Densities and Viscosities of Sugar Alcohol Aqueous Solutions

Chunying Zhu, Youguang Ma,* and Chuanling Zhou

School of Chemical Engineering and Technology, State Key Laboratory of Chemical Engineering, Tianjin University, Tianjin 300072, P. R. China

In this paper, the densities and the viscosities for butane-1,2,3,4-tetrol (erythritol), (2*S*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol (sorbitol), (2*R*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol (mannitol), (2*R*,3*R*,4*S*)-pentane-1,2,3,4,5-pentol (xylitol), and 2-(hydroxymethyl)-6-[4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxane-3,4,5-triol (maltitol) aqueous solutions of various mole concentrations have been determined at T = (293.15, 303.15, 313.15, and 323.15) K. The experimental data for the viscosities of sugar alcohol aqueous solutions present a nonlinear relation to the temperature or concentration. The exponential model was used to correlate the experimental data for viscosities, with the maximum average deviation of 3.7 %. The experimental data for the densities of sugar alcohol aqueous solutions show a linear relation to the temperature or concentration considerably well. The linear equation was used to correlate the data for densities, and the maximum average deviation between the experimental data and the calculated values is 0.056 %.

Introduction

The functional sugar alcohol, including butane-1,2,3,4-tetrol (erythritol), (2*S*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol (sorbitol), (2*R*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol (mannitol), (2*R*,3*R*,4*S*)-pentane-1,2,3,4,5-pentol (xylitol), and 2-(hydroxymethyl)-6-[4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxane-3,4,5-triol (maltitol), and so on, is distinguished owing to its special function in body metastasis and has been widely used in medicine and food industries.[1,2] Chemical and physical properties of functional sugar alcohol are similar to those of sucrose, whereas the heat value of functional sugar alcohol is lower than that of sucrose. Furthermore, the functional sugar alcohol does not result in decayed teeth and is propitious to diabetics because of its small effect on blood sugar levels.[3,4] The density and viscosity are of fundamental importance for the selection and design of equipment related to the processes of heat and/or mass transfer, but there is only limited experimental data regarding those of sugar alcohol solutions in the literature. Banipal et al.[5] reported the densities and viscosities of mannitol and sorbitol in water in the range of (288.15 to 318.15) K. Romero et al.[6] presented the densities and viscosities of erythritol aqueous solutions at the temperatures ranging from (278.15 to 323.15) K. Densities and viscosities of mannitol + water, sorbitol + water, and xylitol + water at 298.15 K were also reported in the literature.[7−10] Up to now, densities and viscosities of sugar alcohol aqueous solutions have not been yet reported systematically in the literature. In this study, the densities and viscosities of aqueous solutions of butane-1,2,3,4-tetrol (erythritol), (2*S*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol (sorbitol), (2*R*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol (mannitol), (2*R*,3*R*,4*S*)-pentane-1,2,3,4,5-pentol (xylitol), and 2-(hydroxymethyl)-6-[4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxane-3,4,5-triol (maltitol) were measured at temperatures between (293.15 and 323.15) K. The experimental data were fitted to obtain the adjustable parameters, and the standard deviation (SD) between the experimental data and fitted values was also calculated.

* Corresponding author. E-mail: ygma@tju.edu.cn. Fax: +86-22-27404772.

Experimental Section

The sugar alcohols used in this work are biochemistry reagents; the mass purities of substances are > 0.998 for butane-1,2,3,4-tetrol (erythritol), > 0.997 for 2-(hydroxymethyl)-6-[4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxane-3,4,5-triol (maltitol), > 0.99 for (2*S*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol (sorbitol), > 0.998 for (2*R*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol (mannitol), and > 0.995 for (2*R*,3*R*,4*S*)-pentane-1,2,3,4,5-pentol (xylitol). Erythritol and maltitol were supplied by Baolingbao Biology Co., Ltd. Sorbitol, mannitol, and xylitol were supplied by Tianjin Kermel Chemical Reagent Co., Ltd. Deionized water was distilled in the experiment. All solutions for the whole mole concentration range at 293.15 K were prepared using a FA2004N balance with a given uncertainty of ± 0.0001 g and a volumetric flask with 1000.0 ± 0.4 mL. The uncertainty of the concentration ΔC was calculated by eq 1. All of the experiments were accomplished at temperatures of (293.15, 303.15, 313.15, and 323.15) K.

$$\Delta C = \left|\frac{1}{VM}\right|\Delta m + \left|\frac{m}{V^2M}\right|\Delta V \qquad (1)$$

where ΔC is the uncertainty of the concentration, V is the volume of the solution, M is the molecular weight of the solute, m is the mass of the solute, Δm is the uncertainty of the mass, and ΔV is the uncertainty of the volume.

The densities of the solutions were measured using the vibrating-tube digital density meter (density/specific gravity meter DA 505, KEM, Japan) with a reproducibility of ± 0.00001 g·cm^{-3}. The uncertainty in the density measurement is ± 0.00005 g·cm^{-3}. The specified repeatability of the integrated temperature is ± 0.01 K. Before each of measurements, the instrument was calibrated at atmospheric pressure with double-distilled water and dry air. Every measurement was repeated three times.

The viscosities of the sugar alcohol aqueous solutions were measured using Ubbelohde viscometers immersed in an insulated jacket, where constant temperature (± 0.01 K) was maintained by circulating water from the thermoelectric control-

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Table 1. Densities ρ and Viscosities η of Sugar Alcohol Aqueous Solutions at 293.15 K

		T/K = 293.15			T/K = 303.15			T/K = 313.15			T/K = 323.15		
C	ΔC	η	$\Delta\eta$	$10^{-3}\ \rho$	η	$\Delta\eta$	$10^{-3}\ \rho$	η	$\Delta\eta$	$10^{-3}\ \rho$	η	$\Delta\eta$	$10^{-3}\ \rho$
$mol\cdot L^{-1}$	$mol\cdot L^{-1}$	$mPa\cdot s$	$mPa\cdot s$	$kg\cdot m^{-3}$	$mPa\cdot s$	$mPa\cdot s$	$kg\cdot m^{-3}$	$mPa\cdot s$	$mPa\cdot s$	$kg\cdot m^{-3}$	$mPa\cdot s$	$mPa\cdot s$	$kg\cdot m^{-3}$
Butane-1,2,3,4-tetrol l (Erythritol)													
				0.99821			0.99565			0.99221			0.98803
0.0000		1.002[6]		0.99820[6]	0.7977[6]		0.99565[6]	0.6532[6]		0.99222[6]	0.5470[6]		0.98804[6]
0.1000	0.0000	1.0468	0.0006	1.00206	0.8541	0.0005	0.99934	0.6807	0.0005	0.99583	0.5663	0.0004	0.99164
0.2000	0.0001	1.0651	0.0006	1.00536	0.8706	0.0005	1.00274	0.7005	0.0005	0.99919	0.5849	0.0004	0.99496
0.3000	0.0001	1.0881	0.0006	1.00937	0.8913	0.0005	1.00674	0.7210	0.0005	1.00309	0.5986	0.0004	0.99881
0.4000	0.0002	1.1104	0.0006	1.01265	0.9110	0.0006	1.00958	0.7430	0.0005	1.00630	0.6171	0.0004	1.00194
0.5000	0.0002	1.1385	0.0006	1.01616	0.9366	0.0006	1.01333	0.7611	0.0005	1.00963	0.6351	0.0005	1.00523
0.6000	0.0002	1.1691	0.0006	1.01938	0.9634	0.0006	1.01667	0.7827	0.0005	1.01243	0.6520	0.0005	1.00841
0.7000	0.0003	1.2126	0.0007	1.02378	1.0018	0.0006	1.02080	0.8067	0.0005	1.01582	0.6734	0.0005	1.01227
0.8000	0.0003	1.2575	0.0007	1.02682	1.0446	0.0006	1.02420	0.8339	0.0005	1.01915	0.6909	0.0005	1.01563
0.9000	0.0004	1.3057	0.0007	1.03190	1.0869	0.0006	1.02780	0.8610	0.0006	1.02323	0.7057	0.0005	1.01938
1.0000	0.0004	1.3381	0.0007	1.03432	1.1372	0.0006	1.03118	0.8965	0.0006	1.02724	0.7251	0.0005	1.02264
(2*R*,3*R*,4*R*,5*R*)-Hexane-1,2,3,4,5,6-hexol (Mannitol)													
0.1000	0.0000	1.0964	0.0006	1.00482	0.8694	0.0005	1.00213	0.6961	0.0005	0.99828	0.5782	0.0004	0.99421
0.2000	0.0001	1.1432	0.0006	1.01089	0.9398	0.0005	1.00814	0.7468	0.0005	1.00450	0.6062	0.0004	0.99982
0.3000	0.0001	1.2031	0.0006	1.01696	0.9860	0.0006	1.01415	0.7918	0.0005	1.01072	0.6356	0.0004	1.00523
0.4000	0.0002	1.2854	0.0006	1.02303	1.0361	0.0006	1.02016	0.8201	0.0005	1.01694	0.6706	0.0005	1.01102
0.5000	0.0002	1.3360	0.0007	1.02910	1.0845	0.0006	1.02617	0.8642	0.0005	1.02316	0.7104	0.0005	1.01733
0.6000	0.0002	1.3997	0.0007	1.03517	1.1420	0.0006	1.03218	0.8954	0.0006	1.02938	0.7458	0.0005	1.02445
0.7000	0.0003	1.4719	0.0007	1.04124	1.1972	0.0007	1.03819	0.9383	0.0006	1.03560	0.7849	0.0005	1.03032
0.8000	0.0003	1.5532	0.0007	1.04731	1.2534	0.0007	1.04420	0.9934	0.0006	1.04182	0.8456	0.0005	1.03678
(2*S*,3*R*,4*R*,5*R*)-Hexane-1,2,3,4,5,6-hexol (Sorbitol)													
0.1000	0.0000	1.0881	0.0006	1.00476	0.8619	0.0005	1.00212	0.6892	0.0005	0.99858	0.5711	0.0004	0.99432
0.2000	0.0001	1.1135	0.0006	1.01123	0.8842	0.0005	1.00852	0.7109	0.0005	1.00489	0.5983	0.0004	1.00054
0.3000	0.0001	1.1677	0.0006	1.01764	0.9329	0.0006	1.01483	0.7399	0.0005	1.01114	0.6199	0.0004	1.00675
0.4000	0.0002	1.2195	0.0006	1.02407	0.9794	0.0006	1.02115	0.7849	0.0005	1.01737	0.6596	0.0005	1.01293
0.5000	0.0002	1.2748	0.0007	1.02989	1.0291	0.0006	1.02688	0.8127	0.0005	1.02301	0.6841	0.0005	1.01850
0.6000	0.0002	1.3299	0.0007	1.03694	1.0785	0.0006	1.03382	0.8573	0.0006	1.02990	0.7037	0.0005	1.02533
0.7000	0.0003	1.3940	0.0007	1.04332	1.1363	0.0007	1.04011	0.8885	0.0006	1.03608	0.7392	0.0005	1.03144
0.8000	0.0003	1.4663	0.0007	1.04936	1.2015	0.0007	1.04604	0.9310	0.0006	1.04195	0.7779	0.0005	1.03725
0.9000	0.0004	1.5312	0.0008	1.05616	1.2599	0.0007	1.05272	0.9849	0.0006	1.04848	0.8178	0.0005	1.04379
1.0000	0.0004	1.6081	0.0008	1.06252	1.3294	0.0007	1.05899	1.0298	0.0006	1.05472	0.8541	0.0006	1.04992
(2*R*,3*R*,4*S*)-Pentane-1,2,3,4,5-pentol (Xylitol)													
0.1000	0.0000	1.0675	0.0005	1.00331	0.8580	0.0005	1.00096	0.6850	0.0005	0.99716	0.5687	0.0004	0.99272
0.2000	0.0001	1.0893	0.0005	1.00850	0.8774	0.0005	1.00578	0.7057	0.0005	1.00218	0.5916	0.0004	0.99777
0.3000	0.0001	1.1279	0.0006	1.01342	0.9121	0.0006	1.01064	0.7305	0.0005	1.00699	0.6093	0.0004	1.00255
0.4000	0.0002	1.1650	0.0006	1.01854	0.9452	0.0006	1.01565	0.7640	0.0005	1.01195	0.6384	0.0005	1.00751
0.5000	0.0002	1.2067	0.0006	1.02359	0.9829	0.0006	1.02049	0.7869	0.0005	1.01686	0.6596	0.0005	1.01243
0.6000	0.0002	1.2495	0.0006	1.02866	1.0210	0.0006	1.02538	0.8250	0.0005	1.02178	0.6779	0.0005	1.01734
0.7000	0.0003	1.3133	0.0006	1.03372	1.0791	0.0006	1.03028	0.8476	0.0006	1.02670	0.7063	0.0005	1.02226
0.8000	0.0003	1.3619	0.0007	1.03878	1.1231	0.0007	1.03517	0.8825	0.0006	1.03162	0.7344	0.0005	1.02717
0.9000	0.0004	1.4235	0.0007	1.04384	1.1784	0.0007	1.04006	0.9230	0.0006	1.03654	0.7618	0.0005	1.03208
1.0000	0.0004	1.4731	0.0007	1.04890	1.2233	0.0007	1.04499	0.9632	0.0006	1.04146	0.7896	0.0005	1.03700
2-(Hydroxymethyl)-6-[4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxane-3,4,5-triol (Maltitol)													
0.1000	0.0000	1.2744	0.0006	1.00945	0.8869	0.0005	1.00732	0.6982	0.0005	1.00378	0.6083	0.0004	0.99968
0.2000	0.0001	1.3811	0.0007	1.01837	0.9747	0.0006	1.01624	0.7706	0.0005	1.01270	0.6520	0.0005	1.00860
0.3000	0.0001	1.5134	0.0007	1.02729	1.1039	0.0006	1.02516	0.8464	0.0005	1.02162	0.7175	0.0005	1.01752
0.4000	0.0002	1.6603	0.0008	1.03621	1.2254	0.0007	1.03408	0.9455	0.0006	1.03054	0.7827	0.0005	1.02644
0.5000	0.0002	1.8478	0.0008	1.04513	1.3609	0.0007	1.04300	1.0600	0.0006	1.03946	0.8723	0.0006	1.03536
0.6000	0.0002	2.0090	0.0009	1.05405	1.5362	0.0008	1.05192	1.1765	0.0007	1.04838	0.9616	0.0006	1.04428
0.7000	0.0003	2.1728	0.0009	1.06297	1.6843	0.0008	1.06084	1.3011	0.0007	1.05730	1.0612	0.0006	1.05320
0.8000	0.0003	2.3045	0.0010	1.07189	1.8254	0.0009	1.06976	1.4381	0.0008	1.06622	1.1502	0.0007	1.06212
0.9000	0.0004	2.4897	0.0010	1.08081	1.9468	0.0010	1.07868	1.5912	0.0008	1.07514	1.2423	0.0007	1.07104
1.0000	0.0004	2.6799	0.0011	1.08973	2.1322	0.0010	1.08760	1.7411	0.0009	1.08406	1.3849	0.0007	1.07996

ler at the required temperature. The flow times of the solutions were recorded by using an electronic digital stopwatch with a readability of ± 0.01 s. The flow times were larger than 150 s for water. Experiments were repeated four times, and the deviation was less than 0.2 s. The viscosity η of the solutions was then calculated from the following equation:[11]

$$\frac{\eta}{\eta_w} = \frac{\rho t}{\rho_w t_w} \tag{2}$$

where η, ρ, and t and η_w, ρ_w, and t_w are the viscosity, density, and flow time of the mixture and pure water, respectively. The viscosity and density of pure water were obtained from Lange's Handbook of Chemistry.[12] The uncertainty of the viscosity $\Delta\eta$ was calculated by eq 3.

$$\Delta\eta = \left|\frac{\rho t}{\rho_w t_w}\right|\Delta\eta_w + \left|\frac{\eta_w t}{\rho_w t_w}\right|\Delta\rho + \left|\frac{\eta_w \rho}{\rho_w t_w}\right|\Delta t + \left|\frac{\eta_w \rho t}{\rho_w^2 t_w}\right|\Delta\rho_w + \left|\frac{\eta_w \rho t}{\rho_w t_w^2}\right|\Delta t_w \tag{3}$$

where $\Delta\eta$ is the uncertainty of the viscosity, $\Delta\eta_w$ is the uncertainty of the viscosity of pure water, $\Delta\rho$ is the uncer-

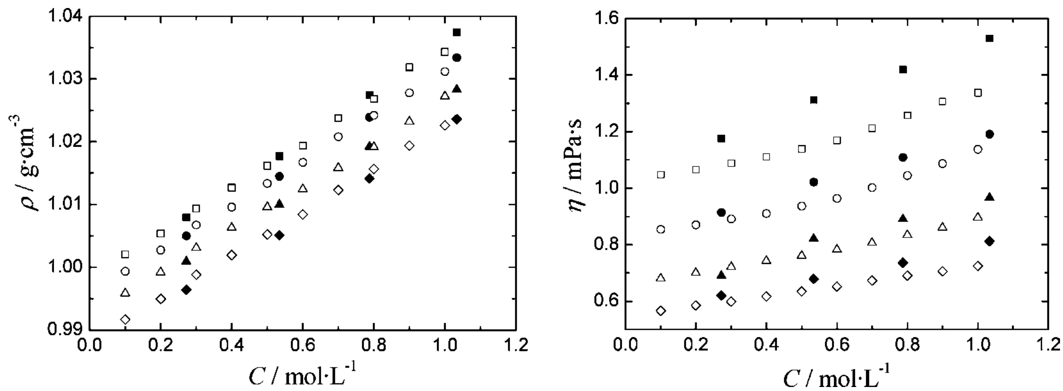

Figure 1. Comparison of densities ρ and viscosities η between the experimental data and the values in the literature for butane-1,2,3,4-tetrol (erythritol) aqueous solutions. Symbols: open symbols, the data in this work; filled symbols, the data in the literature.[7] □, 293.15 K; ○, 303.15 K; △, 313.15 K; ◇, 323.15 K.

Table 2. Parameters in Equation 7 for Sugar Alcohol Aqueous Solutions

	A_1	A_2	A_3	A_4	AD/%	SD/mPa·s
erythritol	0.0126	873.56	60.89	93.14	1.3	0.017
mannitol	0.0752	285.28	59.52	183.94	1.8	0.022
sorbitol	0.0547	365.20	59.25	168.02	1.8	0.022
xylitol	0.0140	807.30	77.12	103.86	1.1	0.016
maltitol	0.0182	695.51	161.13	123.49	3.7	0.058

Table 3. Parameters in Equation 10 for Sugar Alcohol Aqueous Solutions

	B_1	B_2	$10^3\ B_3$	AD/%	SD/kg·m^{-3}
erythritol	1.1086	0.0351	−0.3732	0.044	0.54
mannitol	1.1064	0.0611	−0.3663	0.056	0.71
sorbitol	1.1121	0.0628	−0.3842	0.041	0.51
xylitol	1.1087	0.0495	−0.3734	0.032	0.39
maltitol	1.0974	0.0892	−0.3285	0.047	0.52

tainty of the density, and Δt is the uncertainty of the flow time.

Results and Discussion

Experimental data for the densities and viscosities of binary mixtures of {butane-1,2,3,4-tetrol, (2*S*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol, (2*R*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol, (2*R*,3*R*,4*S*)-pentane-1,2,3,4,5-pentol, and 2-(hydroxymethyl)-6-[4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxane-3,4,5-triol} + water, at $T = (293.15$ to $323.15)$ K, are displayed in Table 1. The comparison of densities and viscosities of butane-1,2,3,4-tetrol (erythritol) aqueous solutions between the experimental data and those in literature[6] is shown in Figure 1. The measured densities are in good agreement with those in the literature. Serious discrepancies were shown for the viscosity data at 293.15 K, which can be due to the difference of erythritol purity.

For a specific molar concentration of sugar alcohol, the densities and viscosities decrease with the increase of temperature. When the solution is heated, the thermal energy of molecules increases, and the intermolecular distances increase, leading to the decrease of density and viscosity. At a certain temperature, the density and the viscosity increase with increasing solute concentration.

In the range of temperature studied, the viscosities of sugar alcohols decrease nonlinearly with the increase of temperature, while the densities of sugar alcohol decrease linearly with increasing the temperature. However, some authors have found that the density decreases nonlinearly with the temperature over a wide range of temperatures.[13]

Carbon molecule numbers of erythritol, xylitol, mannitol (sorbitol), and maltitol increase gradually, and so do molecular weights and volumes, respectively, leading to the increase of viscosities and densities of solutions for a specific molar concentration and temperature.

Gonzáles-Tello et al.[14] proposed an equation to correlate the viscosity of polymeric solutions:

$$(\eta/\text{mPa·s}) = A_1 \exp\left(\frac{A_2 + A_3 w}{(T/\text{K}) - A_4}\right) \tag{4}$$

where A_1, A_2, A_3, and A_4 are the dimensionless empirical constants and w is the mass fraction of the solute.

Rao[15] correlated viscosity with temperature and concentration:

$$\eta(T, C) = \eta_0(C) \exp\left[\frac{E_a(C)}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] \tag{5}$$

Both the pre-exponential parameter $\eta_0(C)$ and activation energy $E_a(C)$ were assumed to be dependent on the molar concentration C, and T_0 was assumed to be 293 K. In eq 5, it is difficult to determine activation energy $E_a(C)$.

Laliberté[16] developed a model to calculate the viscosity of aqueous solutions:

$$(\eta/\text{mPa·s}) = \exp\left(\frac{v_1 w^{v_2} + v_3}{(v_4(t/°\text{C}) + 1)(v_5 w^{v_6} + 1)}\right) \tag{6}$$

where v_1 to v_6 are empirical dimensionless constants. Parameters for 74 solutes were established based on a review of the literature. However, parameters in eq 6 are more than those in eq 4. Therefore, eq 4 was used to correlate the experimental data in the present work, and the mole concentration is substituted for the mass fraction of solute:

$$(\eta/\text{mPa·s}) = A_1 \exp\left[\frac{A_2 + A_3(C/\text{mol·L}^{-1})}{(T/\text{K}) - A_4}\right] \tag{7}$$

A_1, A_2, A_3, and A_4 were obtained by using nonlinear regression method. The values of the SD and the average deviation (AD) were calculated by eqs 8 and 9, respectively.

$$\mathrm{SD} = \sqrt{\frac{\sum_{i=1}^{n} (\eta_{\mathrm{exp},i} - \eta_{\mathrm{cal},i})^2}{n - m}} \quad (8)$$

$$\mathrm{AD} = \left[\sum_{i=1}^{n}\left(\frac{|\eta_{\mathrm{exp},i} - \eta_{\mathrm{cal},i}|}{\eta_{\mathrm{exp},i}}\right)\right]\frac{100}{n} \quad (9)$$

where n is the total number of experimental values and m is the number of parameters.

The experimental data of the density were fitted by using eq 10 proposed by Guimarães et al.:[17]

$$(10^{-3}\rho/\mathrm{kg{\cdot}m^{-3}}) = B_1 + B_2(C/\mathrm{mol{\cdot}L^{-1}}) + B_3(T/\mathrm{K}) \quad (10)$$

where B_1, B_2, and B_3 are dimensionless empirical constants determined by fitting experimental data.

The parameters in eqs 7 and 10 were obtained by fitting the experimental data for several sugar alcohols as shown in Tables 2 and 3, respectively, as well as the values of SD and AD. It can be observed that for viscosities, the values of SD and AD are less than 0.058 mPa·s and 3.7 %, respectively, and for densities, the values of SD and AD are inferior to 0.71 $\mathrm{kg{\cdot}m^{-3}}$ and 0.056 %, respectively.

Conclusions

The viscosities and densities of butane-1,2,3,4-tetrol (erythritol), (2*S*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol (sorbitol), (2*R*,3*R*,4*R*,5*R*)-hexane-1,2,3,4,5,6-hexol (mannitol), (2*R*,3*R*,4*S*)-pentane-1,2,3,4,5-pentol (xylitol), and 2-(hydroxymethyl)-6-[4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxane-3,4,5-triol (maltitol) were measured, and the influence of the temperature [(293.15, 303.15, 313.15, and 323.15) K] and the concentration of the sugar alcohols on the viscosity and density of aqueous solutions was studied.

The maximum values of the SD and AD between the data of this work and the values calculated by the Gonzáles-Tello et al. correlation (eq 7) are 0.058 mPa·s and 3.7 %, respectively. The maximum values of the SD and AD between the experimental densities and those calculated by Guimarães et al. correlation (eq 10) are 0.71 $\mathrm{kg{\cdot}m^{-3}}$ and 0.056 %, respectively. The results show that eqs 7 and 10 can yield good predictions for the viscosities and the densities, respectively, over the range of temperatures in this work.

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