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## Measurement of Volumetric and Viscometric Properties of Binary Mixtures of Methyl *tert*-butyl Ether (MTBE) + 1-Alcohol from 293.15 to 308.15 K and at Atmospheric Pressure

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Densities and viscosities of binary mixtures of methyl *tert*-butyl ether (MTBE) with 1-alkanols, or +1-pentanol, or +1-hexanol, or +1-heptanol were measured as a function of composition from 293.15 to 308.15 K at atmospheric pressure. The temperatures studied were 293.15, 298.15, 303.15 and 308.15 K. The experimental results have been used to calculate the viscosity deviation  $\Delta\eta$  and volumetric properties such as  $V_\phi$ ,  $\bar{V}$  and  $\bar{V}^\infty$ . Both  $V_m^E$  and  $\Delta\eta$  values were negative over the entire range of mole fraction for all temperatures and systems studied. The results for all volumetric and viscometric properties are discussed on the basis of molecular interactions between the components of the mixtures.

**Keywords:** Volumetric properties, Viscometric properties, Ether, Alcohols

### INTRODUCTION

Volumetric and viscometric properties such as excess molar volume and viscosity deviation are of particular importance to interpret intermolecular phenomena in mixtures. By using viscosity and density values, engineering can predict the behaviors of systems containing chemical mixtures. Access to these properties are a primary factor in designing systems and chemical processes [1]. In recent decade, methyl *tert*-butyl ether (MTBE) has been widely used in the chemical and petrochemical industry as an octane booster for gasoline and as an organic solvent.

In this work, we report density and viscosity of methyl *tert*-butyl ether (MTBE) + 1-butanol, or +1-pentanol, or +1-hexanol, or +1-heptanol over the complete composition range at the temperatures of 293.15, 298.15, 303.15 and 308.15 K and at atmospheric pressure.

Addition of MTBE reduces exhaust fumes, especially

unburned hydrocarbons, carbon monoxide, polycyclic aromatics and particulate carbon [2]. The 1-alkanols, 1-butanol is used widely as a solvent for painting, coating, etc., 1-pentanol as a fuel, due to its similar properties with gasoline, and 1-hexanol as a dissolvable in a wide range of industries.

Volumetric and viscometric properties of binary liquid mixtures of ethers with alcohols have been reported by a few authors [2-19].

However, to the best of our knowledge, there is no report on the viscosity deviation and excess molar at several temperatures (293.15 to 308.15 K) for all systems studied in this work.

### EXPERIMENTAL

Methyl *tert*-butyl ether (Merck, mole fraction purity > 0.998), 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol (Merck, mole fraction purity > 0.99) were used without subsequent purification. The purity of each component was

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**Table 1.** Comparison of Measured Values of Density and Viscosity of the Pure Substance with those in Literature at Different Temperatures and Atmospheric Pressure

Component	<i>T</i> (K)	<i>ρ</i> (g cm <sup>-3</sup> )		<i>η</i> (mPa s)	
		Experimental	Literature	Experimental	Literature
Methyl tert-butyl ether	293.15	0.74068	0.74065 [20]	0.34202	0.3861 [21]
	298.15	0.73541	0.7356 [22]	0.32101	0.3354 [23]
	303.15	0.73011	0.7301 [20]	0.29902	0.349 [25]
	308.15	0.72477	0.72482 [20]	0.28901	0.38 [24]
1-Butanol	293.15	0.80962	0.80956 [27]	2.9789	2.941 [34]
	298.15	0.80579	0.8055 [33]	2.6061	2.5723 [26]
	303.15	0.80199	0.80195 [27]	2.2892	2.2705 [26]
	308.15	0.79836	0.7985 [28]	2.0075	1.982 [28]
1-Pentanol	293.15	0.81452	0.81462 [29]	4.0309	4.0321 [29]
	298.15	0.81079	0.8151 [33]	3.4923	3.5190 [29]
	303.15	0.80709	0.80723 [30]	3.0365	2.959 [30]
	308.15	0.80335	0.80345 [29]	2.6515	2.6387 [29]
1-Hexanol	293.15	0.81876	0.81882 [29]	5.3695	5.3614 [29]
	298.15	0.81516	0.8151 [33]	4.5823	4.4029 [22]
	303.15	0.81179	0.81200 [31]	3.9371	3.8951 [32]
	308.15	0.80822	0.80834 [29]	3.4019	3.6045 [29]
1-Heptanol	293.15	0.82120	-	7.0284	-
	298.15	0.81869	0.8187 [33]	5.9243	-
	303.15	0.81517	-	5.0329	-
	308.15	0.81159	-	4.3051	-

evaluated with the corresponding values available in Table 1 from measurements of density (*ρ*) and viscosity (*η*) by comparing the empirical data of the pure liquid.

All binary systems were prepared by weight measuring the pure components on A&D Phoenix Analytical (Model

GH-252) balance. The binary mixtures containing MTBE and 1-alkanols were prepared taking due precautions to minimize the evaporation losses and the instability in the mole fraction is estimated to be  $\pm 1 \times 10^{-4}$ . The viscosities and densities of pure components and their solutions

(MTBE with 1-alkanols) were measured at various temperatures and atmospheric pressure with an Anton Paar (SVM) Model 3000 density-viscosity meter calibrated by distilled n-hexane. The uncertainty of the measurements was calculated to be  $\pm 1 \times 10^{-4}$  g cm<sup>-3</sup>, the excess molar volume was  $\pm 1 \times 10^{-3}$  cm<sup>3</sup> mol<sup>-1</sup> and viscosity deviation was  $\pm 2 \times 10^{-4}$  mPa s. The average reproducibility in the viscosity estimations was  $\pm 0.30\%$ . The viscometer can set a steady temperature with uncertainty about  $\pm 0.01$  K.

## RESULTS AND DISCUSSION

The excess molar volume can be calculated by the following equation:

$$V_m^E = x_1 M_1 \left( \frac{1}{\rho} - \frac{1}{\rho_1} \right) + x_2 M_2 \left( \frac{1}{\rho} - \frac{1}{\rho_2} \right) \quad (1)$$

where  $\rho_1$  and  $\rho_2$  are the densities of components 1 and 2,  $M_1$  and  $M_2$  are the molar mass and  $\rho$  is the density of the mixture.

Empirical results for density and volumetric properties of (MTBE + 1-alkanol) mixtures over the whole mole fraction composition for various temperatures (293.15 to 308.15 K) and atmospheric pressure are reported in Table 2. The viscosity deviation is calculated by the following equation:

$$\Delta\eta = \eta - (x_1\eta_1 + x_2\eta_2) \quad (2)$$

in which  $\eta$  represents the dynamic viscosity of a mixture containing one mole of (MTBE + 1-alkanol),  $x_1$  and  $x_2$  are the mole fractions of components 1 (MTBE) and 2 (1-alkanol), respectively, and  $\eta_1$  and  $\eta_2$  are the dynamic viscosities of pure components.

The estimations of  $V_m^E$  and  $\Delta\eta$  for all systems have been fitted to the Redlich-Kister polynomial equation which is discussed in following:

$$Y^E = x_1 (1 - x_1) \sum_{i=0}^n A_i (1 - 2x_1)^i \quad (3)$$

where  $A_i$  are the polynomial coefficients obtained through fitting the equation to the empirical data with a least-squares regression method. The correlated results are reported in Tables 3 and 4, along with the standard deviations determined from the equation:

$$\sigma = \sqrt{\frac{(Y_{\text{exp}}^E - Y_{\text{cal}}^E)^2}{N-n}} \quad (4)$$

where  $N$  is the number of measurements and  $n$  is the number of estimated parameters.

The partial molar volumes,  $\bar{V}_1$  and  $\bar{V}_2$ , were calculated by using the following equations:

$$\bar{V}_1 = V_m^E + V_1^0 - x_2 (\partial V_m^E / \partial x_2)_{p,T} \quad (5)$$

$$\bar{V}_2 = V_m^E + V_2^0 - x_1 (\partial V_m^E / \partial x_1)_{p,T} \quad (6)$$

By using Eqs. (3), (5) and (6), the partial molar volumes,  $\bar{V}_1$  and  $\bar{V}_2$ , would be:

$$\bar{V}_1 = V_1^0 + x_2^2 \sum_{j=0}^{j=n} A_j (1 - 2x_2)^j + 2x_2^2 (1 - x_2) \sum_{j=0}^{j=n} A_j (j) (1 - 2x_2)^{j-1} \quad (7)$$

and

$$\bar{V}_2 = V_2^0 + (1 - x_2)^2 \sum_{j=0}^{j=n} A_j (1 - 2x_2)^j - 2x_2 (1 - x_2)^2 \sum_{j=0}^{j=n} A_j (j) (1 - 2x_2)^{j-1} \quad (8)$$

where the partial molar volumes of MTBE and 1-alkanol are  $\bar{V}_1$  and  $\bar{V}_2$ , respectively.

Because of the importance of partial molar volume at infinite dilution, in this study, we report these data for all binary systems containing MTBE + 1-alkanol.

Accordingly, by setting  $x_1 = 0$  and  $x_2 = 1$  in Eq. (7):

$$\bar{V}_1^\infty = V_1^0 + \sum_{j=0}^{j=n} A_j (-1)^j \quad (9)$$

**Table 2.** Experimental Densities, Viscosities, Viscosity Deviations, Excess Molar Volume, Partial Molar Volume and Partial Molar Volume in Infinite Dilution of the (MTBE + 1-Alkanol) Mixtures at Different Temperatures and Atmospheric Pressure

$x_1$	P (g cm <sup>-3</sup> )	$V_m^E$ (cm <sup>3</sup> mol <sup>-1</sup> )	$V_{\phi 1}$ (cm <sup>3</sup> mol <sup>-1</sup> )	$V_{\phi 2}$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\bar{V}_1$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\bar{V}_2$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\eta$ (mPa s)	$\Delta\eta$ (mPas)
$x_1$ MTBE + $x_2$ 1-Butanol								
T = 293.15 K								
0	0.8093	0	-	-	-	-	2.93	0
0.0807	0.8043	-0.234	116.48	91.32	116.65	91.52	2.28	-0.448
0.1595	0.7992	-0.413	116.74	91.15	117.02	91.48	1.79	-0.731
0.2403	0.794	-0.571	117.00	90.88	117.49	91.38	1.44	-0.881
0.3499	0.7867	-0.711	117.27	90.60	117.91	91.23	1.11	-0.933
0.4415	0.7805	-0.784	117.51	90.33	118.26	91.06	0.93	-0.879
0.5579	0.7724	-0.779	117.76	90.02	118.54	90.82	0.73	-0.784
0.6498	0.7661	-0.731	117.99	89.70	118.74	90.52	0.61	-0.671
0.7384	0.7598	-0.624	118.26	89.31	118.89	90.07	0.55	-0.502
0.8491	0.752	-0.432	118.51	88.88	118.97	89.50	0.46	-0.309
0.9399	0.7455	-0.215	118.81	88.43	119.01	88.70	0.42	-0.116
1	0.7409	0	-	-	-	-	0.39	0
T = 298.15 K								
0	0.8055	0	-	-	-	-	2.93	0
0.0807	0.8006	-0.261	117.27	91.75	117.40	91.95	2.28	-0.448
0.1595	0.7955	-0.465	117.50	91.56	117.80	91.91	1.79	-0.731
0.2403	0.7903	-0.641	117.77	91.28	118.31	91.81	1.44	-0.881
0.3499	0.783	-0.814	118.04	90.90	118.74	91.67	1.11	-0.933
0.4415	0.7766	-0.874	118.30	90.70	119.08	91.47	0.93	-0.879
0.5579	0.7683	-0.865	118.55	90.38	119.36	91.22	0.73	-0.784
0.6498	0.7617	-0.811	118.79	90.04	119.57	90.89	0.61	-0.671
0.7384	0.7553	-0.701	119.07	89.64	119.73	90.42	0.55	-0.502

**Table 2.** Continued

0.8491	0.7471	-0.471	119.34	89.23	119.81	89.85	0.46	-0.309
0.9399	0.7404	-0.227	119.65	88.72	119.86	89.04	0.42	-0.116
1	0.7357	0	-	-	-	-	0.39	0
<b>T = 303.15 K</b>								
0	0.8016	0	-	-	-	-	2.27	0
0.0807	0.7967	-0.292	118.02	92.18	118.17	92.39	1.82	-0.297
0.1595	0.7917	-0.513	118.28	91.99	118.59	92.35	1.46	-0.501
0.2403	0.7863	-0.693	118.56	91.69	119.12	92.24	1.19	-0.621
0.3499	0.7789	-0.881	118.83	91.39	119.56	92.09	0.91	-0.686
0.4415	0.7726	-0.969	119.10	91.09	119.92	91.89	0.74	-0.678
0.5579	0.764	-0.947	119.36	90.79	120.21	91.62	0.63	-0.571
0.6498	0.7572	-0.881	119.62	90.41	120.42	91.28	0.53	-0.492
0.7384	0.7506	-0.761	119.91	90.00	120.59	90.80	0.48	-0.367
0.8491	0.7423	-0.525	120.19	89.59	120.6	90.21	0.41	-0.228
0.9399	0.7354	-0.274	120.52	89.08	120.72	89.38	0.38	-0.085
1	0.7304	0	-	-	-	-	0.35	0
<b>T = 308.15 K</b>								
0	0.7978	0	-	-	-	-	2.01	0
0.0807	0.7929	-0.313	118.81	92.62	118.97	92.84	1.62	-0.253
0.1595	0.7878	-0.551	119.07	92.42	119.40	92.80	1.31	-0.429
0.2403	0.7824	-0.756	119.36	92.11	119.95	92.68	1.08	-0.519
0.3499	0.7749	-0.954	119.65	91.80	120.41	92.53	0.86	-0.561
0.4415	0.7684	-1.05	119.93	91.49	120.78	92.32	0.73	-0.533
0.5579	0.7596	-1.031	120.20	91.17	121.07	92.03	0.59	-0.479
0.6498	0.7526	-0.949	120.47	90.78	121.30	91.67	0.51	-0.411
0.7384	0.7459	-0.821	120.77	90.36	121.47	91.18	0.46	-0.304
0.8491	0.7372	-0.555	121.07	8.95	121.57	90.57	0.4	-0.184
0.9399	0.7301	-0.275	121.40	89.43	121.61	89.73	0.35	-0.081
1	0.725	0	-	-	-	-	0.33	0

**Table 2.** Continued

x <sub>1</sub> MTBE + x <sub>2</sub> 1-Pentanol									
T = 293.15 K									
0	0.8145	0	-	-	-	-	-	4.03	0
0.0814	0.8094	-0.192	116.37	108.00	116.45	108.21	3.08	-0.654	
0.1599	0.8045	-0.373	116.61	107.82	116.88	108.16	2.45	-1.001	
0.2384	0.7995	-0.527	116.89	107.53	117.44	108.07	1.95	-1.207	
0.3504	0.7918	-0.661	117.15	107.25	117.88	107.94	1.45	-1.306	
0.4402	0.7854	-0.716	117.41	106.90	118.26	107.73	1.13	-1.295	
0.5598	0.7764	-0.709	117.62	106.57	118.52	107.48	0.9	-1.093	
0.6497	0.7695	-0.663	117.90	106.19	118.73	107.13	0.72	-0.947	
0.7391	0.7625	-0.572	118.13	105.71	118.88	106.68	0.6	-0.736	
0.8493	0.7536	-0.386	118.48	105.15	118.99	105.93	0.49	-0.441	
0.9385	0.7462	-0.191	118.78	104.52	119.01	104.96	0.42	-0.186	
1	0.7409	0	-	-	-	-	0.39	0	
T = 298.15 K									
0	0.8108	0	-	-	-	-	3.49	0	
0.0814	0.8056	-0.204	117.16	108.48	117.26	108.69	2.71	-0.524	
0.1599	0.8008	-0.418	117.35	108.28	117.69	108.65	2.14	-0.853	
0.2384	0.7956	-0.569	117.65	107.98	118.25	108.55	1.76	-0.986	
0.3504	0.7878	-0.711	117.90	107.68	118.68	108.42	1.31	-1.083	
0.4402	0.7813	-0.781	118.17	107.32	119.07	108.19	1.04	-1.075	
0.5598	0.7721	-0.766	118.41	106.97	119.33	107.92	0.83	-0.913	
0.6497	0.765	-0.705	118.69	106.58	119.56	107.55	0.67	-0.793	
0.7391	0.7578	-0.592	118.94	106.94	119.71	107.09	0.56	-0.619	
0.8493	0.7487	-0.414	119.30	105.51	119.83	106.31	0.47	-0.373	
0.9385	0.7412	-0.203	119.62	104.89	119.86	105.32	0.4	-0.159	
1	0.7357	0	-	-	-	-	0.37	0	
T = 298.15 K									
0	0.8108	0	-	-	-	-	3.49	0	

**Table 2.** Continued

0.0814	0.8056	-0.204	117.16	108.48	117.26	108.69	2.71	-0.524
0.1599	0.8008	-0.418	117.35	108.28	117.69	108.65	2.14	-0.853
0.2384	0.7956	-0.569	117.65	107.98	118.25	108.55	1.76	-0.986
0.3504	0.7878	-0.711	117.90	107.68	118.68	108.42	1.31	-1.083
T = 303.15 K								
0	0.8071	0	-	-	-	-	3.04	0
0.0814	0.8022	-0.265	117.90	108.97	118.04	109.19	2.39	-0.424
0.1599	0.7971	-0.465	118.12	108.76	118.47	109.15	1.89	-0.713
0.2384	0.7918	-0.627	118.40	108.44	119.04	109.04	1.56	-0.841
0.3504	0.784	-0.796	118.67	108.13	119.50	108.90	1.14	-0.951
0.4402	0.7773	-0.868	118.96	107.75	119.90	108.66	0.93	-0.921
0.5598	0.7679	-0.849	119.21	107.39	120.18	108.38	0.7	-0.831
0.6497	0.7607	-0.796	119.50	106.97	120.41	107.99	0.62	-0.667
0.7391	0.7533	-0.675	119.77	106.46	120.58	107.50	0.53	-0.522
0.8493	0.7439	-0.468	120.15	105.87	120.70	106.68	0.44	-0.316
0.9385	0.7362	-0.249	120.48	105.20	120.72	105.66	0.38	-0.132
1	0.7304	0	-	-	-	-	0.35	0
T = 308.15 K								
0	0.8033	0	-	-	-	-	2.65	0
0.0814	0.7985	-0.304	118.69	109.46	118.84	109.70	2.13	-0.335
0.1599	0.7932	-0.503	118.88	109.24	119.27	109.65	1.71	-0.571
0.2384	0.7881	-0.704	119.18	108.91	119.86	109.54	1.41	-0.683
0.3504	0.7801	-0.885	119.47	108.58	120.33	109.39	1.09	-0.746
0.4402	0.7732	-0.951	119.77	108.18	120.75	109.14	0.89	-0.738
0.5598	0.7637	-0.945	120.03	107.80	121.04	108.84	0.72	-0.635
0.6497	0.7563	-0.881	120.33	107.37	121.29	108.43	0.59	-0.555
0.7391	0.7488	-0.765	120.61	106.84	121.46	107.92	0.5	-0.432
0.8493	0.739	-0.516	121.02	106.24	121.59	107.07	0.42	-0.258
0.9385	0.7309	-0.248	121.36	105.55	121.62	106.01	0.37	-0.106

**Table 2.** Continued

1	0.725	0	-	-	-	-	0.33	0
$x_1$ MTBE + $x_2$ 1-Hexanol								
T = 293.15 K								
0	0.8187	0	-	-	-	-	5.37	0
0.0813	0.8138	-0.174	116.46	124.56	116.63	124.76	4.1	-0.861
0.1605	0.8089	-0.341	116.60	124.35	117.02	124.72	3.23	-1.337
0.2409	0.8037	-0.464	116.85	124.03	117.53	124.63	2.51	-1.657
0.3499	0.796	-0.569	117.08	123.71	117.93	124.48	1.81	-1.815
0.4405	0.7893	-0.606	117.30	123.37	118.25	124.29	1.41	-1.762
0.5605	0.7799	-0.601	117.59	122.94	118.56	123.96	1.07	-1.507
0.6493	0.7726	-0.563	117.82	122.56	118.75	123.62	0.85	-1.284
0.7399	0.7649	-0.481	118.10	122.04	118.90	123.09	0.69	-0.992
0.8498	0.7551	-0.327	118.43	121.40	118.99	122.29	0.53	-0.605
0.9392	0.7469	-0.162	118.76	120.76	119.02	121.23	0.44	-0.253
1	0.7409	0	-	-	-	-	0.39	0
T = 298.15 K								
0	0.8151	0	-	-	-	-	4.58	0
0.0813	0.8101	-0.191	117.14	125.09	117.31	125.30	3.57	-0.671
0.1605	0.8053	-0.389	117.33	124.87	117.73	125.26	2.85	-1.054
0.2409	0.7999	-0.515	117.58	124.53	118.29	125.16	2.22	-1.352
0.3499	0.7922	-0.632	117.82	124.19	118.72	125.01	1.64	-1.471
0.4405	0.7853	-0.676	118.05	123.84	119.05	124.81	1.29	-1.435
0.5605	0.7757	-0.661	118.36	123.38	119.37	124.45	0.98	-1.239
0.6493	0.7683	-0.621	118.60	122.98	119.57	124.09	0.79	-1.059
0.7399	0.7604	-0.535	118.89	122.45	119.74	123.54	0.64	-0.821
0.8498	0.7504	-0.371	119.24	121.78	119.84	122.71	0.5	-0.503
0.9392	0.7419	-0.189	119.59	121.09	119.86	121.60	0.41	-0.213
1	0.7357	0	-	-	-	-	0.37	0

**Table 2.** Continued

T = 303.15 K									
0	0.8115	0	-	-	-	-	-	3.94	0
0.0813	0.8067	-0.234	117.89	125.63	118.08	125.86	3.11	-0.535	
0.1605	0.8017	-0.429	118.07	125.40	118.51	125.81	2.45	-0.911	
0.2409	0.7962	-0.573	118.32	125.04	119.08	125.71	1.95	-1.125	
0.3499	0.7885	-0.72	118.59	124.69	119.53	125.55	1.46	-1.221	
0.4405	0.7815	-0.777	118.83	124.32	119.87	125.33	1.16	-1.195	
0.5605	0.7717	-0.764	119.15	123.84	120.22	124.96	0.9	-1.025	
0.6493	0.7641	-0.712	119.40	123.41	120.43	124.57	0.73	-0.879	
0.7399	0.7559	-0.609	119.71	122.85	120.60	124.00	0.6	-0.683	
0.8498	0.7456	-0.421	120.08	122.16	120.70	123.13	0.47	-0.421	
0.9392	0.7369	-0.221	120.44	121.43	120.73	121.97	0.38	-0.184	
1	0.7304	0	-	-	-	-	0.35	0	
T = 308.15 K									
0	0.8079	0	-	-	-	-	-	3.4	0
0.0813	0.8032	-0.281	118.64	126.18	118.86	126.42	2.73	-0.425	
0.1605	0.798	-0.466	118.82	125.94	119.30	126.38	2.19	-0.721	
0.2409	0.7926	-0.651	119.09	125.56	119.89	126.26	1.74	-0.924	
0.3499	0.7847	-0.801	119.36	125.19	120.35	126.09	1.32	-1.007	
0.4405	0.7776	-0.862	119.61	124.80	120.72	125.87	1.06	-0.988	
0.5605	0.7676	-0.859	119.95	124.29	121.08	125.48	0.82	-0.861	
0.6493	0.7598	-0.801	120.22	123.85	121.30	125.07	0.68	-0.724	
0.7399	0.7514	-0.689	120.55	123.25	121.48	124.46	0.57	-0.561	
0.8498	0.7407	-0.467	120.94	122.54	121.59	123.54	0.44	-0.347	
0.9392	0.7317	-0.237	121.32	121.78	121.62	122.33	0.32	-0.195	
1	0.725	0	-	-	-	-	0.33	0	
x <sub>1</sub> MTBE + x <sub>2</sub> 1-Heptanol									
T = 293.15 K									
0	0.8222	0	-	-	-	-	-	7.03	0

**Table 2.** Continued

0.0812	0.8174	-0.149	116.52	137.32	116.71	137.41	5.36	-1.129
0.1599	0.8125	-0.266	116.70	137.08	116.94	137.37	4.23	-1.741
0.2404	0.8073	-0.373	116.89	136.84	117.29	137.15	3.31	-2.121
0.3506	0.7996	-0.474	117.07	136.66	117.48	137.08	2.33	-2.367
0.4399	0.7929	-0.513	117.31	136.09	117.71	136.86	1.75	-2.358
0.5601	0.7832	-0.509	117.56	135.70	117.94	136.47	1.22	-2.088
0.6558	0.775	-0.469	117.79	135.19	118.26	136.06	0.91	-1.763
0.7399	0.7674	-0.407	117.97	134.75	118.52	135.45	0.76	-1.356
0.8498	0.7567	-0.27	118.29	134.15	118.79	135.33	0.56	-0.821
0.9399	0.7474	-0.123	118.44	133.68	118.98	135.22	0.45	-0.336
1	0.7409	0	-	-	-	-	0.39	0
T = 298.15 K								
0	0.8187	0	-	-	-	-	5.92	0
0.0812	0.8139	-0.166	117.26	137.86	117.43	137.98	4.59	-0.887
0.1599	0.8091	-0.325	117.38	137.63	117.62	137.91	3.63	-1.401
0.2404	0.8038	-0.443	117.59	137.35	117.80	137.72	2.89	-1.701
0.3506	0.796	-0.556	117.75	137.19	117.98	137.63	2.06	-1.916
0.4399	0.7891	-0.582	117.94	136.89	118.18	137.42	1.57	-1.909
0.5601	0.7792	-0.575	118.13	136.68	118.34	137.06	1.1	-1.714
0.6558	0.7708	-0.537	118.31	136.49	118.57	136.71	0.84	-1.439
0.7399	0.7629	-0.462	118.48	136.30	118.79	136.29	0.64	-1.171
0.8498	0.7521	-0.332	118.65	136.09	118.94	135.71	0.53	-0.671
0.9399	0.7426	-0.169	118.82	135.88	119.16	135.14	0.43	-0.274
1	0.7357	0	-	-	-	-	0.37	0
T = 303.15 K								
0	0.8152	0	-	-	-	-	5.03	0
0.0812	0.8105	-0.209	117.98	138.34	118.18	138.59	3.95	-0.705
0.1599	0.8056	-0.376	118.10	138.11	118.37	138.52	3.13	-1.157
0.2404	0.8002	-0.504	118.31	137.83	118.55	138.33	2.5	-1.411

**Table 2.** Continued

0.3506	0.7923	-0.627	118.46	137.66	118.72	138.23	1.85	-1.541
0.4399	0.7854	-0.686	118.65	137.36	118.92	138.02	1.44	-1.531
0.5601	0.7752	-0.679	118.84	137.15	119.08	137.66	1	-1.411
0.6558	0.7666	-0.621	119.01	136.96	119.30	137.30	0.78	-1.184
0.7399	0.7585	-0.538	119.18	136.76	119.52	136.88	0.62	-0.951
0.8498	0.7473	-0.377	119.35	136.55	119.67	136.29	0.5	-0.555
0.9399	0.7376	-0.201	119.52	136.34	119.88	135.72	0.4	-0.228
1	0.7304	0	-	-	-	-	0.35	0
T = 308.15 K								
0	0.8116	0	-	-	-	-	4.3	0
0.0812	0.807	-0.248	118.72	138.84	118.93	139.19	3.42	-0.562
0.1599	0.802	-0.427	118.84	138.61	119.12	139.12	2.74	-0.929
0.2404	0.7966	-0.582	119.05	138.33	119.30	138.93	2.2	-1.151
0.3506	0.7886	-0.721	119.19	138.15	119.46	138.82	1.57	-1.341
0.4399	0.7815	-0.773	119.38	137.85	119.66	138.61	1.27	-1.287
0.5601	0.7711	-0.761	119.57	137.64	119.82	138.25	0.95	-1.131
0.6558	0.7622	-0.696	119.73	137.45	120.03	137.88	0.75	-0.951
0.7399	0.7539	-0.603	119.90	137.24	120.25	137.46	0.62	-0.743
0.8498	0.7424	-0.413	120.07	137.03	120.40	136.86	0.48	-0.449
0.9399	0.7323	-0.207	120.23	136.82	120.60	136.29	0.38	-0.183
1	0.725	0	-	-	-	-	0.33	0

$$\overline{V_2^\infty} = V_2^0 + \sum_{j=0}^{j=n} A_j \quad (10)$$

and

$$V_{\phi 2} = (V_m - x_1 V_1^0) / x_2 \quad (12)$$

where the partial molar volumes at infinite dilution of MTBE is  $\overline{V_1^\infty}$ , and 1-alkanol is  $\overline{V_2^\infty}$ . We have additionally computed partial molar volume at infinite dilution through apparent molar volumes by the following equations:

$$V_{\phi 1} = (V_m - x_2 V_2^0) / x_1 \quad (11)$$

where apparent molar volume of MTBE in 1-alkanol is  $V_{\phi 1}$ , and the apparent molar volume of alcohols in MTBE is  $V_{\phi 2}$ .

By merging Eqs. of (1), (11) and (12):

$$V_{\phi 1} = V_1^0 + (V_m^E / x_1) \quad (13)$$

**Table 3.** Coefficients  $A_j$  of the Fitting Equation (3) and Standard Deviations  $\sigma$  for Excess Molar Volume at Different Temperatures

T (K)	$A_0$ (cm <sup>3</sup> mol <sup>-1</sup> )	$A_1$ (cm <sup>3</sup> mol <sup>-1</sup> )	$A_2$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\sigma$ (cm <sup>3</sup> mol <sup>-1</sup> )
$x_1$ MTBE + $x_2$ 1-butanol				
293.15	-3.152	0.168	0.212	0.023
298.15	-3.535	0.112	-0.16	0.009
303.15	-3.85	0.155	-0.307	0.018
308.15	-4.188	0.11	-0.149	0.015
$x_1$ MTBE + $x_2$ 1-pentanol				
293.15	-2.902	0.131	-0.025	0.012
298.15	-3.124	0.047	0.007	0.016
303.15	-3.463	0.099	-0.271	0.016
308.15	-3.848	0.103	-0.245	0.011
$x_1$ MTBE + $x_2$ 1-hexanol				
293.15	-2.459	0.021	-0.179	0.009
298.15	-2.716	0.024	-0.318	0.014
303.15	-3.112	0.067	-0.292	0.013
308.15	-3.483	0.073	-0.337	0.011
$x_1$ MTBE + $x_2$ 1-heptanol				
293.15	-2.079	0.064	-0.029	0.005
298.15	-2.357	0.064	-0.288	0.014
303.15	-2.738	0.089	-0.313	0.013
308.15	-3.098	0.019	-0.305	0.011

and

have computed partial molar volumes at infinite dilution:

$$V_{\phi 2} = V_2^0 + (V_m^E / x_2) \quad (14)$$

$$V_m^E / x_1 x_2 = (V_{\phi 1} - V_1^0) / x_2 \quad (15)$$

extrapolations of  $V_{\phi 1}$  to  $x_1 = 0$  and  $V_{\phi 2}$  to  $x_2 = 0$  lead to  $\overline{V_1^\infty}$  and  $\overline{V_2^\infty}$ , respectively.

Through modifying the Eq. (13) and deviation by  $x_2$ , we

Linear extrapolations represented by  $V_m^E / x_1 x_2$  to  $x_1 = 0$  and  $V_m^E / x_1 x_2$  to  $x_2 = 0$  lead to  $\overline{V_1^\infty}$  and  $\overline{V_2^\infty}$ , respectively.

The partial molar volume and apparent molar volume

**Table 4.** Coefficients  $A_j$  of the Fitting Equation (3) and Standard Deviations  $\sigma$  for Viscosity Deviation at Different Temperatures

T (K)	$A_0$ (mPa.s)	$A_1$ (mPa.s)	$A_2$ (mPa.s)	$\sigma$ (mPa.s)
$x_1 \text{MTBE} + x_2 \text{1-butanol}$				
293.15	-3.385	-2.151	-1.145	0.015
298.15	-2.907	-1.765	-0.801	0.012
303.15	-2.534	-1.466	-0.423	0.008
308.15	-2.06	-1.215	-0.548	0.008
$x_1 \text{MTBE} + x_2 \text{1-pentanol}$				
293.15	-4.814	-2.884	-1.501	0.019
298.15	-4.006	-2.335	-1.265	0.018
303.15	-3.515	-1.987	-0.675	0.014
308.15	-2.789	-1.535	-0.689	0.009
$x_1 \text{MTBE} + x_2 \text{1-hexanol}$				
293.15	-6.619	-3.907	-1.739	0.016
298.15	-5.429	-3.009	-1.215	0.014
303.15	-4.505	-2.524	-1.113	0.009
308.15	-3.732	-1.961	-0.823	0.021
$x_1 \text{MTBE} + x_2 \text{1-heptanol}$				
293.15	-8.949	-4.671	-1.779	0.038
298.15	-7.313	-3.531	-1.341	0.031
303.15	-5.941	-2.847	-1.241	0.026
308.15	-4.935	-2.522	-0.625	0.016

values are reported in Table 2. The partial molar volumes at infinite dilution of MTBE and 1-alkanol using other methods are shown in Tables 5 and 6.

The values of excess molar volume ( $V_m^E$ ) for the binary systems containing MTBE and 1-alkanol using Eq. (3) and at  $T = 298.15$  K are shown in Fig. 1. For all binary systems studied, over the whole composition range,  $V_m^E$  is negative and around 0.45 to 0.55 mole fraction of MTBE and it becomes more negative in sequence: 1-hexanol < 1-heptanol < 1-pentanol < 1-butanol. Negative values of  $V_m^E$  can be due to three types of interactions between molecular components of liquid mixtures: 1) physical interaction 2) chemical interaction 3) structural contribution [2,10,14]. The values of excess molar volume for binary liquid mixtures containing MTBE and 1-alkanols have been related with hydrogen bonding and formation of complex between MTBE, 1-alkanol and structural effects [10,14,35-38]. By expanding alkyl chain length alcohol, the

chemical interactions get to be weaker.

The values of viscosity deviation ( $\Delta\eta$ ) for the binary systems containing MTBE and 1-alkanol using Eq. (3) and at  $T = 298.15$  K are shown in Fig. 2. The values of viscosity deviations are negative for all binary liquid systems studied and the values diminish in the arrangement: 1-butanol < 1-pentanol < 1-hexanol < 1-heptanol. The negative values of viscosity deviation have been reported in different forms by many authors [19,20,37,39]. By comparing binary mixtures containing MTBE and pure form of 1-alkanols can be found that due to strong intermolecular force reduction, 1-alkanols molecular can move easier in mixture mode [40]. Huge amount of negative values of viscosity deviation may be due to demolition of orientation order [40,41].

The partial molar volumes at infinite dilution and excess partial molar volumes at infinite dilution of each component for all binary systems are reported in Tables 5 and 6. The partial molar volume at infinite dilution of each component

**Table 5.** Partial Molar Volumes at Infinite Dilution of MTBE in 1-Alkanols at Different Temperatures and Atmospheric Pressure

T (K)	$V_i^0$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\overline{V}_i^\infty$ from Eq. (9)	$\overline{V}_i^\infty$ from Eq. (13)	$\overline{V}_i^\infty$ from Eq. (15)	$\overline{V}_i^{E,\infty}$ from Eq. (7)
$x_1$ MTBE + $x_2$ 1-butanol					
293.15	119.01	115.58	115.16	115.17	-2.791
298.15	119.86	116.27	115.85	115.80	-2.931
303.15	120.73	117.03	116.71	116.74	-3.046
308.15	121.62	117.82	117.38	117.39	-3.157
$x_1$ MTBE + $x_2$ 1-pentanol					
293.15	119.01	114.79	114.53	114.47	-3.083
298.15	119.85	115.47	115.36	115.36	-3.114
303.15	120.72	116.18	116.06	116.03	-3.214
308.15	121.61	116.90	116.93	116.87	-3.329
$x_1$ MTBE + $x_2$ 1-hexanol					
293.15	119.01	114.42	115.67	115.67	-2.823
298.15	119.86	115.02	115.95	116.01	-3.031
303.15	120.73	115.67	116.86	116.82	-3.146
308.15	121.62	116.33	117.75	117.74	-3.274
$x_1$ MTBE + $x_2$ 1-heptanol					
293.15	119.01	113.84	114.12	114.12	-2.941
298.15	119.86	114.43	114.38	114.43	-3.121
303.15	120.72	115.08	115.25	115.21	-3.194
308.15	121.61	115.73	116.11	116.10	-3.283

( $\overline{V}_i$  and  $\overline{V}_2^\infty$ ) is a little lower than the molar volumes of the pure ones ( $V_i$  and  $V_2$ ).

## CONCLUSIONS

In this work, density and viscosity data are reported for

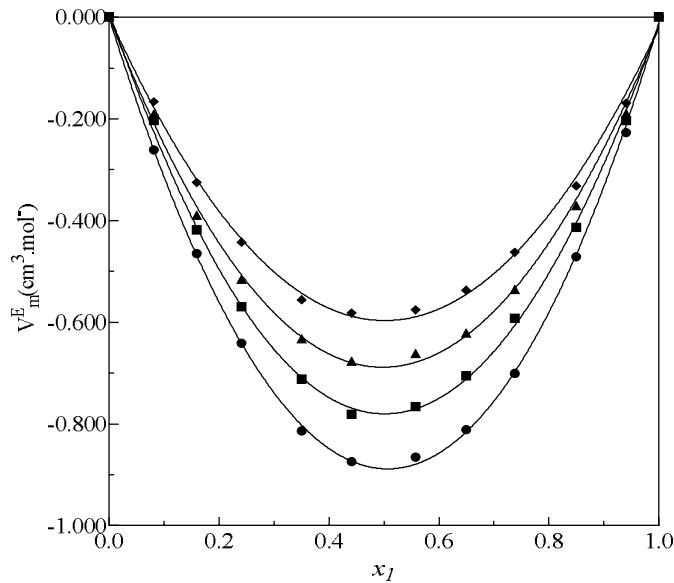
four binary mixtures of MTBE with 1-butanol, 1-pentanol, 1-hexanol or 1-heptanol. Data are taken at the temperature range from 293.15-308.15 K covering the composition range at atmospheric pressure. For the whole composition and temperature ranges, the excess molar volume ( $V^E$ ) and the viscosity deviation ( $\Delta\eta$ ) showed negative values.

**Table 6.** Partial Molar Volumes at Infinite Dilution of 1-Alkanols in MTBE at Different Temperatures and Atmospheric Pressure

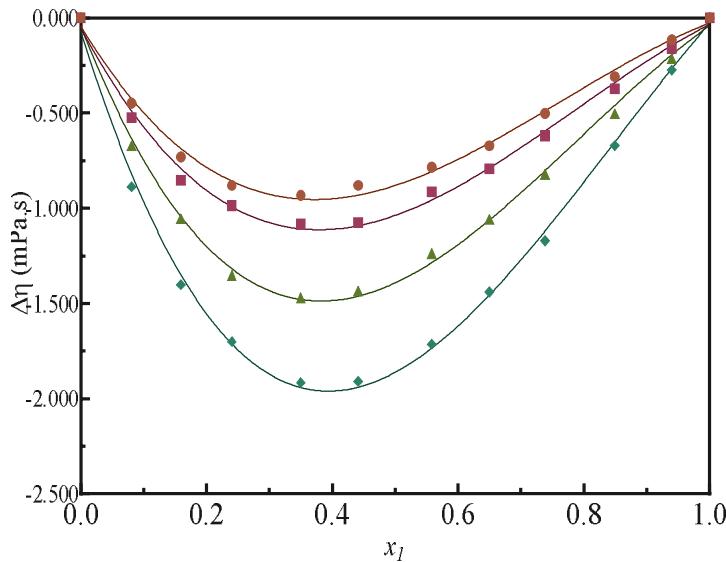
T (K)	$V_2^0$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\overline{V}_2^\infty$ from Eq. (9)	$\overline{V}_2^\infty$ from Eq. (13)	$\overline{V}_2^\infty$ from Eq. (15)	$\overline{V}_2^{E,\infty}$ from Eq. (8)
$x_1$ MTBE + $x_2$ 1-butanol					
293.15	91.55	88.75	87.62	87.61	-3.401
298.15	91.98	89.05	87.99	88.06	-3.457
303.15	92.42	89.37	88.37	88.37	-3.651
308.15	92.87	89.71	88.79	88.76	-3.752
$x_1$ MTBE + $x_2$ 1-pentanol					
293.15	108.24	105.16	103.24	103.25	-4.114
298.15	108.72	105.61	103.56	103.53	-4.275
303.15	109.22	106.00	103.81	103.79	-4.441
308.15	109.72	106.39	104.10	104.07	-4.610
$x_1$ MTBE + $x_2$ 1-hexanol					
293.15	124.78	121.95	119.95	119.99	-4.499
298.15	125.32	122.29	120.17	120.21	-4.727
303.15	125.88	122.73	120.35	120.40	-4.954
308.15	126.44	123.16	120.58	120.52	-5.189
$x_1$ MTBE + $x_2$ 1-heptanol					
293.15	138.01	136.89	135.23	135.26	-4.784
298.15	138.56	135.64	133.75	133.78	-4.928
303.15	139.21	134.81	132.57	132.61	-5.124
308.15	139.84	134.19	131.69	131.62	-5.219

Generally, the physical or dispersive interactions are dominant, mainly due to breaking the hydrogen bonds. These data are also complemented with the partial molar

obtained from Redlich-Kister polynomials. These new results can improve the knowledge of interactions among polar and non-polar compositions in binary mixtures.



**Fig. 1.** Plot of excess molar volume as a function of mole fraction of MTBE for  $x_1$  MTBE +  $x_2$  1-alkanol mixtures at  $T = 298.15\text{ K}$  and  $p = 0.1\text{ MPa}$ : ●,  $x_1$  MTBE +  $x_2$  1-butanol; ■,  $x_1$  MTBE +  $x_2$  1-pentanol; ▲,  $x_1$  MTBE +  $x_2$  1-heptanol; ♦,  $x_1$  MTBE +  $x_2$  1-hexanol. The solid lines have been drawn from Eq. (3) using parameters listed in Table 3.



**Fig. 2.** Plot of viscosity deviation as a function of mole fraction of MTBE for  $\{x_1\text{ MTBE} + x_2\text{ alcohol}\}$  mixtures at  $T = 298.15\text{ K}$  and  $p = 0.1\text{ MPa}$ : ●,  $x_1$  MTBE +  $x_2$  1-butanol; ■,  $x_1$  MTBE +  $x_2$  1-pentanol; ▲,  $x_1$  MTBE +  $x_2$  1-heptanol; ♦,  $x_1$  MTBE +  $x_2$  1-hexanol. The solid lines have been drawn from Eq. (3) using parameters listed in Table 4.

## Nomenclature

$A_i$	coefficients of the Redlich-Kister polynomial
$N$	number of experimental data
$n$	number of estimated parameters
$R$	universal gas constant
$T$	absolute temperature, K
$V$	molar volume mixture, $\text{cm}^3 \text{ mol}^{-1}$
$V^E$	excess volume, $\text{cm}^3 \text{ mol}^{-1}$
$V_i$	molar volume of species i, $\text{cm}^3 \text{ mol}^{-1}$
$\overline{V}_i$	partial molar volumes of species i, $\text{cm}^3 \text{ mol}^{-1}$
$\overline{V}_i^E$	excess partial molar volumes of species i, $\text{cm}^3 \text{ mol}^{-1}$
$\overline{V}_i^\infty$	partial molar volume at infinite dilution of species i, $\text{cm}^3 \text{ mol}^{-1}$
$\overline{V}_i^{E,\infty}$	excess partial molar volume at infinite dilution of species i, $\text{cm}^3 \text{ mol}^{-1}$
$x_i$	mole fraction of species i, $\text{mol mol}^{-1}$
$Y^E$	dependent variable
$\Delta\eta$	dynamic viscosity deviations, $\text{mPa s}$
$\eta$	dynamic viscosity of the mixture, $\text{mPa s}$
$\eta_i$	dynamic viscosity of pure component i, $\text{mPa s}$
$\rho$	densities of the mixture, $\text{g cm}^{-3}$
$\rho_i$	densities of species i, $\text{g cm}^{-3}$
$\sigma$	Standard deviation

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