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Densities of dilute aqueous solutions of 1-butanol and 1-pentanol at atmospheric pressure and temperatures in the range 283.15 to 353.15 K

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Abstract

Mass densities of dilute aqueous solutions of 1-butanol and 1-pentanol (with alcohol concentrations between 0.07 to 0.7 mol·kg⁻¹ and 0.006 to 0.06 mol·kg⁻¹, respectively) were determined at atmospheric pressure and temperatures in the range of 283.15 to 353.15 K using a custom-built volume dilatometer. The dilatometer was first calibrated using water, and then benchmarked using water and aqueous solutions of ethanol. Evaporation in the experiments with water and the alcohol solutions was prevented by adding a small amount of oil (about 0.2 ml) over the liquid surface that was exposed to the ambient air. The density data complement and extend those available in the published literature. They also show that at alcohol concentrations less than 0.01 mol·kg⁻¹, the density of such solutions may be reasonably assumed to be the same as that of water or calculated using the ideal-solution assumption. For solutions with higher alcohol concentrations, however, the aforementioned assumptions are inappropriate as they lead

to density values that differ from the data presented in this paper by amounts that exceed the expanded uncertainty of the underlying measurements.

Keywords: Mass density measurement; volume dilatometer; dilute aqueous solutions; 1-butanol; 1-pentanol; water

1. Introduction

The values of the mass density (referred to simply as 'density' from this point on) of dilute aqueous solutions of 1-butanol and 1-pentanol at atmospheric pressure and temperatures ranging from 283.15 to 353.15 K, in 10 K increments (nominal), are presented and discussed in this paper. The qualification 'dilute' is used here to indicate solutions with alcohol concentrations less than or equal to approximately 0.7 mol·kg⁻¹ (mass fraction \leq 5%). The density of three different aqueous solutions of 1-butanol and three of 1-pentanol, with alcohol concentration in the range 0.07 to 0.7 mol·kg⁻¹ and 0.006 to 0.06 mol·kg⁻¹, respectively, were determined using measurements obtained from a custom-built volume dilatometer. A brief description of some practical applications of such solutions, a statement of the main underlying motivation for this work, and a concise review of the literature are presented in the remainder of this section. In the following sections, the details of this experimental investigation (descriptions of the alcohols, water, the custom-built volume dilatometer, and the procedures used), results and discussions, concluding remarks, and a listing of the references are provided.

Dilute aqueous solutions of long-chain alcohols (such as 1-butanol and 1-pentanol) have been proposed as working fluids for heat pipes and vapor-chamber spreaders, which are passive devices (devices with no moving mechanical parts) that employ liquid-vapor phase-change and surface-tension driven phenomena to achieve continuous (cyclical) operation at high heat fluxes with relatively low temperature differences between the heated (evaporator) and cooled (condenser) sections.¹⁻⁷ Such devices are very useful (and commonly used) for thermal management of electronic devices and illumination systems based on light-emitting diodes (LEDs).^{1-4,8} Dilute aqueous solutions of 1-butanol and 1-pentanol (and also 1-hexanol and 1-heptanol) are of interest as working fluids in above-mentioned thermal-management devices as they exhibit a positive gradient of surface tension with temperature (at about 313.15 K and higher; depending on the alcohol), which enhances the return of the liquid phase from the cooled to the heated sections.⁵⁻⁷

Mathematical models of heat pipes and vapor-chamber spreaders require data on several thermophysical properties of the working fluid (such as density, dynamic viscosity, specific heat at constant pressure, and thermal conductivity of the liquid and vapor phases; and the surface tension at the interface between these phases).^{1,3,4,9-12} However, the bulk of the published data on the density of dilute aqueous solutions of the above-mentioned long-chain alcohols pertains to temperatures of either 293.15 or 298.15 K. Thus, the available density data are rather sparse over the temperature range 283.15 to 353.15 K, which roughly corresponds to the operating temperature range of many commonly used electronic devices and LED illumination systems.^{1,2,4,8,11} In this context, it should also be noted that data on the density of these solutions is a required input for the determination of their surface tension using either the pendant drop or maximum bubble pressure methods.¹³ Thus, there is an important practical need for such density

data. The authors' desire to contribute to the fulfillment of this need is the main underlying motivation for the work reported in this paper.

The thermophysical properties of aqueous solutions of 1-hexanol and 1-heptanol with concentrations less than 0.01 mol·kg⁻¹ are sometimes assumed to be those of pure water.^{5,6,14} Another assumption that is sometimes invoked for determining the density of dilute aqueous solutions of alcohols is that they can be approximated as ideal solutions (the volume of an ideal solution is equal to the sum of the volumes of its components).^{7,15} For example, the idealsolution assumption was used in a recent study by Cheng and Park⁷ for calculating the densities of aqueous solutions of 1-butanol, 1-pentanol, and 1-hexanol at alcohol concentrations of approximately 0.07 to 0.9 mol·kg⁻¹, 0.01 to 0.2 mol·kg⁻¹, and 0.005 to 0.05 mol·kg⁻¹, respectively. However, the ideal-solution assumption is not always valid. For instance, when ethanol and water are mixed together, an overall decrease in volume is known to occur due to hydrogen bonding.¹⁶⁻²⁰ This change in volume is typically expressed in terms of the excess molar volume, which is the difference between the actual molar volume of the solution and that if it were an ideal solution (that is, the mole-fraction-weighted average of the molar volumes of the pure components).¹⁹⁻²² The excess molar volume is negative for aqueous solutions of ethanol at all concentrations^{16,19,23,24}; in other words, the actual density of these solutions is higher than that obtained using the ideal-solution assumption. Aqueous solutions of both 1-butanol and 1pentanol have also exhibited negative values of the excess molar volume.^{24,25}

For the experimental determination of the density of liquids, hydrometers, hydrostatic balances, pycnometers, volume dilatometers, and vibrating-tube density meters, are commonly used.²⁶⁻²⁹ Compared to current state-of-the-art vibrating-tube density meters, the other abovementioned instruments are lower-cost options; however, the liquid in these other instruments is exposed to the atmospheric air, so erroneous measurements can result due to evaporation, especially at elevated temperatures, unless proper precautions are taken to limit the related loss of mass. Vibrating-tube density meters do not suffer from such evaporative losses, and they require a lower volume of solution and significantly reduced measurement time.²⁸

Vibrating-tube density meters were used in most experimental investigations of the density of dilute aqueous solutions of 1-butanol and 1-pentanol reported in the published literature, and very impressive uncertainties were claimed ($\leq 0.005 \text{ kg} \cdot \text{m}^{-3}$). However, it should also be noted that in other recent studies in which vibrating-tube density meters were used, more conservative standard uncertainty estimates have been reported (0.1 to 2.0 kg·m⁻³).^{25,30-34} Pycnometers³⁵⁻³⁹ have also been used to determine the density of dilute aqueous solutions of 1-butanol and 1-pentanol, with reported uncertainties ranging from 0.01 to 5 kg·m⁻³.

In a large proportion of the experimental investigations of the density of aqueous solutions of 1-butanol and 1-pentanol reported in the literature, the temperatures were below 323.15 K, and there is a dearth of such density measurements at higher temperatures.^{35,39-46} To the knowledge of the authors, in only four investigations were density measurements performed at temperatures exceeding 323.15 K, namely, Ling and Van Winkle⁴¹, Origlia and Woolley⁴², Inglese and Robert⁴⁵, and Cárdenas et al.⁴³ In these investigations, the measurements were either affected by evaporation⁴¹, performed at elevated pressures⁴², done at only one temperature⁴⁵ greater than 323.15 K, or only performed for a single concentration at the solubility limit.⁴³

As was stated earlier, the values of the density of dilute aqueous solutions of 1-butanol and 1-pentanol at atmospheric pressure and temperatures ranging from 283.15 to 353.15 K, in 10 K increments (nominal), are presented and discussed in this paper. The density of three different aqueous solutions of 1-butanol (with alcohol concentration in the range 0.07 to 0.7 mol·kg⁻¹) and three different aqueous solutions of 1-pentanol (with alcohol concentration in the range 0.006 to 0.06 mol·kg⁻¹) were determined using a custom-built volume dilatometer. The concentrations of all alcohol solutions considered here remained below their respective solubility limits for the entire temperature range investigated, which ensured that the solutions remained homogenous during the measurements.^{47,48} These and even lower concentrations are of interest as the gradient of surface tension with concentration of alcohol is negative for these solutions (water has a greater surface tension than the alcohols).⁵⁻⁷ In the work reported in this paper, the thermal expansion of the volume dilatometer was taken into account.⁴⁹⁻⁵¹ In addition, a simple (but effective) technique was used to prevent evaporative losses that could otherwise compromise the accuracy of the density data.

It is worth noting here that the custom-built dilatometer described in this work could be used for measurements of the density of solids, granular materials, and encapsulated substances by immersing them in water or other liquids (within the dilatometer; provided they do not dissolve in the water or the other liquids) for which accurate data on the variation of density with temperature in the range of interest are available. It could also be used for measuring the density of slurries of micro-encapsulated solid-liquid phase-change materials suspended in water (in temperature ranges in which the solid-liquid phase-change takes place). Such slurries are being investigated for potential use in thermosyphons for cooling high-heat-flux devices.⁵²

2. Experimental Investigation

Descriptions of the alcohols and water used in this work, the custom-built volume dilatometer, the procedure used for preparing the aqueous solutions of the alcohols, the experimental procedure for determining the density of the liquids of interest, and a note on the calibration of the volume dilatometer are presented in this section. For conciseness, the volume dilatometer will be referred to as the dilatometer in the remainder of this paper.

2.1 Alcohols and Water

The alcohols used in this work were all of reagent grade, used in the forms supplied by the manufacturers (without further purification). The ethanol was obtained from Commercial Alcohols by Greenfield Global; and the 1-butanol, 1-pentanol, and water (purified, all-glass-distilled) were obtained from A&C American Chemicals Ltd. Details and specifications of these alcohols and the water are presented in Table 1. The suppliers have also indicated that water is the primary impurity in the alcohols listed in Table 1.

Table 1. Details of the alcohols and water

Chemical Name	CAS No.	Source	Initial Mole Fraction Purity	Purification Method	Analysis Method ^a	Molar Mass ^b ∕g∙mol ⁻¹
Ethanol CH3CH2OH	64-17-5	Commercial Alcohols	0.9995°	-	Density	46.07
1-butanol	71-36-3	A&C American	0.999	-	GC	74.12

CH ₃ (CH ₂) ₃ OH		Chemicals Ltd.						
1-pentanol CH ₃ (CH ₂) ₃ CH ₂ OH	71-41-0	A&C American Chemicals Ltd.	0.999	-	GC	88.15		
Water H2O	7732- 18-5	A&C American Chemicals Ltd.	1.0	-	-	18.016		
^a Analysis performed by the supplier: density (digital density meter); GC (gas chromatography) ^b Molar masses values taken from Perry ⁵³ ^c Equivalent mole fraction (99.98% purity by volume specified by Commercial Alcohols); see Supporting Information for details								

2.2 Dilatometer

The dilatometer used in this work was made mainly of borosilicate glass (Type I, Class A, lowexpansion borosilicate glass) and fabricated in-house by a master glassblower, using a combination of custom-made and modified commercially available parts.

The dilatometer was comprised of three sections: a main body, a filling section, and a measurement section. A photograph of these three sections (disconnected from each other) is shown in Figure 1 and the full measurement section is depicted in Figure 2. The main body of the dilatometer (about 155 mm in height) was custom-blown and had a cylindrical lower portion (approximately 55 mm in diameter) and a conical top portion. The filling section consisted of a modified commercially available valve (Chemglass model CG-960-01; Chem-Vac valve and Teflon Chem-Cap), with its lower glass tube fused to the male portion of a Rodaviss joint that was used to attach it to the curved side of the lower cylindrical portion of the main body of the dilatometer. The measurement section was formed by modifying a commercially available

burette (ChemScience model 114.202.01F; 10 ml total volume with 0.02 ml subdivisions at 293.15 K). This burette was cut at the 8.00 ml mark on its scale and fused to the male portion of another Rodaviss joint that was used to attach the measurement section to the conical top portion of the main body of the dilatometer. In this configuration, the 0.00 ml mark on the scale of the burette was located near the top of the measurement section. The length of the measurement section was approximately 500 mm. Thus, the assembled dilatometer had a total height of approximately 650 mm.

The dilatometer depicted in Figure 1 and described in the previous paragraph was designed with the following requirements in mind: 1) easy assembly, disassembly, cleaning, and drying of its three sections; 2) convenient bottom-up filling with the liquids of interest without entrapment of air; and 3) effective use of the full range of the burette for the liquids of interest over the temperature range 283.15 to 353.15 K. To achieve the last of these requirements, the volume of the dilatometer (up to the reference mark of 7.50 ml on the scale of the burette) at a reference temperature of $T_{ref} = 293.15$ K was chosen to be $V_{ref@T_{ref}} \approx 225$ ml (the actual value of this reference volume of the dilatometer is given in Subsection 2.5 and was determined using a calibration procedure described in the Supporting Information portion of this paper) using the following rationale: when this dilatometer is filled with 225 ml of water at 293.15 K, then an increase of about 7 ml in the volume of this water is obtained when its temperature is changed from 283.15 to 358.15 K (which corresponds to the lower limit and 5 K above the upper limit, respectively, of the temperature range of interest). A support structure facilitated the immersion of the dilatometer into (and its removal from) a specially designed and constructed cylindrical acrylic water-tower that was connected to a refrigerated/recirculating constant-temperature bath

(Neslab RTE 211; temperature stability \pm 0.01 K). This water-tower allowed the dilatometer and its contents to be maintained at the various desired temperatures in the range 283.15 to 353.15 K during the density measurements (procedure described in Subsection 2.4).



Figure 1. Three sections of the dilatometer: main body, filling section, and a portion of the measurement section.



Figure 2. Full measurement section of the dilatometer.

2.3 Procedure for Preparation of the Aqueous Solutions of the Alcohols

The water used in this study was degassed by boiling it for 30 mins^{54,55} and then immediately poured into glass storage bottles (previously cleaned and dried) such that when capped, no air gap was present above the liquid level inside the bottle. Each solution was prepared to the desired alcohol concentration (by weight) using a Sartorius BP 210 S analytical laboratory balance (readability: 0.1 mg) just prior to filling the dilatometer and performing density measurements. Details of the calculation of the alcohol concentrations are provided in the Supporting Information portion of the paper. These solutions were prepared in custom-blown glass bottles and thoroughly mixed for 45 minutes using a magnetic stirrer. The air that could be dissolved in the solution during this mixing process was then expelled by placing the closed bottles in an ultrasonic water-bath for about 10 seconds just prior to pouring the solution into the dilatometer.

2.4 Procedure for Determining Density

Prior to filling any of the liquids of interest (water and the dilute aqueous alcohol solutions) in the dilatometer, it was fully assembled and its empty mass ($m_{emptydilatometer}$) was measured using a Sartorius Practum1102-1S laboratory balance (readability: 0.01 g). The dilatometer was then filled with approximately 225 ml of liquid and the mass of the filled dilatometer was measured on the same balance ($m_{filled dilatometer}$). These measurements were used to determine the mass of the liquid in the filled dilatometer ($m_{liquid} = m_{filled dilatometer} - m_{emptydilatometer}$). To prevent evaporation of the liquid in the dilatometer during measurements for the determination of density at the temperatures of interest, about 0.2 ml of Edwards Ultra Grade 19 vacuum-pump oil was added (with a dropper) on top of the surface of the liquid within the burette (which would otherwise be exposed to the ambient air). The Edwards Ultra Grade 19 oil is primarily mineral oil ($w_{mineral oil} = 0.98 \text{ kg} \cdot \text{kg}^{-1}$); which is insoluble in water, ethanol⁵⁶, and 1-butanol⁵⁶. Although it is soluble in 1-pentanol⁵⁶, this solubility had no noticeable effects on the density measurements, given the low concentrations of 1-pentanol in the dilute aqueous solutions used in this work and the 5 mm diameter bore of the burette used to construct the measurement section of the dilatometer (total volume of the liquids in dilatometer is about 225 ml). As this oil was less dense than the liquids of interest (specific gravity: 0.86 at 15 °C; see Supporting Information for additional specifications), it remained on the top of the surface of the liquid in the burette. It also did not react with the water or the dilute aqueous alcohol solutions investigated in this work, and the liquid-oil interface in the burette remained sharp and clear throughout the measurements.

After filling the dilatometer and adding the oil layer, it was placed in an acrylic water-tower such that the entire scale on the burette was fully submerged (with only a small portion of the burette above the water level in the tower). The water-tower was connected to a refrigerated/recirculating constant-temperature bath (Neslab RTE-211; temperature stability of \pm 0.01 K) via a closed water circuit. For each temperature setpoint, two hours were allotted for the filled dilatometer to reach thermal equilibrium with the water in the tower (this two-hour time period was determined to be sufficient in preliminary experiments). The temperature of the filled dilatometer was determined using measurements from 10 calibrated Type-E thermocouples placed inside the water-tower (combined standard uncertainty: 0.06 K). The ambient pressure was determined using a mercury-in-glass barometer (NovaLynx model 230-7410; standard uncertainty of 30 Pa). The measured pressures were all approximately one standard atmosphere (*P* = 101.3 kPa; combined standard uncertainty of $u_c(P) = 1$ kPa). In the temperature range

considered in this work (283.15 to 353.15 K), changes in pressure of \pm 1 kPa (or less) about one standard atmosphere have effectively no influence on the density of dilute aqueous solutions of 1-butanol and 1-pentanol.

The values of volume indicated by the scale of the burette used in the construction of the measurement section of the dilatometer were calibrated at a temperature of 293.15 K, which was therefore chosen to be the reference temperature (T_{ref}) for measurements herein. The 7.50 ml subdivision on the scale of the burette (above the 8.00 ml mark where it was cut and fused to the male portion of a Rodaviss joint) was taken as the volume-reference mark for the dilatometer: the corresponding *total* volume of the dilatometer at the reference temperature is denoted as $V_{ref@T_{ref}}$; the value of $V_{ref@T_{ref}}$ was determined using a special calibration procedure. A note on this calibration procedure is provided in the next subsection, and it is described in detail in the Supporting Information portion of this paper.

For any particular run, the absolute temperature of the dilatometer is denoted by T; the *apparent* volume of the liquid *in the burette of the dilatometer <u>above</u> its volume-reference mark* (obtained using the scale on the burette which corresponds to $T_{ref} = 293.15$ K) is denoted by $\Delta V_{B@T_{ref}}$ (its value would be negative if the level of the liquid in the burette were <u>below</u> the volume-reference mark); and m_{liquid} is used to denote the total mass of the liquid in the dilatometer. Compensating for the thermal volumetric expansion of the borosilicate glass of which the dilatometer is primarily made, the actual total volume of the liquid in the dilatometer and the density of this liquid are given by the following two equations:

$$V = \left[V_{ref @ T_{ref}} + \Delta V_{B @ T_{ref}} \right] \left[1 + \beta \left(T - T_{ref} \right) \right]$$
(1)

$$\rho = m_{liquid} / V \tag{2}$$

In Eq. (1), $\beta = 9.75 \cdot 10^{-6} \text{ K}^{-1}$, is the thermal volumetric expansion coefficient for borosilicate glass (Type I, Class A, low-expansion borosilicate glass) which is three times the value of its linear thermal expansion coefficient, $\beta_{linear} = 3.25 \cdot 10^{-6} \text{ K}^{-1}$, as reported in the ASTM E-438 standard⁵⁷ for temperatures in the range 273.15 to 573.15 K.

Following the practices outlined in Refs. 58 and 59, it was estimated that the density of the liquids of interest determined using this procedure has an expanded uncertainty, $U(\rho)$, of 0.2 kg·m⁻³ (for a level of confidence of 0.95; coverage factor, k = 2). Details of the uncertainty analysis are provided in the Supporting Information portion of this paper.

2.5 Calibration of the Dilatometer

The dilatometer was calibrated using purified all-glass-distilled water (see Table 1 for additional details) to determine the reference volume of the dilatometer, $V_{ref@T_{ref}}$, at the chosen reference temperature, $T_{ref} = 293.15$ K. Details of the procedure for calibrating the dilatometer are presented in the Supporting Information portion of this paper. After performing several calibration runs, the value of the reference volume of the dilatometer at $T_{ref} = 293.15$ K was determined to be $V_{ref@T_{ref}} = 224.40$ ml.

3. Results and Discussion

In this section, first, the benchmarking measurements with water and two aqueous ethanol solutions are presented. After that, the values of density obtained for dilute aqueous solutions of 1-butanol and 1-pentanol are presented.

The difference between a value determined experimentally in this work, X, and the corresponding reference value, X_{ref} , obtained from the National Institute of Standards and Technology (NIST) or some other suitable published data was calculated as follows:

$$\Delta X = X - X_{ref} \tag{3}$$

The average absolute difference, $|\Delta X|_{avg}$, the maximum absolute difference, $|\Delta X|_{max}$, the absolute relative error, $|e_{ref}|_{avg}$, and the average absolute relative error, $|e_{ref}|_{avg}$, for N values of ΔX were calculated as follows:

$$\left|\Delta X\right|_{avg} = \sum_{i}^{N} \left|\Delta X_{i}\right| / N \tag{4}$$

$$\left|\Delta X\right|_{\max} = \max\left(\left|\Delta X_{i}\right|\right) \tag{5}$$

$$\left|e_{ref}\right| = \left|\Delta X / X_{ref}\right| \tag{6}$$

$$\left|e_{ref}\right|_{avg} = \sum_{i}^{N} \left|e_{ref}\right|_{i} / N \tag{7}$$

3.1 Benchmarking Measurements

The dilatometer was benchmarked with water and aqueous solutions of ethanol at atmospheric pressure and temperatures ranging from 283.15 to 353.15 K.

Two sets of benchmarking runs were performed with water. The experimentally determined values of the density of water were compared to the corresponding NIST values obtained using REFPROP (V9.1).⁶⁰ The results are given in Table S2 of the Supporting Information portion of this paper. The relative uncertainty in the NIST values of the density of water at atmospheric pressure⁶¹ is $U_r(\rho_{H_{2}O,NIST})=1\cdot10^{-6}$; the stated uncertainty in Ref. 61 is assumed to be the expanded value for a level of confidence of 0.95 (k = 2). The differences ($\Delta \rho$) between the values of density determined in these benchmarking runs with water and the corresponding NIST values are presented graphically in Figure 3: the average of the absolute values of these differences is $|\Delta \rho|_{arg} = 0.03 \text{ kg} \cdot \text{m}^{-3}$; the maximum value of these absolute differences is $|\Delta \rho|_{arg} = 0.003\%$; and these differences are all within the expanded uncertainty of the dilatometer, $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$.



Figure 3. Differences (\bullet) between the values of density determined in benchmarking runs with water and the corresponding NIST (REFPROP V9.1)⁶⁰ values at atmospheric pressure and

temperatures in the range 283.15 to 353.15 K. Numerical values of the differences are given in Table S2 of the Supporting Information portion of this paper.

Additional benchmarking runs were performed with aqueous solutions of ethanol and the experimentally determined densities were compared to the corresponding NIST values obtained using REFPROP (V9.1).⁶⁰ These results are given in Tables S3 and S4 of the Supporting Information portion of this paper. The relative uncertainty in the NIST values of the density of aqueous solutions of ethanol, as stated in the works of Lemmon and Jacobsen⁶² and Schroeder⁶³, $U_r(\rho_{H_2O-ethanol,NIST}) = 0.002$, which gives an uncertainty approximately is of $U(\rho_{H_2O-ethanol,NIST}) = 2.0 \text{ kg} \cdot \text{m}^{-3}$; the stated uncertainties in Refs. 62 and 63 are assumed to be the expanded values for a level of confidence of 0.95 (k = 2). Two concentrations of ethanol were considered, 0.1091 and 1.142 mol·kg⁻¹ (ethanol mass fractions: 0.5% and 5%). The differences $(\Delta \rho)$ between the values of density of these two aqueous solutions of ethanol determined in these benchmarking runs and the corresponding NIST values are presented graphically in Figure 4: the average of the absolute values of these differences ($|\Delta \rho|_{avg}$) are 0.17 kg·m⁻³ and 0.49 kg·m⁻³; the maximum values of these absolute differences ($|\Delta \rho|_{max}$) are 0.77 kg·m⁻³ and 1.04 kg·m-3; and the average absolute relative errors (expressed here as percentage values) are $|e_{ref}|_{avg} = 0.02\%$ and 0.05%, for the 0.1091 mol·kg⁻¹ and 1.142 mol·kg⁻¹ solutions, respectively. Some of these differences are larger than the expanded uncertainty of the dilatometer, $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$; however, they (the differences) are considered to be satisfactory as they fall well within the expanded uncertainty of the corresponding NIST values.



Figure 4. Differences between the values of density determined in the benchmarking runs with two aqueous solutions of ethanol, $m_2 = 0.1091$ (**I**) and 1.142 (**A**) mol·kg⁻¹, and the corresponding NIST values (REFPROP V9.1)⁶⁰ values at atmospheric pressure and temperatures in the range 283.15 to 353.15 K. Numerical values of the differences are given in Tables S3 and S4 of the Supporting Information portion of this paper.

3.2 Density of Dilute Aqueous Solutions of 1-Butanol and 1-Pentanol

The values of density (ρ) of the dilute aqueous solutions of 1-butanol and 1-pentanol for the concentration and temperature ranges of interest were determined using the procedure described in Subsection 2.4 and are presented in Tables 2 and 3, respectively. Only for comparison purposes, the differences between these values of density and the corresponding values for pure water (denoted as $\Delta \rho_{H_2O}$) and the values calculated invoking the ideal-solution assumption (denoted as $\Delta \rho_{ideal}$) are also presented in Tables 2 and 3. To facilitate the comparison of these results with similar results in the published literature, the values of the alcohol concentration are given in Tables 2 and 3 in terms of molality (m_2), mole fraction (x_2), and percentage mass

fraction (w_2) . The corresponding ideal-solution values of the density were calculated (again, only for comparison purposes) assuming that the total volume of the solution is equal to the sum of the volumes of each component of the solution, water (1) and alcohol (2) here, as follows:

$$\rho_{ideal} = \frac{\sum x_i M_i}{\sum \frac{x_i M_i}{\rho_i}} = \frac{x_1 M_1 + x_2 M_2}{\frac{x_1 M_1}{\rho_1} + \frac{x_2 M_2}{\rho_2}}$$
(8)

where, x_i and M_i are the mole fraction and molar mass of each component, respectively. For each case, the densities of the water and alcohol were calculated at the same temperature and pressure (atmospheric) as the experimentally determined densities in this work. For the density of water, the NIST values calculated with REFPROP (V9.1)⁶⁰ were used; the relative uncertainty in these NIST values⁶¹ is $U_r(\rho_{H_{20},NIST}) = 1 \cdot 10^{-6}$. The density values for the alcohols were calculated from empirical correlations given in Frenkel et al.⁶⁴, who stated that the uncertainties for the densities of 1-butanol (p.26 of Ref. 64) and 1-pentanol (p.48 of Ref. 64) were $3.5754 \cdot 10^{-1}$ kg·m⁻³ and $7.5696 \cdot 10^{-1}$ kg·m⁻³, respectively, which were taken as the standard deviations of the difference between their calculated values and selected literature values.

Table 2. Density of dilute solutions of water (1) and 1-butanol (2) at atmospheric pressure (P = 101.3 kPa) and various values of temperatures (T) and alcohol concentration (values expressed in terms of molality, m_2 ; mole fraction, x_2 ; and percentage mass fraction, w_2): values determined experimentally in this work (ρ) ; the differences between these values and the corresponding values for pure water $(\Delta \rho_{H_2O})$ and the values calculated invoking the ideal-solution assumption $(\Delta \rho_{ideal})^a$

T/K	$m_2/\mathrm{mol}\cdot\mathrm{kg}^{-1}$	<i>x</i> ₂	w ₂ /%	$ ho/\mathrm{kg}\cdot\mathrm{m}^{-3}$	$\Delta ho_{H_2O}/\mathrm{kg}\cdot\mathrm{m}^{-3}$	$\Delta ho_{ideal}/{ m kg} \cdot { m m}^{-3}$
283.17	0.06780	0.001220	0.500	999.12	-0.59	0.53
293.14	0.06780	0.001220	0.500	997.59	-0.62	0.55
303.18	0.06780	0.001220	0.500	994.97	-0.67	0.53
313.14	0.06780	0.001220	0.500	991.52	-0.70	0.54
323.19	0.06780	0.001220	0.500	987.27	-0.75	0.52
333.18	0.06780	0.001220	0.500	982.45	-0.73	0.57
343.20	0.06780	0.001220	0.500	977.04	-0.70	0.62
353.17	0.06780	0.001220	0.500	971.01	-0.77	0.57
283.16	0.2055	0.003688	1.500	997.51	-2.19	1.15
293.14	0.2055	0.003688	1.500	995.95	-2.26	1.22
303.15	0.2055	0.003688	1.500	993.29	-2.36	1.23
313.14	0.2055	0.003688	1.500	989.72	-2.50	1.20
323.18	0.2055	0.003688	1.500	985.35	-2.67	1.12
333.16	0.2055	0.003688	1.500	980.59	-2.60	1.27
343.19	0.2055	0.003688	1.500	975.24	-2.51	1.44
353.16	0.2055	0.003688	1.500	969.01	-2.77	1.25
283.12	0.7101	0.01263	5.000	992.78	-6.93	4.11
293.12	0.7101	0.01263	5.000	990.82	-7.39	4.10
303.18	0.7101	0.01263	5.000	987.86	-7.78	4.10
313.18	0.7101	0.01263	5.000	984.05	-8.16	4.06
323.18	0.7101	0.01263	5.000	979.44	-8.58	3.94
333.15	0.7101	0.01263	5.000	974.41	-8.79	4.00
343.17	0.7101	0.01263	5.000	968.88	-8.88	4.16
353.15	0.7101	0.01263	5.000	962.74	-9.05	4.21
^a Combine	ed standard unce	rtainties: $u_c(H)$	P) = 1 kPa	$u_c(T) = 0.00$	6 K.	L

Relative combined standard uncertainties: $u_r(m_2, x_2, w_2) = 0.001$. Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).

Table 3. Density of dilute solutions of water (1) and 1-pentanol (2) at atmospheric pressure (P = 101.3 kPa) and various values of temperatures (T) and alcohol concentration (values expressed in terms of molality, m_2 ; mole fraction, x_2 , and percentage mass fraction, w_2): values determined experimentally in this work (ρ) ; the differences between these values and the corresponding values for pure water $(\Delta \rho_{H_2O})$ and the values calculated invoking the ideal-solution assumption $(\Delta \rho_{ideal})^a$

T/K	$m_2/\mathrm{mol}\cdot\mathrm{kg}^{-1}$	<i>x</i> ₂	w ₂ /%	$ ho/\mathrm{kg}\cdot\mathrm{m}^{-3}$	$\Delta ho_{H_2O}/\mathrm{kg}\cdot\mathrm{m}^{-3}$	$\Delta ho_{ideal}/\mathrm{kg}\cdot\mathrm{m}^{-3}$
283.18	0.005675 ^b	0.0001022 ^b	0.050 ^b	999.65	-0.05	0.06
293.14	0.005675 ^b	0.0001022 ^b	0.050 ^b	998.13	-0.08	0.03
303.18	0.005675 ^b	0.0001022 ^b	0.050 ^b	995.55	-0.09	0.03
313.16	0.005675 ^b	0.0001022 ^b	0.050 ^b	992.15	-0.06	0.06
323.19	0.005675 ^b	0.0001022 ^b	0.050 ^b	987.94	-0.08	0.05
333.17	0.005675 ^b	0.0001022 ^b	0.050 ^b	983.25	0.07	0.19
343.18	0.005675 ^b	0.0001022 ^b	0.050 ^b	977.67	-0.08	0.05
353.20	0.005675 ^b	0.0001022 ^b	0.050 ^b	971.85	0.09	0.22
283.15	0.01704	0.0003069	0.150	999.61	-0.10	0.23
293.14	0.01704	0.0003069	0.150	998.04	-0.17	0.17
303.18	0.01704	0.0003069	0.150	995.46	-0.18	0.17
313.16	0.01704	0.0003069	0.150	992.06	-0.16	0.20
323.19	0.01704	0.0003069	0.150	987.81	-0.21	0.15
333.19	0.01704	0.0003069	0.150	982.51	-0.67	-0.29

343.23	0.01704	0.0003069	0.150	977.61	-0.11	0.27			
353.20	0.01704	0.0003069	0.150	971.75	-0.01	0.38			
283.16	0.05701	0.001026	0.500	999.12	-0.59	0.49			
293.14	0.05701	0.001026	0.500	997.51	-0.70	0.42			
303.19	0.05701	0.001026	0.500	994.93	-0.71	0.45			
313.16	0.05701	0.001026	0.500	991.48	-0.73	0.46			
323.19	0.05701	0.001026	0.500	987.23	-0.79	0.43			
333.19	0.05701	0.001026	0.500	982.50	-0.68	0.57			
343.21	0.05701	0.001026	0.500	977.17	-0.56	0.71			
353.19	0.05701	0.001026	0.500	971.18	-0.58	0.71			
^a Combine	ed standard unce	rtainties: $u_c(F)$	$\mathbf{r}) = 1 \text{ kPa}$	$u_c(T) = 0.00$	6 K.				
Relative combined standard uncertainties: $u_r(m_2, x_2, w_2) = 0.001$.									
Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).									
^b Relative	combined stand	ard uncertainti	les: $u_r(m_2$	$(x_2, w_2) = 0.00$)3.				

The values of $\Delta \rho_{H_2O}$ given in Tables 2 and 3 show that the density of the dilute aqueous solutions is overpredicted in almost all of the cases considered here if it is assumed to be the same as the density of pure water at the same temperature (as indicated by the negative values of $\Delta \rho_{H_2O}$). This finding confirms what was expected, as the densities of the alcohols considered here are lower than that of water. The only two positive values of $\Delta \rho_{H_2O}$ reported in Table 3 correspond to the lowest concentration of 1-pentanol investigated, and these two positive values are within the expanded uncertainty of the measurements. The values of $\Delta \rho_{ideal}$ given in Tables 2 and 3 generally show that the ideal-solution assumption underpredicts the density of the dilute aqueous solutions of the alcohols considered here (as indicated by the positive values of $\Delta \rho_{ideal}$).

The averages of the absolute values of $\Delta \rho_{H_2O}$ and $\Delta \rho_{ideal}$ in Tables 2 and 3 ($|\Delta \rho_{H_2O}|_{avg}$ and $|\Delta \rho_{ideal}|_{avg}$) over all values of the temperature considered for each of the concentrations of 1-butanol and 1-pentanol investigated here are presented graphically in Figure 5; and these results for values of alcohol concentration less than 0.08 mol·kg⁻¹ are presented graphically with an expanded concentration scale in Figure 6. The results presented in Figure 5 demonstrate that calculating the density of the dilute aqueous alcohols considered herein using the ideal-solution assumption is better than assuming that it is the same as the density of pure water at the same temperature. However, both these assumptions become progressively more inaccurate with increasing values of alcohol concentration. The results presented in Figure 6 demonstrate that for alcohol concentrations less than 0.01 mol·kg⁻¹ for aqueous solutions of 1-butanol and 1-pentanol, the values of both $|\Delta \rho_{H_2O}|_{avg}$ and $|\Delta \rho_{ideal}|_{avg}$ are within the expanded uncertainty of the dilatometer measurements, $U(\rho) = 0.2 \text{ kg·m}^{-3}$; however, this condition is not met for alcohol concentrations greater than about 0.02 mol·kg⁻¹.



Figure 5. Values of $|\Delta \rho_{H_2O}|_{avg,l-butanol}$ (O), $|\Delta \rho_{ideal}|_{avg,l-butanol}$ (X), $|\Delta \rho_{H_2O}|_{avg,l-pentanol}$ (D), and $|\Delta \rho_{ideal}|_{avg,l-pentanol}$ (+) over all values of the temperature (in the range of interest) for each of the values of alcohol concentration of the dilute aqueous solutions of 1-butanol and 1-pentanol investigated here.



Figure 6. Values of $|\Delta \rho_{H_2O}|_{avg,I-butanol}$ (O), $|\Delta \rho_{ideal}|_{avg,I-butanol}$ (X), $|\Delta \rho_{H_2O}|_{avg,I-pentanol}$ (D), and $|\Delta \rho_{ideal}|_{avg,I-pentanol}$ (+) over all values of the temperature (in the range of interest) and values of alcohol concentration less than 0.08 mol·kg⁻¹ for the dilute aqueous solutions of 1-butanol and 1-pentanol investigated here (presented data is the same as in Figure 5; but with an expanded concentration scale). For comparative purposes, the value of $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ is also included and denoted by the dashed line (---).

Where possible, the experimentally determined density values presented in Tables 2 and 3 were also compared to corresponding values available in the published literature (at equivalent or

similar concentrations) for temperatures in the range 283.15 to 323.15 K. Note that the authors could not find any comparable literature data at temperatures greater than 323.15 K. These comparisons are given in Tables S5 to S9 of the Supporting Information portion of this paper; and the interpolated values of density at 298.15 K are given in Tables S10 and S11. The average of the absolute differences between the experimentally determined values of density and the corresponding values in the published literature is 0.12 kg·m-3; this value is well within the expanded uncertainty of the density values determined using the dilatometer measurements, $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (for a level of confidence of 0.95; coverage factor, k = 2). The average of the absolute relative error $(|e_{ref}|_{avg})$ with reference to the literature values (expressed as a percentage value) is 0.01%. These favorable comparisons and the results of the benchmarking runs discussed in Subsection 3.1 (given in Tables S2 - S4 of the Supporting Information portion of this paper) demonstrate that the specially-designed and custom-made dilatometer used in this work is an accurate device for the determination of the density of dilute aqueous solutions of alcohol at atmospheric pressure and the concentration and temperature ranges of interest. In addition, they show that the proposed technique of adding a thin layer of oil on top of the liquid surface in the burette of the measuring section is a simple and very effective way of preventing evaporation of the liquid.

4. Concluding Remarks

The densities of dilute aqueous solutions of 1-butanol and 1-pentanol at atmospheric pressure and temperatures in range of 283.15 to 353.15 K were determined in this work using a specially designed and custom-made dilatometer, after it was calibrated and benchmarked. This dilatometer was made primarily of borosilicate glass, and its thermal volumetric expansion was accounted for in the proposed procedure for determining the density of the liquids of interest. A simple technique, of adding a small amount of a suitable oil (about 0.2 ml of Edwards Ultra Grade 19 vacuum-pump oil) on top of the liquid surface in the burette of the measuring section, was proposed for preventing evaporative losses from the dilatometer and found to be very effective.

The experimentally determined densities of aqueous solutions of 1-butanol, for concentrations of approximately 0.07 to 0.7 mol·kg⁻¹, were presented in Table 2; and those of aqueous solutions of 1-pentanol, for concentrations of approximately 0.006 to 0.06 mol·kg⁻¹, were given in Table 3. These results compare very well with corresponding values in the literature for temperatures in the range 283.15 to 323.15 K. These favorable comparisons, along with the successful benchmarking runs presented and discussed in Section 3.1, confirm that the custom-built dilatometer and the proposed experimental procedures provide a low-cost and accurate option for determining the density of dilute aqueous alcohol solutions.

The results presented in this paper also show the following features for the dilute aqueous solutions of alcohols considered in this work: 1) in general, the values of the density are overpredicted if they are assumed to be those of pure water at the same temperature, and the ideal-solution assumption leads to an underprediction of these values; 2) for alcohol concentrations less than 0.01 mol·kg⁻¹, both of the aforementioned assumptions yield values of the densities that lie within the uncertainty of the present experimental measurements; and 3) at alcohol concentrations of about 0.02 mol·kg⁻¹ and higher, the aforementioned assumptions should <u>not</u> be used, as they yield values of density that become increasingly inaccurate compared

to the values determined experimentally in this work (with the differences exceeding the expanded uncertainty of the present results).

The density data presented in Tables 2 and 3 complement and extend those available in the published literature, with the most significant contribution being the data at temperatures in the range 323.15 to 353.15 K and at concentrations $\geq 0.02 \text{ mol} \cdot \text{kg}^{-1}$. Such data would be especially useful as inputs to mathematical models of heat pipes and vapor-chamber spreaders¹⁻⁷: dilute aqueous solutions of long-chain alcohols such as 1-butanol and 1-pentanol are of interest as working fluids in these high-heat-flux passive thermal-management devices as they exhibit a positive gradient of surface tension with temperature (at about 313.15 K and higher; depending on the alcohol), which enhances the return of the liquid phase from the cooled to the heated sections.⁵⁻⁷ The presented data would also be useful in surface-tension measuring methods (such as the pendant-drop and the maximum-bubble-pressure methods) in which a knowledge of the density of the fluid is required.¹³ If desired, a suitable curve-fit to the density data presented herein could be used to calculate the thermal coefficient of volumetric expansion. The presented data could also be used in conjunction with other similar data reported in the literature (for enhancing the accuracy of the curve-fits by increasing the number of concentrations beyond those considered in this paper) to extrapolate the properties of such solutions (for example, the apparent molar volume) to infinite dilution.

Associated Content

Supporting Information

Notes on calculations of initial mole fraction purity, alcohol concentration, uncertainty analyses, vacuum-pump oil specifications, and the procedure used for calibrating the dilatometer; benchmarking data; and comparisons of experimentally determined density values with available literature values at equivalent or similar concentrations.

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Author Contributions

The experiments were performed and data were collected and analyzed by James I. Medvescek as part of his Ph.D. studies under the supervision of Professors Laurent Mydlarski and Bantwal R. (Rabi) Baliga. The manuscript was primarily written by James I. Medvescek with inputs from both Professors Laurent Mydlarski and Bantwal R. (Rabi) Baliga. All authors have approved the final version of the manuscript.

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SUPPORTING INFORMATION

Densities of dilute aqueous solutions of 1-butanol and 1-pentanol at atmospheric pressure and temperatures in the range 283.15 to 353.15 K

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Calculation of the Initial Mole Fraction Purity of Ethanol

A certificate of analysis of the ethanol used in this work was provided by the supplier, Commercial Alcohols by Greenfield Global. The initial volume fraction purity $(\phi_{purity,ethanol} = V_{ethanol}/V_{total})$ of the ethanol was determined to be 0.9998 m³·m⁻³ and the relative density of the ethanol with respect to water at 20 °C ($\rho_r = \rho_{total}/\rho_{H_2O,NIST,20^\circ C}$) was 0.7908, as measured with a digital density meter. With these two values, the initial mass fraction purity of the ethanol ($w_{purity,ethanol}$) was calculated using Eq. (S1) and the NIST values, obtained using REFPROP (V9.1)¹, of the density of water and ethanol at 20 °C ($\rho_{H_2O,NIST,20^\circ C} = 998.21$ kg·m⁻³ and $\rho_{ethanol,NIST,20^\circ C} = 789.42$ kg·m⁻³).

$$w_{purity,ethanol} = \frac{m_{ethanol}}{m_{total}} = \frac{V_{ethanol} \times \rho_{ethanol,NIST,20^{\circ}C}}{V_{total} \times \rho_{total}}$$

$$= \frac{\phi_{purity,ethanol} \times \rho_{ethanol,NIST,20^{\circ}C}}{\rho_r \times \rho_{H_2O,NIST,20^{\circ}C}} = 0.9998 / \text{kg} \cdot \text{kg}^{-1}$$
(S1)

With the value of the initial mass fraction purity of ethanol ($w_{purity,ethanol}$) and assuming the only impurity present in the ethanol is water, the initial mole fraction purity of the ethanol

 $(x_{purity,ethanol})$ can be calculated using Eq. (S2) and the molar masses of ethanol and water $(M_{ethanol})$ and $M_{H_{2}O}$ that are presented in Table 1 of the paper.

$$x_{purity,ethanol} = \frac{w_{purity,ethanol} / M_{ethanol}}{w_{purity,ethanol} / M_{ethanol} + (1 - w_{purity,ethanol}) / M_{H_2O}} = 0.9995 / \text{mol} \cdot \text{mol}^{-1}$$
(S2)

Calculation of Alcohol Concentration

The alcohol solutions were prepared to the desired concentration (by weight) using a Sartorius BP 210 S analytical laboratory balance. Aqueous solutions were prepared in custom-blown glass bottles with an internal volume of approximately 165 ml. Custom bottles were made such that the mass of the bottle was minimized (approximately 50 g), as compared to commercially available glass bottles, to maximize the amount (mass) of the solution that could be prepared while using the 210 g analytical balance. The approximate total mass of a prepared solution ($m_{total} = m_{H_2O} + m_{alcohol}$) is 130 g; where m_{H_2O} and $m_{alcohol}$, are the masses of the water and the alcohol, respectively. The alcohol concentration, expressed in terms of molality (m_2), mole fraction (x_2), and mass fraction (w_2), can be calculated using the following equations:

$$m_2 = \frac{n_{alcohol}}{m_{H_2O}} = \frac{m_{alcohol}/M_{alcohol}}{m_{H_2O}}$$
(S3)

$$x_{2} = \frac{n_{alcohol}}{n_{total}} = \frac{n_{alcohol}}{n_{H_{2}O} + n_{alcohol}} = \frac{m_{alcohol}/M_{alcohol}}{m_{H_{2}O}/M_{H_{2}O} + m_{alcohol}/M_{alcohol}}$$
(S4)

$$w_2 = \frac{m_{alcohol}}{m_{total}} = \frac{m_{alcohol}}{m_{H_2O} + m_{alcohol}}$$
(S5)

where, n and M, are the number of moles and the molar mass, respectively. The molar masses of the alcohols and water are presented in Table 1 of the paper.

Concentration Uncertainty Analyses and Contributions to the Uncertainties in the Experimentally Determined Values of Density

Noting that the uncertainties associated with the mass of the water, total number of moles, and total mass (denominators of Eqs. (S3)-(S5)) are negligible compared to the uncertainty in the mass of the alcohol ($m_{alcohol}$, the numerators of the same equations), the relative combined standard uncertainty of the alcohol concentrations can be calculated using the following equation:

$$u_r(m_2) = u_r(x_2) = u_r(w_2) = \frac{u_c(m_{alcohol})}{m_{alcohol}}$$
(S6)

The combined standard uncertainty of the mass of the alcohol, $u_c(m_{alcohol})$, can be calculated as follows:

$$u_{c}(m_{alcohol}) = \sqrt{u_{c}(balance_{210g})^{2} + u(purity)^{2}}$$

$$= \sqrt{\left[0.0002\right]^{2} + \left[\left(1 - x_{purity, alcohol}\right)m_{alcohol}\right]^{2}}$$
(S7)

where, $u_c(balance_{210g})$ and $(1-x_{purity,alcohol})$, are the combined standard uncertainty of the mass measured by the 210 g analytical balance (estimated to be 0.2 mg; accounting for readability, repeatability and linearity) and the relative standard uncertainty of the purity of the alcohol. The initial mole fraction purities ($x_{purity,alcohol}$) are presented in Table 1 of the paper. The relative combined standard uncertainty of the alcohol concentrations is $u_r(m_2, x_2, w_2) = 6 \cdot 10^{-4}$ for the 0.1091 mol·kg⁻¹ aqueous solution of ethanol; 0.003 for the 0.005675 mol·kg⁻¹ aqueous solution of 1-pentanol; and $5 \cdot 10^{-4}$, 0.001, and 0.001 for the other aqueous solutions of ethanol, 1-butanol, and 1-pentanol, respectively. The maximum uncertainty of the values of density reported in this work, $u(\rho_{x_2})_{max}$, resulting from the relative combined standard uncertainty of the alcohol concentration can be calculated using the following equation:

$$u(\rho_{x_2})_{\max} = \left| \partial \rho / \partial x_2 \right|_{\max} \cdot u_r(x_2) \cdot x_{2,\max}$$
(S8)

where $|\partial \rho / \partial x_2|_{\text{max}}$ and $x_{2,\text{max}}$ are the maximum absolute value of the density gradient with concentration and the maximum alcohol concentration (both in terms of mole fraction) for each alcohol. The values of density were plotted as a function of the alcohol mole fraction (x_2) for each of the alcohols (ethanol, 1-butanol, and 1-pentanol) and at each nominal temperature investigated in the range of 283.15 to 353.15 K. To obtain an order of magnitude approximation of the density gradient with concentration, linear least squares curve-fits were applied at each nominal temperature and the maximum absolute value of the slopes from these curve-fits was taken to be $|\partial \rho / \partial x_2|_{\text{max}}$. The maximum absolute value of the density gradient with respect to concentration was found to be approximately 500, 700, and 800 kg·m⁻³·mol·mol⁻¹ for the aqueous solutions of ethanol, 1-butanol, and 1-pentanol, respectively.

The values of the maximum uncertainty in the density of the solution calculated using Eq. (S8) were found to be 0.005, 0.009, and $8 \cdot 10^{-4}$ kg·m⁻³ for the aqueous solutions of ethanol, 1-butanol, and 1-pentanol, respectively. These values are negligible in comparison to the expanded uncertainty of the density values determined using the dilatometer measurements, $U(\rho) = 0.2$ kg·m⁻³ (for a level of confidence of 0.95; coverage factor, k = 2).

Vacuum-Pump Oil Specifications

Vapour pressure at 20 °C /mbar	1.0.10-8
Vapour pressure at 100 °C /mbar	1.0.10-3
Molecular weight /g·mol ⁻¹	420
Specific gravity at 15°C	0.86
Viscosity at 20 °C /cSt	143.7
Viscosity at 40 °C /cSt	48.6
Pour point /°C	-16
Flash point /°C	230
Auto ignition point /°C	355
Sulphur content w_{sulfur} /kg·kg ⁻¹	0
Mineral oil content $w_{mineral oil}$ /kg·kg ⁻¹	0.98

 Table S1. Specifications of the Edwards Ultra Grade 19 Vacuum-Pump Oil

Procedure for Calibrating the Dilatometer

The dilatometer was calibrated using purified all-glass-distilled water (see Table 1 of the paper for additional details). The purpose of this calibration was to determine the reference volume of the dilatometer, $V_{ref@T_{ref}}$, at the chosen reference temperature, $T_{ref} = 293.15$ K. For each calibration run, the procedure used consisted of the following steps: 1) the mass of the empty dilatometer, $m_{empty dilatometer}$, was measured and recorded; 2) the dilatometer was filled with water to a desired level in the burette (either below, at, or above the reference mark); 3) the mass of the filled dilatometer, $m_{filled dilatometer}$, was measured and recorded; 4) the mass of the water in the filled dilatometer was determined ($m_{H_2O} = m_{filled \, dilatometer} - m_{empty \, dilatometer}$); 5) a small oil layer was added to the exposed surface of the water in the burette; 6) the dilatometer was placed within the water-tower and, to compensate for the heat losses to (or gains from) the ambient air, the constant-temperature bath (that circulates the water through the water-tower) was set to a temperature just above (or below) the desired dilatometer temperature of 293.15 K; 7) two hours were allowed to elapse to let the filled dilatometer come to thermal equilibrium with the water in the water-tower; 8) the actual temperature, T, of the dilatometer was recorded; 9) using the scale on the burette (which corresponds to $T_{ref} = 293.15$ K), the *apparent* volume of the water *in the* burette of the dilatometer <u>above</u> the chosen volume-reference mark, $\Delta V_{B@T_{ref}}$, was obtained and recorded (a negative value of $\Delta V_{B@T_{ref}}$ would be obtained if the level of the liquid in the burette were <u>below</u> the volume-reference mark); and 10) the NIST value of the density of water at atmospheric pressure and the measured temperature T, $\rho_{H,O@T,NIST}$, was obtained using the computer program REFPROP (V9.1).¹ For the purposes of this calibration, the total volume of water within the dilatometer at the temperature *T*, denoted as $V_{H_2O@T}$, was calculated using the following equation:

$$V_{H_2O@T} = \frac{m_{H_2O}}{\rho_{H_2O@T,NIST}}$$
(S9)

With this calculated volume of water, the thermal volumetric expansion coefficient β for borosilicate glass, and the values of T and $\Delta V_{B@T_{ref}}$, the value of $V_{ref@T_{ref}}$ was obtained using the following equation:

$$V_{H_{2}O@T} = \left(V_{ref@T_{ref}} + \Delta V_{B@T_{ref}}\right) \left\{1 + \beta \left(T - T_{ref}\right)\right\}$$
or
$$V_{ref@T} = \frac{V_{H_{2}O@T}}{\left\{1 + \beta \left(T - T_{ref}\right)\right\}} - \Delta V_{B@T_{ref}}$$
(S10)

Note that the value of the term $\beta (T - T_{ref})$ in this equation would be negligible, as the maximum absolute difference between T and T_{ref} during all calibration runs was 0.05 K. It was nevertheless accounted for in Eq. (S10) for completeness.

Using this procedure, several calibration runs were performed with differing amounts of water added to the dilatometer to cover the full scale of the burette, and the corresponding values of $V_{ref@T_{ref}}$ were determined. The arithmetic mean of these values was taken to be the final value of the reference volume of the dilatometer at $T_{ref} = 293.15$ K: $V_{ref@T_{ref}} = 224.40$ ml.

Uncertainty Analyses of the Experimentally Determined Values of Density

The experimentally determined values of density presented in this work were determined using Eqs. (1) and (2) and following the procedures outlined in Section 2.4 of the paper. The combined

standard uncertainty in the density values, $u_c(\rho)$, can be calculated from the combined standard uncertainty of the mass of the liquid in the dilatometer, $u_c(m_{liquid})$, and the combined standard uncertainty of the volume of the liquid in the dilatometer, $u_c(V)$:

$$\frac{u_{c}(\rho)}{\rho} = \sqrt{\left[\frac{u_{c}(m_{liquid})}{m_{liquid}}\right]^{2} + \left[\frac{u_{c}(V)}{V}\right]^{2}}$$
(S11)

The mass of the liquid was measured using a Sartorius Practum1102-1S laboratory balance. The combined standard uncertainty in the mass measured by the 1100 g laboratory balance, $u_c(m_{liquid})$, is estimated to be the combination (addition in quadrature) of the readability (0.01 g), repeatability (0.01 g) and linearity of the Sartorius Practum1102-1S balance. Based on multiple measurements with known masses, the uncertainty in the linearity was negligible.

With reference to Eq. (1) in Section 2.4 of the paper, the combined standard uncertainty of the volume of the liquid in the dilatometer, $u_c(V)$, can be calculated as follows:

$$u_{c}(V) = \begin{cases} \left[\left(\frac{\partial V}{\partial V_{ref@T_{ref}}} \right) u_{c} \left(V_{ref@T_{ref}} \right) \right]^{2} \\ + \left[\left(\frac{\partial V}{\partial \Delta V_{B@T_{ref}}} \right) u \left(\Delta V_{B@T_{ref}} \right) \right]^{2} + \left[\left(\frac{\partial V}{\partial T} \right) u_{c}(T) \right]^{2} \end{cases} \end{cases}$$
(S12)

In Eq. (S12), $u_c \left(V_{ref @ T_{ref}} \right)$, $u \left(\Delta V_{B @ T_{ref}} \right)$, and $u_c (T)$ are the combined standard uncertainty in the reference volume of the dilatometer (determined later on in this section), the standard uncertainty in the apparent volume of the liquid in the burette above its volume-reference mark (0.01 ml; half of a burette subdivision), and the combined standard uncertainty in the temperature of the

dilatometer (0.06 K). The partial derivatives $\partial V / \partial V_{ref@T_{ref}}$, $\partial V / \partial \Delta V_{B@T_{ref}}$, and $\partial V / \partial T$ of Eq. (1) in Section 2.4 of the paper are determined as follows:

$$\frac{\partial V}{\partial V_{ref@T_{ref}}} = \frac{\partial V}{\partial \Delta V_{B@T_{ref}}} = 1 + \beta \left(T - T_{ref} \right) \approx 1$$
(S13)

$$\frac{\partial V}{\partial T} = \beta \left(V_{ref @ T_{ref}} + \Delta V_{B @ T_{ref}} \right)$$
(S14)

The term, $1 + \beta (T - T_{ref})$, is approximately equal to 1. Noting that the third term in Eq. (S12) is negligible compared to the first two terms, $u_c(V)$ can be determined from $u_c(V_{ref@T_{ref}})$ and $u(\Delta V_{B@T_{ref}})$:

$$u_{c}(V) = \sqrt{\left[u_{c}\left(V_{ref@T_{ref}}\right)\right]^{2} + \left[u\left(\Delta V_{B@T_{ref}}\right)\right]^{2}}$$
(S15)

The reference volume of the dilatometer was determined following the procedures outlined in the previous section. With reference to Eq. (S10), the combined standard uncertainty in this reference volume can be calculated as follows:

$$u_{c}\left(V_{ref@T_{ref}}\right) = \sqrt{\left[u_{c}\left(V_{H_{2}O@T}\right)\right]^{2} + \left[u\left(\Delta V_{B@T_{ref}}\right)\right]^{2} + \left[u\left(\overline{V}_{ref@T_{ref}}\right)\right]^{2}}$$
(S16)

In Eq. (S16), $u_c \left(V_{H_2O@T} \right)$ and $u \left(\overline{V}_{ref@T_{ref}} \right)$ are the standard combined uncertainty in the volume of water in the dilatometer during a calibration run and the standard uncertainty in the average reference volume of the dilatometer taken from the results of several independent calibrations. Referring to Eq. (S9), $u_c \left(V_{H_2O@T} \right)$ can be determined using the following equation:

$$\frac{u_{c}\left(V_{H_{2}O@T}\right)}{V_{H_{2}O@T}} = \sqrt{\left[\frac{u_{c}\left(m_{H_{2}O}\right)}{m_{H_{2}O}}\right]^{2} + \left[\frac{u_{c}\left(\rho_{H_{2}O@T,NIST}\right)}{\rho_{H_{2}O@T,NIST}}\right]^{2}}$$
(S17)

The mass of the water in the dilatometer was measured using the Sartorius Practum1102-1S balance, thus $u_c(m_{H_2O}) = 0.01$ g. Noting that the relative standard uncertainty in the NIST value of the density of water (the second term of Eq. (S17)) is negligible in comparison to the uncertainty in the mass of the water in the dilatometer:

$$u_{c}\left(V_{H_{2}O@T}\right) = \frac{u_{c}\left(m_{H_{2}O}\right)}{\rho_{H_{2}O@T,NIST}} = 0.01\,\mathrm{ml}$$
(S18)

The value of $u(\overline{V}_{ref@T_{ref}}) = SD_{\overline{V}_{ref@T_{ref}}} / \sqrt{N_{cal.}}$ was calculated to be 0.008 ml using the standard deviation, SD, of the reference volumes determined from the number of calibrations that were performed, $N_{cal.}$.

Substituting Eq. (S16) into Eq. (S15), and using the values of $u_c(V_{H_2O@T})$, $u(\Delta V_{B@T_{ref}})$, and $u(\overline{V}_{ref@T_{ref}})$, $u_c(V)$ can be calculated:

$$u_{c}(V) = \sqrt{\left[u_{c}(V_{H_{2}O@T})\right]^{2} + 2\left[u(\Delta V_{B@T_{ref}})\right]^{2} + \left[u(\overline{V}_{ref@T_{ref}})\right]^{2}} = 0.02 \,\mathrm{ml}$$
(S19)

Finally, given that the densities determined in this work were of the order of 1000 kg·m⁻³ (1 g·ml⁻¹), the mass of the liquid in the dilatometer was approximately 225 g, the volume in the dilatometer was approximately 225 ml, $u_c(\rho) = 0.1$ kg·m⁻³ is obtained (following the uncertainty analysis outlined in this section). Thus, the density of the liquids of interest has an expanded uncertainty, $U(\rho) = ku_c(\rho)$, of 0.2 kg·m⁻³ (for a level of confidence of 0.95; coverage factor, k = 2), as determined using the procedure outlined in Section 2.4 of the paper.

Table S2. Density of water at atmospheric pressure (P = 101.3 kPa) and various values of temperatures (T): values determined experimentally in this work (ρ); the corresponding NIST value ($\rho_{H_2O,NIST}$) obtained using REFPROP (V9.1)¹; the differences between these values ($\Delta \rho$); and the absolute relative percentage error $|e_{ref}|^{a}$

Run	T /K	ho /kg·m ⁻³	$ ho_{H_2O,NIST}$ /kg·m ⁻³	Δho /kg·m ⁻³	e _{ref} /%
	293.10	998.22	998.22	0.00	1.0E-04
	303.20	995.64	995.63	0.01	1.0E-04
	313.20	992.19	992.20	-0.01	1.1E-03
1	323.19	988.02	988.02	0.00	2.0E-04
	333.17	983.19	983.19	0.00	8.1E-04
	343.13	977.86	977.78	0.08	8.6E-03
	353.12	971.91	971.81	0.10	1.0E-02
	283.08	999.65	999.71	-0.06	5.7E-03
	293.13	998.18	998.21	-0.03	3.6E-03
	303.17	995.60	995.64	-0.04	4.7E-03
2	313.21	992.15	992.19	-0.04	4.2E-03
2	323.12	988.03	988.05	-0.02	1.6E-03
	333.08	983.21	983.23	-0.02	1.8E-03
	343.02	977.84	977.84	0.00	5.1E-04
	352.97	971.90	971.90	0.00	4.1E-04

^aCombined standard uncertainties: $u_c(P) = 1$ kPa, $u_c(T) = 0.06$ K.

Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).

Relative expanded uncertainty: $U_r(\rho_{H_2O,NIST}) = 1.10^{-6}$ (0.95 level of confidence).

Average absolute relative percentage error with respect to the NIST¹ reference values: 2.9E-03 %

Table S3. Density of dilute solutions of water (1) and ethanol (2) at atmospheric pressure (P = 101.3 kPa) and alcohol concentration of 0.1091 mol·kg⁻¹ (values also expressed in terms of mole fraction, x_2 , and percentage mass fraction, w_2) and various values of temperatures (*T*): values determined experimentally in this work (ρ); the corresponding NIST value $(\rho_{H_2O-ethanol,NIST})$ obtained using REFPROP (V9.1)¹; the differences between these values ($\Delta \rho$); and the absolute relative percentage error $|e_{ref}|^a$

T /K	$m_2 / \text{mol} \cdot \text{kg}^{-1}$	<i>x</i> ₂	W ₂ /%	ho /kg·m ⁻³	$ ho_{_{H_2O-ethanol,NIST}}/\mathrm{kg}\cdot\mathrm{m}^{-3}$	$\Delta \rho$ /kg·m ⁻³	e _{ref} /%
283.13	0.1091	0.001961	0.500	998.80	998.95	-0.15	1.5E-02
293.12	0.1091	0.001961	0.500	997.28	997.42	-0.14	1.3E-02
303.18	0.1091	0.001961	0.500	994.74	994.81	-0.07	6.1E-03
313.14	0.1091	0.001961	0.500	991.30	991.35	-0.05	5.5E-03
323.13	0.1091	0.001961	0.500	987.13	987.15	-0.02	1.5E-03
333.16	0.1091	0.001961	0.500	981.49	982.26	-0.77	7.9E-02
343.18	0.1091	0.001961	0.500	976.93	976.79	0.14	1.5E-02
353.16	0.1091	0.001961	0.500	970.86	970.80	0.06	6.3E-03
^a Combin	ned standard	uncertaintie	s: $u_c(P)$	=1 kPa, u_c	(T) = 0.06 K.		
Relativ	e combined s	standard unc	ertainties	$s: u_r(m_2, x_2,$	$w_2) = 6 \cdot 10^{-4}$.		
Expand	led uncertain	ty: $U(\rho) = 0$	0.2 kg∙m	1 ⁻³ (0.95 leve	el of confidence).		
Relativ	e expanded u	incertainty:	$U_r \left(\rho_{H_2O} \right)$	-ethanol, NIST) =	0.002 (0.95 level	of confiden	ce).

Average absolute relative percentage error with respect to the NIST¹ reference values: 1.8E-02 %

Table S4. Density of dilute solutions of water (1) and ethanol (2) at atmospheric pressure (P = 101.3 kPa) and alcohol concentration of 1.142 mol·kg⁻¹ (values also expressed in terms of mole fraction, x_2 , and percentage mass fraction, w_2) and various values of temperatures (*T*): values determined experimentally in this work (ρ); the corresponding NIST value $(\rho_{H_2O-ethanol,NIST})$ obtained using REFPROP (V9.1)¹; the differences between these values ($\Delta \rho$); and the absolute relative percentage error $|e_{ref}|^a$

T /K	$m_2 / \text{mol} \cdot \text{kg}^{-1}$	<i>x</i> ₂	W ₂ /%0	ho /kg·m ⁻³	$ ho_{H_2O-ethanol,NIST}/\mathrm{kg}\cdot\mathrm{m}^{-3}$	$\Delta \rho$ /kg·m ⁻³	e _{ref} /%			
283.13	1.142	0.02017	5.000	991.26	992.30	-1.04	1.0E-01			
293.12	1.142	0.02017	5.000	989.66	990.33	-0.67	6.8E-02			
303.19	1.142	0.02017	5.000	986.97	987.36	-0.39	4.0E-02			
313.16	1.142	0.02017	5.000	983.42	983.59	-0.17	1.7E-02			
323.16	1.142	0.02017	5.000	978.99	979.08	-0.09	9.6E-03			
333.19	1.142	0.02017	5.000	974.04	973.92	0.12	1.3E-02			
343.17	1.142	0.02017	5.000	967.70	968.19	-0.49	5.0E-02			
353.15	1.142	0.02017	5.000	961.03	961.93	-0.90	9.3E-02			
^a Combin	ned standard u	uncertainties	s: $u_c(P)$	=1 kPa, u_c	(T) = 0.06 K.					
Relative	e combined st	tandard unco	ertainties	$: u_r(m_2, x_2, x_2)$	$(w_2) = 5 \cdot 10^{-4}$.					
Expand	Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).									
Relative	e expanded u	ncertainty: U	$U_r(\rho_{H_2O-}$	$_{ethanol,NIST}) =$	0.002 (0.95 level	of confiden	.ce).			

Average absolute relative percentage error with respect to the NIST¹ reference values: 4.9E-02 %

The densities presented in Tables 2 and 3 of the paper were compared to available values in the literature at equivalent or similar concentrations. Comparative data were only available for temperatures up to 323.15 K and are presented in Tables S5 to S9. The values of density taken from the published literature ($\rho_{lit.}$) were obtained using linear interpolation of the actual reported values (to account for minor differences in concentrations). The cited references are those listed at the end of this document.

Using the values of density presented in Tables 2 and 3 of the paper, interpolated values of the density of dilute aqueous solutions of 1-butanol and 1-pentanol at atmospheric pressure and a temperature of 298.15 K are presented in Tables S10 and S11, respectively. The interpolated values were determined by using linear interpolation (ρ_{linear}), a cubic polynomial least squares curve-fit to the density data ($\rho_{curve-fit}$), and cubic spline interpolation ($\rho_{cubic spline}$).

Table S5. Density of dilute solutions of water (1) and 1-butanol (2) at atmospheric pressure (P = 101.3 kPa) and alcohol concentration of 0.06780 mol·kg⁻¹ (values also expressed in terms of mole fraction, x_2 and percentage mass fraction, w_2) and various values of temperatures (T): values determined experimentally in this work (ρ); available literature values ($\rho_{lit.}$) at nominal temperatures ($T_{nom.}$); the differences between these values ($\Delta \rho$); and the absolute relative percentage error $|e_{ref}|^{a}$

T _{nom.} /K	T /K	$m_2 / \text{mol} \cdot \text{kg}^{-1}$	<i>x</i> ₂	W ₂ /%	ho /kg·m ⁻³	$ ho_{lit.}$ /kg·m ⁻³	$\Delta \rho$ /kg·m ⁻³	e _{ref} /%	
283.15	283.17	0.06780	0.001220	0.500	999.12	998.92 ^b	0.20	2.0E-02	
						997.40 ^b	0.19	1.9E-02	
293.15	293.14	0.06780	0.001220	0.500	997.59	997.46°	0.13	1.3E-02	
						997.39 ^d	0.20	2.0E-02	
303 15	303 18	0.06780	0.001220	0.500	004.07	994.96 ^e	0.01	1.0E-03	
505.15	505.18	0.00780	0.001220	0.500	<u>,,,,</u> ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	994.81 ^d	0.16	1.6E-02	
313 15	313 1/	0.06780	0.001220	0.500	001 52	991.37 ^f	0.15	1.5E-02	
515.15	515.14	0.00780	0.001220	0.500	991.52	991.48°	0.04	4.0E-02	
323.15	323.19	0.06780	0.001220	0.500	987.27	987.30°	-0.03	3.0E-03	
^a Combin	ed standa	rd uncertaint	ies: $u_c(P) =$	1 kPa, <i>i</i>	$u_c(T) = 0.00$	6 K.			
Relative combined standard uncertainties: $u_r(m_2, x_2, w_2) = 0.001$.									
Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).									
^b Ref. 3;	Ref. 4; dF	Ref. 5; ^e Ref. 6	6; ^f Ref. 2						

Average absolute relative percentage error with respect to available literature values: 1.2E-02 %

Table S6. Density of dilute solutions of water (1) and 1-butanol (2) at atmospheric pressure (P = 101.3 kPa) and alcohol concentration of 0.2055 mol·kg⁻¹ (values also expressed in terms of mole fraction, x_2 , and percentage mass fraction, w_2) and various values of temperatures (T): values determined experimentally in this work (ρ); available literature values ($\rho_{lit.}$) at nominal temperatures ($T_{nom.}$); the differences between these values ($\Delta \rho$); and the absolute relative percentage error $|e_{ref}|^{a}$

T _{nom.} /K	T /K	$m_2 / \text{mol} \cdot \text{kg}^{-1}$	<i>x</i> ₂	W ₂ /%	ho /kg·m ⁻³	$ ho_{lit.}$ /kg·m ⁻³	$\Delta \rho$ /kg·m ⁻³	e _{ref} /%
283.15	283.16	0.2055	0.003688	1.500	997.51	997.37 ^b	0.14	1.4E-02
293.15	293.14	0.2055	0.003688	1.500	995.95	995.84 ^b	0.11	1.1E-02
303.15	303.15	0.2055	0.003688	1.500	993.29	993.19°	0.10	1.0E-02
^a Combir	ned standa	ard uncertaintie	es: $u_c(P) = 1$	kPa, <i>u</i> _c	(T) = 0.06	К.		
Relative	e combine	ed standard un	certainties: u	$r_r(m_2, x_2, $	$(w_2) = 0.001$			
Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).								
^b Ref. 7;	°Ref. 8							

Average absolute relative percentage error with respect to available literature values: 1.2E-02 %

Table S7. Density of dilute solutions of water (1) and 1-butanol (2) at atmospheric pressure (P = 101.3 kPa) and alcohol concentration of 0.7101 mol·kg⁻¹ (values also expressed in terms of mole fraction, x_2 , and percentage mass fraction, w_2) and various values of temperatures (T): values determined experimentally in this work (ρ); available literature values ($\rho_{lit.}$) at nominal temperatures ($T_{nom.}$); the differences between these values ($\Delta \rho$); and the absolute relative percentage error $|e_{ref}|^{a}$

T _{nom.} /K	T /K	$m_2 / \text{mol} \cdot \text{kg}^{-1}$	<i>x</i> ₂	W ₂ /%	ho /kg·m ⁻³	$ ho_{lit.}$ /kg·m ⁻³	Δho /kg · m ⁻³	$\left e_{ref} \right _{100}$	
						992.48 ^b	0.30	3.0E-02	
283.15	283.12	0.7101	0.01263	5.000	992.78	992.71°	0.07	7.1E-03	
						992.93 ^d	-0.15	1.5E-02	
						990.58 ^b	0.24	2.4E-02	
293.15	293.12	0.7101	0.01263	5.000	990.82	990.80°	0.02	2.0E-03	
						990.83 ^d	-0.01	1.0E-03	
		0.7101	0.012(2	5.000		987.61 ^b	0.25	2.5E-02	
202 15	202.18				087.86	987.92 ^d	-0.06	6.1E-03	
505.15	505.18		0.01203		987.80	987.87 ^e	-0.01	1.0E-03	
						987.22^{f}	0.64	6.5E-02	
^a Combin	ed standa	rd uncertainti	es: $u_c(P)$	=1 kPa,	$u_c(T) = 0.0$)6 K.			
Relative combined standard uncertainties: $u_r(m_2, x_2, w_2) = 0.001$.									
Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).									
^b Ref. 9; ⁶	² Ref. 3; ^d R	ef. 10; ^e Ref.	6; ^f Ref. 11						

Average absolute relative percentage error with respect to available literature values: 1.8E-02 %

Table S8. Density of dilute solutions of water (1) and 1-pentanol (2) at atmospheric pressure (P = 101.3 kPa) and alcohol concentration of 0.01704 mol·kg⁻¹ (values also expressed in terms of mole fraction, x_2 , and percentage mass fraction, w_2) and various values of temperatures (T): values determined experimentally in this work (ρ); available literature values ($\rho_{lit.}$) at nominal temperatures ($T_{nom.}$); the differences between these values ($\Delta \rho$); and the absolute relative percentage error $|e_{ref}|^{a}$

T _{nom.} /K	T /K	$m_2 / \mathrm{mol} \cdot \mathrm{kg}^{-1}$	<i>x</i> ₂	W2 /%0	ho /kg·m ⁻³	$ ho_{lit.}$ /kg·m ⁻³	$\Delta \rho$ /kg·m ⁻³	e _{ref} /%
283.15	283.15	0.01704	0.0003069	0.150	999.61	999.49 ^b	0.12	1.2E-02
293.15	293.14	0.01704	0.0003069	0.150	998.04	997.97 ^b	0.07	7.0E-03
^a Combined standard uncertainties: $u_c(P) = 1$ kPa, $u_c(T) = 0.06$ K.								
Relative combined standard uncertainties: $u_r(m_2, x_2, w_2) = 0.001$.								
Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).								
^b Ref. 3								

Average absolute relative percentage error with respect to available literature values: 9.5E-03 %

Table S9. Density of dilute solutions of water (1) and 1-pentanol (2) at atmospheric pressure (P = 101.3 kPa) and alcohol concentration of 0.05701 mol·kg⁻¹ (values also expressed in terms of mole fraction, x_2 , and percentage mass fraction, w_2) and various values of temperatures (T): values determined experimentally in this work (ρ); available literature values ($\rho_{lit.}$) at nominal temperatures ($T_{nom.}$); the differences between these values ($\Delta \rho$); and the absolute relative percentage error $|e_{ref}|^{a}$

T _{nom.} /K	T /K	$m_2 / \text{mol} \cdot \text{kg}^{-1}$	<i>x</i> ₂	W ₂ /%0	ρ /kg·m ⁻³	$ ho_{lit.}$ /kg·m ⁻³	$\Delta \rho$ /kg·m ⁻³	e _{ref} /%0
						998.95 ^b	0.17	1.7E-02
283.15	283.16	0.05701	0.001026	0.500	999.12	998.96°	0.16	1.6E-02
						998.97 ^d	0.15	1.5E-02
	293.14	0.05701	0.001026	0.500	997.51	997.44 ^b	0.07	7.0E-03
293.15						997.42°	0.09	9.0E-03
						997.42 ^d	0.09	9.0E-03
						997.48°	0.03	3.0E-03
303.15	303.19	0.05701	0.001026	0.500	994.93	994.85 ^d	0.08	8.0E-03
313.15	313.16	0.05701	0.001026	0.500	991.48	991.39 ^d	0.09	9.1E-03
						991.48 ^e	0.00	0.00E+00
323.15	323.19	0.05701	0.001026	0.500	987.23	987.20 ^d	0.03	3.0E-03
						987.28 ^e	-0.05	5.1E-03
³ Combined standard uncertainties $u(D) = 1$ 1/De $u(T) = 0.06$ V								

^aCombined standard uncertainties: $u_c(P) = 1$ kPa, $u_c(T) = 0.06$ K.

Relative combined standard uncertainties: $u_r(m_2, x_2, w_2) = 0.001$.

Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).

^bRef. 7; ^cRef. 3; ^dRef. 12; ^eRef. 4

Average absolute relative percentage error with respect to available literature values: 8.4E-03 %

Table S10. Interpolated values of density of dilute solutions of water (1) and 1-butanol (2) at atmospheric pressure (P = 101.3 kPa) and temperature (T = 298.15K) and alcohol concentration (values expressed in terms of molality, m_2 ; mole fraction, x_2 ; and percentage mass fraction, w_2): values determined by linear interpolation (ρ_{linear}), a cubic polynomial least squares curve-fit to the density data ($\rho_{curve-fit}$), and by cubic spline interpolation ($\rho_{cubic spline}$)^a

$m_2 / \text{mol} \cdot \text{kg}^{-1}$	<i>x</i> ₂	W ₂ /%	$ ho_{linear}$ /kg·m ⁻³	$ ho_{curve-fit}/\mathrm{kg}\cdot\mathrm{m}^{-3}$	$ ho_{ ext{cubic spline}}\/ ext{kg}\cdot ext{m}^{-3}$		
0.06780	0.001220	0.500	996.28	996.37	996.40		
0.2055	0.003688	1.500	994.62	994.66	994.74		
0.7101	0.01263	5.000	989.34	989.43	989.46		
^a Combined standard uncertainties: $u_c(P) = 1$ kPa, $u_c(T) = 0.06$ K.							
Relative combined standard uncertainties: $u_r(m_2, x_2, w_2) = 0.001$.							
Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).							

Table S11. Interpolated values of density of dilute solutions of water (1) and 1-pentanol (2) at atmospheric pressure (P = 101.3 kPa) and temperature (T = 298.15K) and alcohol concentration (values expressed in terms of molality, m_2 ; mole fraction, x_2 ; and percentage mass fraction, w_2): values determined by linear interpolation (ρ_{linear}), a cubic polynomial least squares curve-fit to the density data ($\rho_{curve-fit}$), and by cubic spline interpolation ($\rho_{cubic spline}$)^a

m_2 /mol·kg ⁻¹	<i>x</i> ₂	W2 /%0	$ ho_{linear}$ /kg·m ⁻³	$ ho_{curve-fit}/\mathrm{kg}\cdot\mathrm{m}^{-3}$	$ ho_{\it cubic spline}\/{ m kg}\cdot{ m m}^{-3}$		
0.005675 ^b	0.0001022 ^b	0.050 ^b	996.84	996.98	996.96		
0.01704	0.0003069	0.150	996.75	996.92	996.87		
0.05701	0.001026	0.500	996.22	996.31	996.34		
^a Combined standard uncertainties: $u_c(P) = 1$ kPa, $u_c(T) = 0.06$ K.							
Relative combined standard uncertainties: $u_r(m_2, x_2, w_2) = 0.001$.							
Expanded uncertainty: $U(\rho) = 0.2 \text{ kg} \cdot \text{m}^{-3}$ (0.95 level of confidence).							
^b Relative combined standard uncertainties: $u_r(m_2, x_2, w_2) = 0.003$.							

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