aqueous alkane-α,ω-diols

complete the information on standard molar volumes of the homologous series of alkane-α,ω-diols from ethane-1,2-diol through nonane-1,9-diol except for heptane-1,7-diol over the wide temperature T = (278 to 573) K and pressure p = (0.1 to 30) MPa ranges. The analysis revealed the dependence of the contribution of the methylene group on the length of the hydrocarbon chain and thus the results indicate a need of the structural contribution to be incorporated into the group additivity scheme. Dependences of standard molar volumes on temperature and pressure were also analyzed; the results confirmed the general behaviour related to the ratio between hydrophobic and hydrophilic parts of the solute molecules as observed for other classes of organic solutes. Compared to monohydric alkane-1-ols the presence of the second hydroxyl brings significant and well justified effects on the standard molar volumes and derived quantities of aqueous alkane-α,ω-diols.

Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at doi: xx.xxx/.......

References

[1] P. Hynčica, L. Hnědkovský, I. Cibulka, J. Chem. Thermodyn. 38 (2006) 801-809.

[2] P. Hynčica, L. Hnědkovský, I. Cibulka, J. Chem. Thermodyn. 38 (2006) 1085-1091.

[3] L. Hnědkovský, I. Cibulka, J. Chem. Thermodyn. 39 (2007) 833-840.

[4] L. Hnědkovský, I. Cibulka, J. Chem. Eng. Data (submitted, MS je-2013-001203).

[5] T. Katriňák, L. Hnědkovský, I. Cibulka, J. Chem. Eng. Data 57 (2012) 1152-1159.

[6] L. Hnědkovský, I. Cibulka, J. Chem. Eng. Data 58 (2013) 388-397.

[7] V. Hynek, L. Hnědkovský, I. Cibulka, J. Chem. Thermodyn. 29 (1997) 1237-1252.

[8] L. Hnědkovský, I. Cibulka, Int. J. Thermophys. 25 (2004) 1135-1142.

[9] W. Wagner, A. Pruss, J. Phys. Chem. Ref. Data 31 (2002) 387-535.

[10] R.T. Jacobsen, R.B. Stewart, M. Jahangiri, J. Phys. Chem. Ref. Data 15 (1986) 735-909.

[11] I. Cibulka, L. Hnědkovský J. Chem. Thermodyn. 41 (2009) 489-498.

[12] I. Cibulka, J. Chem. Thermodyn. 42 (2010) 502-512.

[13] S. Wurzburger, R. Sartorio, V. Elia, C. Cascella, J. Chem. Soc., Faraday Trans. 86 (1990) 3891-3895.

[14] J.T. Edward, P.G. Farrell, F. Shahidi, J. Chem. Soc., Faraday Trans.1 73 (1977) 705- 714.

[15] A.W. Hakin, H. Høiland, Phys. Chem. Chem. Phys. 7 (2005) 2199-2207.

[16] S. Cabani, P. Gianni, V. Mollica, L. Lepori, J. Solution Chem. 10 (1981) 563-595.

[17] H. Høiland, E. Vikingstad, Acta Chem. Scand. A, 30 (1976) 182-186.

[18] H. Høiland in Thermodynamic Data for Biochemistry and Biotechnology (H.-J. Hinz, Editor). Chap. 2, Partial Molar Volumes of Biochemical Model Compounds in Aqueous Solutions, pp. 17-44; Springer-Verlag: Berlin, 1986.

[19] K. Spildo, H. Høiland, J. Solution Chem. 31 (2002) 149-164.

[20] T. Nakajima, T. Komatsu, T. Nakagawa, Bull. Chem. Soc. Jpn. 48 (1975) 783-787.

[21] H. Høiland, J. Solution Chem. 9 (1980) 857-866.

[22] M.D. Schulte, E.L. Shock, M. Obšil, V. Majer, J. Chem. Thermodyn. 31 (1999) 1195-1129.

[23] I. Cibulka, L. Hnědkovský, J. Chem. Thermodyn. 43 (2011) 1215-1223.

[24] P. Hynčica, L. Hnědkovský, I. Cibulka, J. Chem. Thermodyn.36 (2004) 1095-1103.

[25] P. Hynčica, L. Hnědkovský, I. Cibulka, J. Chem. Thermodyn.38 (2006) 418-426.

[26] S. Cabani, P. Gianni, V. Mollica, L. Lepori, J. Solution Chem. 10 (1981) 563-595.

[27] I. Cibulka, C. Alexiou, J. Chem. Thermodyn. 42 (2010) 274-285.

[28] I. Cibulka, L. Šimurka, L. Hnědkovský , A. Bolotov, J. Chem. Thermodyn. 43 (2011) 1028-1035.

[29] L. Šimurka, I. Cibulka, L. Hnědkovský, J. Chem. Eng. Data 57 (2012) 1570-1580.

[30] L. Šimurka, I. Cibulka, L. Hnědkovský, J. Chem. Eng. Data 56 (2011) 4564–4576.

Figure captions.

Figure 1.

Plot of experimental standard molar volumes $V_{m,2}^0$ **at low pressures against temperature** *T*. **The lines are to aid the eye. Integer numbers denote the numbers of methylene groups** *n* **(carbon atoms C**$_n$**) in the solute molecule.**
●, **ethane-1,2-diol [1,4];** ○, **propane-1,3-diol [1,5];** ■, **butane-1,4-diol [2,6];** □, **pentane-1,5-diol [4,this work];** ▲, **hexane-1,6-diol [3,4];** Δ, **octane-1,8-diol [4,this work];** ▼, **nonane-1,9-diol [4,this work].**

Figure 2.

Plot of the contribution of the methylene group
$V_m^0\left(-CH_2-\right) = V_{m,2}^0\left[HO-\left(CH_2\right)_{n+1}-OH\right] - V_{m,2}^0\left[HO-\left(CH_2\right)_n-OH\right]$ **to standard molar volume at saturation vapour pressure of water against** *n*. **Due to the lack of data for** *n* **= 7 the averages over two homologous neighbours (C**$_{n+2}$ **− C**$_n$**) are shown for the pair C**$_8$**/C**$_6$ **(**n **= 6); for details see text. Horizontal dotted lines represent the values of the contribution reported in ref. [23] for respective temperatures starting from 298.15 K (the lowest line).**
●, **278.15 K;** ○, **298.15 K;** ▲, **323.15 K;** Δ, **373.15 K;** □, **423.15 K;** ■, **473.15 K;** ▼, **523.15 K;** ▽, **573.15 K.**

Figure 3.

Plot of isobaric expansivity $\alpha_{p,2}^0 = \left(1 / V_{m,2}^0\right)\left(\partial V_{m,2}^0 / \partial T\right)_p$ **at saturation vapour pressure of water calculated from the fits using equation (3) against temperature** *T*.
n **= 2, ethane-1,2-diol;** *n* **= 3, propane-1,3-diol;**
n **= 4, butane-1,4-diol;** *n* **= 5, pentane-1,5-diol;**
n **= 6, hexane-1,6-diol;** *n* **= 8, octane-1,8-diol;**
n **= 9, nonane-1,9-diol.**

Figure 4.

Plot of isobaric expansivity $\alpha_{p,2}^0 = \left(1 / V_{m,2}^0\right)\left(\partial V_{m,2}^0 / \partial T\right)_p$ **at saturation vapour pressure of water calculated from the fits using equation (3) against the number of methylene groups** *n* **(carbon atoms C**$_n$**) in the solute molecule.**
Full lines, alkane-α,ω-diols; dashed lines - alkane-1-ols [23-25].
○, **298.15 K;** Δ, **373.15 K;** ■, **473.15 K;** ▼, **523.15 K;**
▽, **573.15 K.**

Figure 5.

Plot of $\left(\partial c_{p,\mathrm{m},2}^{0} / \partial p\right)_{T} = -T\left(\partial^2 V_{\mathrm{m},2}^{0} / \partial T^2\right)_{p}$ **at saturation vapour pressure of water calculated from the fits using equation (3) against temperature** *T*.

n **= 2, ethane-1,2-diol;** *n* **= 3, propane-1,3-diol;**
n **= 4, butane-1,4-diol;** *n* **= 5, pentane-1,5-diol;**
n **= 6, hexane-1,6-diol;** *n* **= 8, octane-1,8-diol;**
n **= 9, nonane-1,9-diol.**

Figure 6.

Plot of isothermal compressibility $\kappa_{T,2}^{0} = -(1 / V_{\mathrm{m},2}^{0})\left(\partial V_{\mathrm{m},2}^{0} / \partial p\right)_{T}$ **at saturation vapour pressure of water calculated from the fits using equation (3) against temperature** *T*.

n **= 2, ethane-1,2-diol;** *n* **= 3, propane-1,3-diol;**
n **= 4, butane-1,4-diol;** *n* **= 5, pentane-1,5-diol;**
n **= 6, hexane-1,6-diol;** *n* **= 8, octane-1,8-diol;**
n **= 9, nonane-1,9-diol.**

Figure 7.

Plot of isothermal compressibility $\kappa_{T,2}^{0} = -(1 / V_{\mathrm{m},2}^{0})\left(\partial V_{\mathrm{m},2}^{0} / \partial p\right)_{T}$ **at saturation vapour pressure of water calculated from the fits using equation (3) against the number of methylene groups** *n* **(carbon atoms** C_n**) in the solute molecule.**

Full lines, alkane-α,ω-diols; dashed lines - alkane-1-ols [23-25].
○, 298.15 K; Δ, 373.15 K; ■, 473.15 K; ▼, 523.15 K;
∇, 573.15 K.
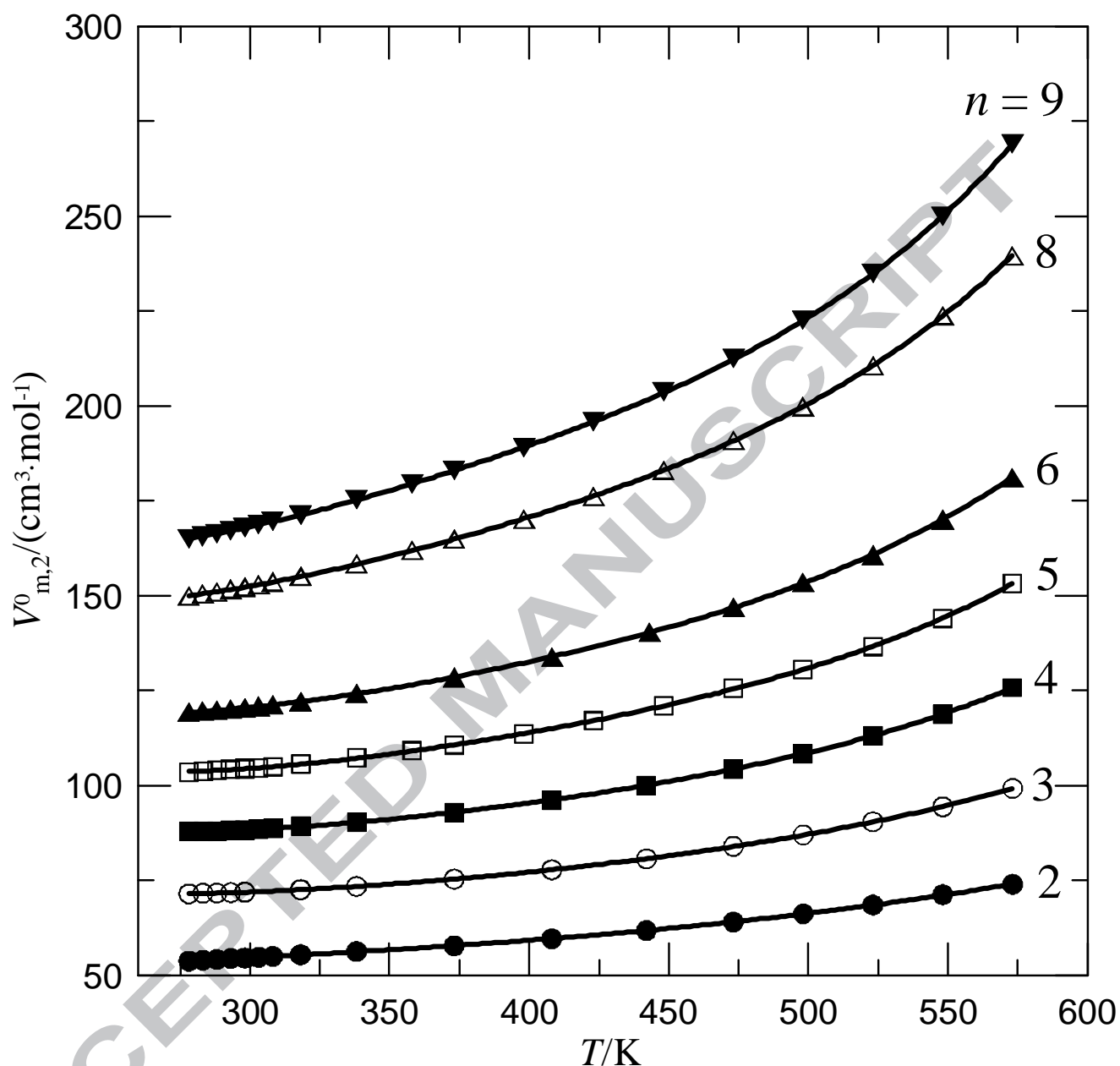
Figure 1.

Plot of experimental standard molar volumes $V_{m,2}^0$ at low pressures against temperature T. The lines are to aid the eye. Integer numbers denote the numbers of methylene groups n (carbon atoms C_n) in the solute molecule.

●, ethane-1,2-diol [1,4]; ○, propane-1,3-diol [1,5]; ■, butane-1,4-diol [2,6]; □, pentane-1,5-diol [4,this work]; ▲, hexane-1,6-diol [3,4]; △, octane-1,8-diol [4,this work]; ▼, nonane-1,9-diol [4,this work].
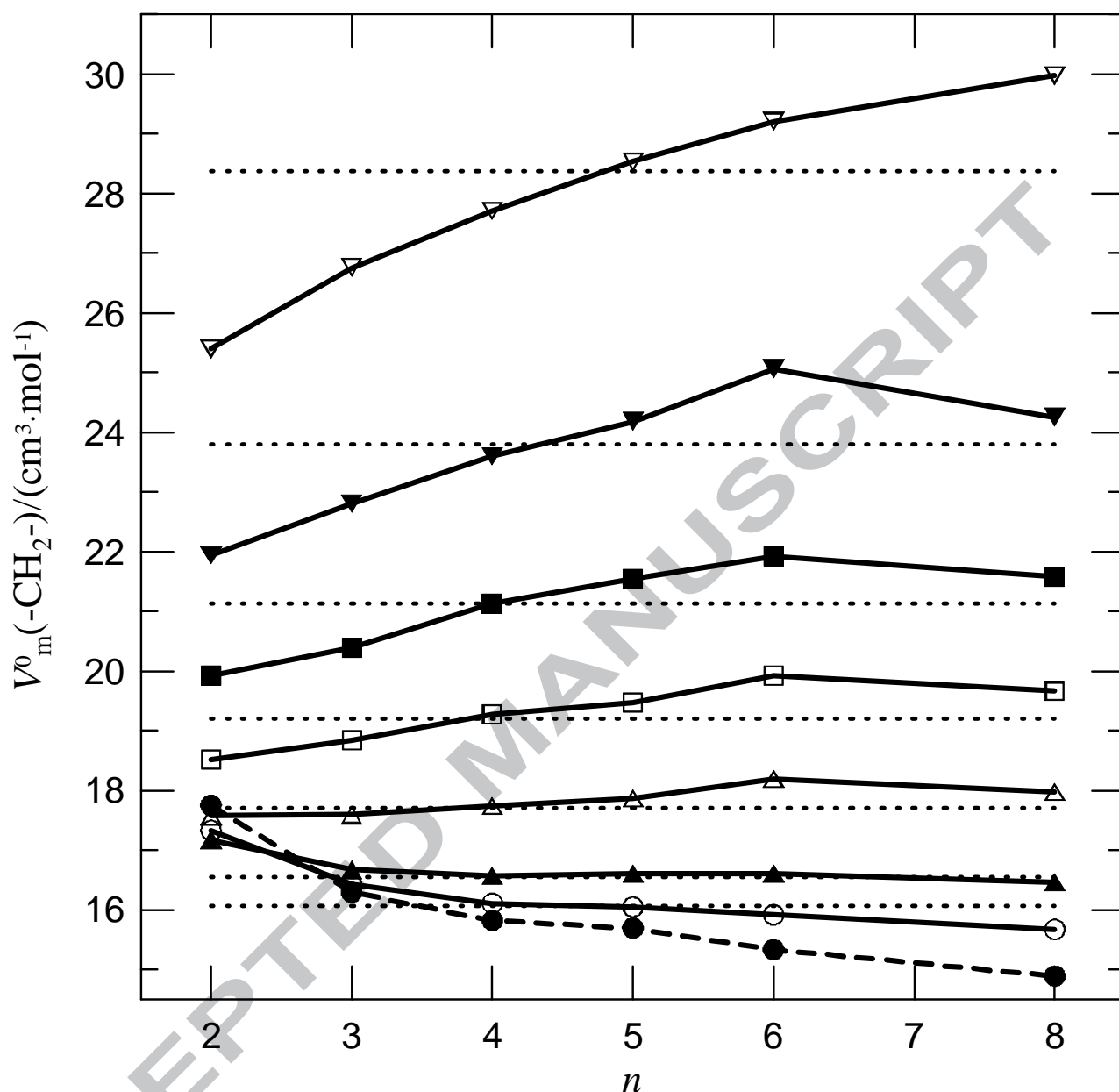
Figure 2.
Plot of the contribution of the methylene group
$V_{\mathrm{m}}^{0}(-CH_2-) = V_{\mathrm{m,2}}^{0}\left[HO-(CH_2)_{n+1}-OH\right] - V_{\mathrm{m,2}}^{0}\left[HO-(CH_2)_n-OH\right]$ to standard molar volume at saturation vapour pressure of water against n. Due to the lack of data for $n = 7$ the averages over two homologous neighbours ($C_{n+2} - C_n$) are shown for the pair C_8/C_6 ($n = 6$); for details see text. Horizontal dotted lines represent the values of the contribution reported in ref. [23] for respective temperatures starting from 298.15 K (the lowest line).

●, 278.15 K; ○, 298.15 K; ▲, 323.15 K; △, 373.15 K; □, 423.15 K;
■, 473.15 K; ▼, 523.15 K; ∇, 573.15 K.

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Figure 3.
Plot of isobaric expansivity $\alpha_{p,2}^0 = \left(1/V_{m,2}^0\right)\left(\partial V_{m,2}^0 / \partial T\right)_p$ at saturation vapour pressure of water calculated from the fits using equation (3) against temperature T.
n = 2, ethane-1,2-diol; n = 3, propane-1,3-diol;
n = 4, butane-1,4-diol; n = 5, pentane-1,5-diol;
n = 6, hexane-1,6-diol; n = 8, octane-1,8-diol;
n = 9, nonane-1,9-diol.

Figure 4.

Plot of isobaric expansivity $\alpha_{p,2}^{0} = \left(1/V_{m,2}^{0}\right)\left(\partial V_{m,2}^{0}/\partial T\right)_{p}$ at saturation vapour pressure of water calculated from the fits using equation (3) against the number of methylene groups n (carbon atoms C_n) in the solute molecule.

Full lines, alkane-α,ω-diols; dashed lines - alkane-1-ols [23-25].
○, 298.15 K; △, 373.15 K; ■, 473.15 K; ▼, 523.15 K;
∇, 573.15 K.

Figure 5.

Plot of $\left(\partial c_{p,\mathrm{m},2}^{0} \, / \, \partial p \right)_{T} = - T \left(\partial^{2} V_{\mathrm{m},2}^{0} \, / \, \partial T^{2} \right)_{p}$ at saturation vapour pressure of water calculated from the fits using equation (3) against temperature T.

n = 2, ethane-1,2-diol; n = 3, propane-1,3-diol;
n = 4, butane-1,4-diol; n = 5, pentane-1,5-diol;
n = 6, hexane-1,6-diol; n = 8, octane-1,8-diol;
n = 9, nonane-1,9-diol.

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Figure 6.
Plot of isothermal compressibility $\kappa_{T,2}^{0} = -(1/V_{m,2}^{0})(\partial V_{m,2}^{0}/\partial p)_{T}$ at saturation vapour pressure of water calculated from the fits using equation (3) against temperature T.
$n = 2$, ethane-1,2-diol; $n = 3$, propane-1,3-diol;
$n = 4$, butane-1,4-diol; $n = 5$, pentane-1,5-diol;
$n = 6$, hexane-1,6-diol; $n = 8$, octane-1,8-diol;
$n = 9$, nonane-1,9-diol.

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Figure 7.

Plot of isothermal compressibility $\kappa_{T,2}^0 = -\left(1/V_{m,2}^0\right)\left(\partial V_{m,2}^0/\partial p\right)_T$ at saturation vapour pressure of water calculated from the fits using equation (3) against the number of methylene groups n (carbon atoms C_n) in the solute molecule.

Full lines, alkane-α,ω-diols; dashed lines - alkane-1-ols [23-25].
$\circ$, 298.15 K; $\triangle$, 373.15 K; $\blacksquare$, 473.15 K; $\blacktriangledown$, 523.15 K;
∇, 573.15 K.

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TABLE 1

Specifications of Chemical Samples of Solutes. All Samples Were
from Sigma Aldrich and Were Used as Supplied.

Chemical name	Formula	CAS RN	Mass Fraction Purity[a]	Mass Fraction of Water[b]
Pentane-1,5-diol	$C_5H_{12}O_2$	111-29-5	0.97	0.00028, 0.00034[c]
Octane-1,8-diol	$C_8H_{18}O_2$	629-41-4	0.98	
Nonane-1,9-diol	$C_9H_{20}O_2$	3937-56-2	0.98	

[a] Declared by the supplier. [b] Determined by the Karl Fischer
method. [c] Two solute samples were used.

TABLE 2
Density ρ_1 of water [9], coefficients a, b, and c of equation (1) and standard molar volumes $V_{m,2}^{\circ}$ of organic solutes for {pentane-1,5-diol(2) or octane-1,8-diol(2) or nonane-1,9-diol(2) + water(1)}. The standard deviations $\sigma(a)$, $\sigma(b)$, and $\sigma(c)$ refer to the coefficients a, b, and c of equation (1), $\sigma(V_{m,2}^{\circ})$ represents the total estimated uncertainty.

$\dfrac{T}{K}$	$\dfrac{p}{MPa}$	$\dfrac{\rho_1}{kg \cdot m^{-3}}$	$\dfrac{a}{kg^2 \cdot m^{-3} \cdot mol^{-1}}$	$\sigma(a)$	$\dfrac{b}{kg^3 \cdot m^{-3} \cdot mol^{-2}}$	$\sigma(b)$	$\dfrac{c}{kg^4 \cdot m^{-3} \cdot mol^{-3}}$	$\sigma(c)$	$\dfrac{V_{m,2}^{0}}{cm^3 \cdot mol^{-1}}$	$\sigma\left(V_{m,2}^{0}\right)$
					Pentane-1,5-diol (aq)					
298.15	0.51	997.232	-0.066	0.066	1.360	0.301	-0.729	0.335	104.50	0.07
318.18	0.52	990.381	-0.488	0.105	0.568	0.405	-0.103	0.465	105.66	0.11
338.18	0.52	980.717	-1.019	0.090	0.443	0.363	-0.108	0.414	107.25	0.09
358.16	0.52	968.797	-1.552	0.078	0.473	0.308	-0.233	0.356	109.16	0.08
373.18	0.51	958.523	-1.908	0.054	0.294	0.103			110.73	0.06
398.14	1.88	939.872	-2.506	0.055	0.336	0.104			113.65	0.06
423.16	1.86	917.781	-3.027	0.055	0.402	0.102			117.07	0.07
448.16	1.86	892.895	-3.485	0.053	0.516	0.098			121.01	0.07
473.23	1.83	864.778	-3.830	0.055	0.591	0.099			125.55	0.07
498.12	3.05	834.244	-4.047	0.074	0.677	0.137			130.65	0.11
523.19	5.03	800.060	-4.180	0.054	0.825	0.099			136.70	0.09
548.16	7.05	760.694	-4.138	0.068	0.968	0.124			144.06	0.12
573.18	10.05	715.327	-3.899	0.092	1.243	0.179			153.21	0.18
298.15	15.17	1003.740	-0.572	0.079	1.251	0.292	-0.362	0.310	104.33	0.08
318.17	15.14	996.674	-0.775	0.059	0.577	0.090			105.28	0.06
338.18	15.19	987.045	-1.232	0.052	0.495	0.091			106.78	0.05
358.16	15.12	975.279	-1.617	0.052	0.358	0.091			108.49	0.06
373.15	15.19	965.288	-1.940	0.055	0.341	0.106			109.97	0.06
398.12	15.17	946.484	-2.436	0.054	0.350	0.103			112.76	0.06
423.15	15.14	925.107	-2.852	0.051	0.371	0.093			115.91	0.06
448.19	15.28	901.270	-3.203	0.051	0.468	0.093			119.50	0.06
473.22	15.13	874.508	-3.434	0.053	0.514	0.100			123.58	0.07
498.12	15.11	844.833	-3.595	0.059	0.612	0.107			128.31	0.08

523.19   15.12   811.100   −3.634   0.054   0.740   0.096   133.93   0.08

TABLE 2 (*continued*)

$\dfrac{T}{\text{K}}$	$\dfrac{p}{\text{MPa}}$	$\dfrac{\rho_1}{\text{kg}\cdot\text{m}^{-3}}$	$\dfrac{a}{\text{kg}^2\cdot\text{m}^{-3}\cdot\text{mol}^{-1}}$	$\sigma(a)$	$\dfrac{b}{\text{kg}^3\cdot\text{m}^{-3}\cdot\text{mol}^{-2}}$	$\sigma(b)$	$\dfrac{c}{\text{kg}^4\cdot\text{m}^{-3}\cdot\text{mol}^{-3}}$	$\sigma(c)$	$\dfrac{V_{m,2}^0}{\text{cm}^3\cdot\text{mol}^{-1}}$	$\sigma\left(V_{m,2}^0\right)$
548.16	15.04	772.200	−3.428	0.060	0.667	0.100			140.62	0.10
573.18	15.22	725.915	−3.281	0.087	0.953	0.172			149.70	0.17
298.16	30.13	1010.180	−1.072	0.079	1.346	0.292	−0.393	0.208	104.15	0.07
318.17	30.23	1002.960	−1.135	0.109	0.802	0.445	−0.257	0.507	104.97	0.11
338.16	30.16	993.297	−1.544	0.138	0.972	0.623	−0.480	0.782	106.42	0.14
358.14	30.04	981.664	−1.729	0.060	0.404	0.118			107.89	0.06
373.17	30.18	971.889	−1.990	0.061	0.375	0.114			109.27	0.07
398.13	30.14	953.582	−2.368	0.064	0.336	0.127			111.82	0.07
423.15	30.12	932.924	−2.729	0.051	0.393	0.094			114.77	0.06
448.18	30.03	909.930	−2.996	0.052	0.472	0.095			118.08	0.06
473.22	29.98	884.529	−3.152	0.054	0.560	0.099			121.77	0.07
498.11	30.10	856.762	−3.151	0.053	0.535	0.096			125.85	0.07
523.18	30.05	825.564	−3.046	0.052	0.617	0.093			130.62	0.08
548.16	30.04	790.662	−2.734	0.057	0.611	0.093			136.10	0.09
573.19	30.09	750.712	−2.179	0.070	0.602	0.140			142.60	0.12
				Octane-1,8-diol (aq)						
298.15	0.51	997.234	−5.577	0.162	0.869	0.918			152.24	0.16
318.18	0.52	990.381	−7.287	0.200					155.08	0.20
338.18	0.52	980.716	−8.942	0.093					158.40	0.10
358.16	0.52	968.796	−10.333	0.086					161.95	0.09
373.18	0.52	958.524	−11.335	0.079					164.89	0.09
398.14	1.88	939.871	−12.933	0.164	1.430	1.125			170.22	0.19
423.16	1.86	917.781	−14.255	0.164	2.043	1.064			176.25	0.20
448.16	1.85	892.892	−15.457	0.162	3.384	1.091			183.16	0.21
473.23	1.83	864.781	−16.378	0.156	3.569	1.017			190.99	0.21
498.12	3.05	834.244	−17.098	0.183	7.388	1.548			199.85	0.27
523.19	5.03	800.061	−17.840	0.158	9.658	1.081			210.64	0.25
548.16	7.05	760.691	−18.277	0.181	10.307	1.203			223.82	0.32
573.18	10.05	715.333	−17.986	0.285	6.536	2.065			239.57	0.56

TABLE 2 (*continued*)

$\dfrac{T}{\mathrm{K}}$	$\dfrac{p}{\mathrm{MPa}}$	$\dfrac{\rho_1}{\mathrm{kg \cdot m^{-3}}}$	$\dfrac{a \qquad \sigma(a)}{\mathrm{kg^2 \cdot m^{-3} \cdot mol^{-1}}}$		$\dfrac{b \qquad \sigma(b)}{\mathrm{kg^3 \cdot m^{-3} \cdot mol^{-2}}}$		$\dfrac{c \qquad \sigma(c)}{\mathrm{kg^4 \cdot m^{-3} \cdot mol^{-3}}}$		$\dfrac{V_{\mathrm{m,2}}^0 \qquad \sigma\left(V_{\mathrm{m,2}}^0\right)}{\mathrm{cm^3 \cdot mol^{-1}}}$	
298.16	15.17	1003.740	−6.629	0.194	2.949	1.233			152.26	0.19
318.17	15.14	996.674	−7.658	0.149					154.43	0.15
338.18	15.19	987.045	−9.154	0.092					157.54	0.10
358.16	15.12	975.279	−10.332	0.086					160.80	0.09
373.15	15.19	965.287	−11.230	0.083					163.54	0.09
398.12	15.17	946.484	−12.676	0.164	1.820	1.131			168.65	0.18
423.15	15.14	925.108	−13.738	0.173	1.683	1.204			174.12	0.20
448.19	15.28	901.271	−14.635	0.159	2.250	1.054			180.26	0.20
473.22	15.13	874.511	−15.314	0.171	2.561	1.130			187.24	0.23
498.12	15.11	844.837	−16.085	0.152	8.155	0.969			195.62	0.22
523.19	15.13	811.102	−16.452	0.159	8.612	1.020			205.29	0.25
548.16	15.04	772.194	−16.394	0.167	7.341	0.788			216.86	0.29
573.18	15.22	725.911	−16.246	0.202	4.484	1.328			232.27	0.39
298.16	30.13	1010.180	−7.489	0.205	3.467	1.426			152.09	0.20
318.17	30.23	1002.960	−8.187	0.104					153.94	0.10
338.16	30.16	993.297	−9.481	0.118					156.82	0.12
358.14	30.03	981.663	−10.399	0.087					159.75	0.09
373.17	30.19	971.891	−11.171	0.086					162.28	0.09
398.13	30.14	953.582	−12.284	0.164	0.770	1.064			166.85	0.18
423.15	30.12	932.924	−13.395	0.165	2.398	1.136			172.13	0.19
448.18	30.03	909.932	−14.059	0.192	2.216	1.125			177.68	0.23
473.22	29.99	884.529	−14.647	0.154	3.570	0.999			184.04	0.20
498.11	30.09	856.760	−14.883	0.165	6.683	1.146			190.95	0.23
523.18	30.04	825.554	−14.989	0.173	7.785	1.212			199.12	0.26
548.16	30.05	790.669	−14.563	0.183	7.171	1.174			208.24	0.30
573.19	30.09	750.712	−13.670	0.193	4.757	1.337			219.04	0.35

TABLE 2 (*continued*)

$\dfrac{T}{K}$	$\dfrac{p}{MPa}$	$\dfrac{\rho_1}{kg \cdot m^{-3}}$	$\dfrac{a \qquad \sigma(a)}{kg^2 \cdot m^{-3} \cdot mol^{-1}}$	$\dfrac{b \qquad \sigma(b)}{kg^3 \cdot m^{-3} \cdot mol^{-2}}$	$\dfrac{c \qquad \sigma(c)}{kg^4 \cdot m^{-3} \cdot mol^{-3}}$	$V_{m,2}^0 \qquad \sigma\left(V_{m,2}^0\right)$ $\dfrac{}{cm^3 \cdot mol^{-1}}$
				Nonane-1,9-diol (aq)		
298.15	0.51	997.233	−7.276 0.233			168.02 0.23
318.19	0.51	990.378	−9.389 0.407			171.38 0.42
338.18	0.52	980.715	−11.481 0.202			175.34 0.21
358.16	0.51	968.794	−13.158 0.139			179.44 0.15
373.18	0.52	958.525	−14.456 0.149			182.92 0.17
398.14	1.88	939.870	−16.262 0.184			188.92 0.21
423.16	1.86	917.780	−17.884 0.178			195.84 0.22
448.16	1.85	892.893	−19.345 0.177			203.74 0.23
473.23	1.84	864.781	−20.309 0.199			212.47 0.27
498.13	3.05	834.237	−21.202 0.226			222.56 0.33
523.19	5.04	800.061	−22.144 0.216			234.90 0.34
548.16	7.05	760.683	−22.739 0.213			249.97 0.38
573.18	10.05	715.319	−23.027 0.253			269.03 0.50
298.16	15.16	1003.730	−8.227 0.256			167.83 0.25
318.17	15.14	996.675	−9.802 0.352			170.66 0.36
338.17	15.19	987.047	−11.754 0.223			174.42 0.23
358.15	15.12	975.281	−13.161 0.132			178.15 0.14
373.15	15.19	965.287	−14.296 0.192			181.36 0.21
398.13	15.15	946.465	−15.913 0.176			187.08 0.20
423.15	15.14	925.103	−17.265 0.189			193.40 0.22
448.18	15.23	901.250	−18.323 0.170			200.37 0.21
473.22	15.13	874.513	−19.092 0.238			208.21 0.32
498.12	15.11	844.832	−19.809 0.230			217.44 0.33
523.19	15.13	811.106	−20.339 0.246			228.49 0.38
548.19	15.05	772.162	−20.515 0.260			241.94 0.44
573.19	15.22	725.891	−21.150 0.248			260.91 0.48
298.16	30.11	1010.170	−9.246 0.239			167.70 0.24
318.17	30.24	1002.960	−10.364 0.253			170.09 0.25
338.16	30.15	993.291	−12.034 0.170			173.53 0.17

TABLE 2 (*continued*)

$\dfrac{T}{K}$	$\dfrac{p}{MPa}$	$\dfrac{\rho_1}{kg \cdot m^{-3}}$	$\dfrac{a \qquad \sigma(a)}{kg^2 \cdot m^{-3} \cdot mol^{-1}}$	$\dfrac{b \qquad \sigma(b)}{kg^3 \cdot m^{-3} \cdot mol^{-2}}$	$\dfrac{c \qquad \sigma(c)}{kg^4 \cdot m^{-3} \cdot mol^{-3}}$	$\dfrac{V_{m,2}^0 \qquad \sigma\left(V_{m,2}^0\right)}{cm^3 \cdot mol^{-1}}$
358.14	30.06	981.679	-13.182 0.134			176.93 0.14
373.17	30.19	971.894	-14.226 0.180			179.95 0.19
398.12	30.16	953.597	-15.488 0.184			185.09 0.21
423.15	30.12	932.926	-16.765 0.175			191.04 0.20
448.18	30.04	909.935	-17.567 0.227			197.33 0.28
473.22	30.01	884.547	-18.174 0.219			204.40 0.28
498.11	30.09	856.757	-18.531 0.215			212.29 0.30
523.18	30.05	825.552	-18.640 0.222			221.47 0.33
548.16	30.07	790.700	-18.403 0.232			232.11 0.38
573.19	30.07	750.685	-17.785 0.215			245.04 0.39

Standard uncertainties are $u(T)$ = 0.02 K at T = 298 K increasing to $u(T)$ = 0.1 K at T = 573 K, $u(p)$ = 0.01 MPa at $p \leq$ 10 MPa and $u(p)$ = 0.03 MPa at $p >$ 10 MPa.

TABLE 3
Comparison of measured values of standard molar volume with the values at p = 0.1 MPa taken from the literature.

	This work[a]	Literature		
T K	$V_{m,2}^0$ cm^3·mol^{-1}	$V_{m,2}^0$ cm^3·mol^{-1}	ref	dev.[b] cm^3·mol^{-1}
		Pentane-1,5-diol (aq)		
298.15	104.50 ±0.07[c]	104.47 ±0.03	[4]	0.03
	(104.46)	104.15	[13]	0.35
		104.2 ±0.1	[14]	0.30
		104.29	[15]	0.21
		104.35 ±0.1	[16,17]	0.15
		104.39 ±0.1	[18]	0.11
		104.4 ±0.3	[19]	0.10
		104.43	[20]	0.07
313.15	105.34[e]	105.27	[21]	0.07
318.18	105.66 ±0.11[c]	105.66 ±0.03[d]	[4]	0.00
	(105.68)	105.63[c]	[20]	0.03
		Octane-1,8-diol (aq)		
298.15	152.24 ±0.16[c]	152.34 ±0.10	[4]	-0.10
	(152.34)	152.6 ±0.1	[14,16,18]	-0.36
318.18	155.08 ±0.20[c]	155.05 ±0.14[d]	[4]	0.03
	(155.09)			

[a] Values in parentheses were calculated from equation (3) for p = 0.1 MPa. [b] Deviation between this work and the literature value. [c] At p = 0.5 MPa. [d] At T = 318.15 K. [e] Interpolated using equation (3).

TABLE 4

Comparison of smoothed values of standard molar volume of aqueous pentane-1,5-diol (equation (3)) at elevated pressures with the values from the literature

		This work (eq 3)	Literature		
T	P	$V_{m,2}^0$	$V_{m,2}^0$	ref	dev[a]
K	MPa	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$		$cm^3 \cdot mol^{-1}$
298.15	20.00	104.28	104.07	15	0.21
301.80	0.13	104.66	104.4 ±0.4	22	0.26
301.84	28.02	104.30	104.0 ±0.3	22	0.30
373.50	28.01	109.40	109.1 ±0.3	22	0.30
423.70	28.00	114.98	115.1 ±0.3	22	-0.12
473.21	28.00	121.99	122.1 ±0.2	22	-0.11
521.31	6.88	135.60	138.2 ±1.6	22	-2.60
521.37	28.00	130.62	132.8 ±1.1	22	-2.18

[a] Deviation between this work and the literature value.

Highlights

↗Standard molar volumes of three alkane-α,ω-diols (C$_5$, C$_8$, C$_9$) in water are presented. ↗Data were obtained in the range T from (298 to 573) K and p up to 30 MPa. ↗Dependences on carbon atom number, temperature, and pressure are analyzed.