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Liquid Densities and Excess Volumes of Diisopropyl Ether (DIPE) + 1-Butanol Mixtures from 273 to 473 K and Pressures up to 35 MPa

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Densities of five gravimetrically prepared diisopropyl ether + 1-butanol mixtures in the liquid state at different compositions have been measured with a computer-controlled high-temperature high-pressure vibrating tube densimeter system (DMA-HDT). The uncertainty in the density measurement was estimated to be lower than ±0.2 $kg \cdot m^{-3}$. The densities were measured for temperatures from 273 K to 473 K and pressures up to 35 MPa (~320 data points for each mixture), which covered a density range between (518 and 830) $kg \cdot m^{-3}$ and an excess volume range between (−0.02 and −5) $cm^3 \cdot mol^{-1}$. Densities of 1-butanol were also measured in the same temperature and pressure ranges. The experimental data were correlated with the new three-dimensional density correlation system (TRIDEN); excess volumes were calculated using the densities already published for diisopropyl ether. The excess volumes and the densities of 1-butanol are compared with published data.

Introduction

For the density measurements as a function of temperature and pressure, a computer-controlled high-temperature high-pressure vibrating tube densimeter system (DMA-HDT) was developed.[1−3] Densities for several pure components for the compressed liquid and the supercritical states have already been published.[1−5] In this work the densities of diisopropyl ether + 1-butanol mixtures were measured with the objective to check the accuracy of the experimental technique for the reliable determination of excess volumes.

For this purpose densities of five gravimetrically prepared diisopropyl ether (1) + 1-butanol (2) mixtures with $x_1 = 0.2001$, 0.3508, 0.5001, 0.6503, and 0.8000 have been investigated. The densities were measured for temperatures from 273 K to 473 K and pressures up to 35 MPa (~320 data points for each mixture). Additionally, the required pure component densities of 1-butanol were measured. The required densities of DIPE have already been published.[5] The experimental data were correlated with the new three-dimensional density correlation system (TRIDEN); excess volumes were calculated, and the results were compared with published data. Details of the measurement system, the calibration, and the correlation model can be found in refs 1 and 2.

Experimental Section

Diisopropyl ether (DIPE, $C_6H_{14}O$, $M = 102.18$ $g \cdot mol^{-1}$, CAS-RN 108-20-3) and 1-butanol ($C_4H_{10}O$, $M = 74.12$ $g \cdot mol^{-1}$, CAS-RN 71-36-3) were both obtained from Aldrich. All compounds were stored over 3 Å molecular sieves and degassed by distillation. The final purities were checked by gas chromatography (DIPE and 1-butanol: >99.8 mass %) and by Karl Fischer titration (water content of DIPE: <10 ppm; of 1-butanol: <15 ppm).

A computer-operated vibrating tube densimeter system for high temperatures and pressures (temperatures from 273 K to 623 K and pressures up to 40 MPa) was used for the measurement of the density data for the five DIPE + 1-butanol mixtures and for the pure 1-butanol. The automated equipment can be used for the determination of densities in the sub- and supercritical states. With this apparatus, a large number of data points can be obtained in a rather short time with a minimum of manual effort. A temperature and pressure program can be driven to obtain a complete $P\rho T$ field for the desired component or mixture. The measurement system was developed in the thesis of Ihmels.[3] Densities of several liquids and liquefied gases (e.g. toluene, carbon dioxide, carbonyl sulfide, hydrogen sulfide, sulfur hexafluoride, dinitrogen monoxide, and R227ea) have already been published.[1−4] The comparison with reference equations of state (EoS's) for toluene, CO_2, and SF_6 demonstrated the high accuracy and suitability of this measurement system.

The apparatus and procedure of the measurements were described in detail by Ihmels and Gmehling.[1,2] A prototype of a high-pressure high-temperature vibrating tube densimeter (DMA-HDT) is the essential part of the experimental setup. The temperature is measured using a Pt100 resistance thermometer, and the pressure is monitored by means of a calibrated external pressure sensor (model PDCR 911, pressure range 60 MPa, Druck). The density values are obtained from the periods of oscillation of the vibrating tube. For the calibration, the period of oscillation at zero pressure and the two reference substances water and butane were used. The reference densities were calculated using the reference EoS from Pruss and Wagner[6,7] for water and the EoS from Younglove and Ely[8] for butane. The uncertainty of the temperature is estimated to be ±0.03 K, and the pressure has an estimated uncertainty of ±6 kPa. For density measurements in the temperature and pressure ranges covered (273 K to 473 K; 0.3 MPa to 35 MPa) a maximum error of ±0.2 $kg \cdot m^{-3}$ is estimated.

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Table 1. Parameters for the TRIDEN Correlation Model for Diisopropyl Ether (DIPE) (1) + 1-Butanol (2) Mixtures: Temperature Range, Pressure Range, Number of Data Points, Tait Parameters, Rackett Parameters, and Absolute (RMSD) and Relative (RMSDr) Root Mean Square Deviations, and the Mean Deviation (bias) as Statistical Values for the TRIDEN Fit

	$x_1 = 0.2001$	$x_1 = 0.3508$	$x_1 = 0.5001$	$x_1 = 0.6503$	$x_1 = 0.8000$
T_{min}/K	273	273	273	273	273
T_{max}/K	473	473	473	473	473
P_{min}/MPa	0.35	0.32	0.35	0.34	0.34
P_{max}/MPa	35	35	35	35	35
ρ_{min}/kg·m^{-3}	591.5	564.0	542.7	518.0	497.1
ρ_{max}/kg·m^{-3}	829.8	818.7	808.6	797.5	787.6
data points	328	314	328	328	328
C_T	0.083 016 6	0.083 104 2	0.083 711 6	0.083 808 5	0.083 857 3
b_0/MPa	411.272	300.368	361.622	344.773	360.601
b_1/MPa	−178.973	−99.2811	−153.303	−148.693	−167.387
b_2/MPa	26.9397	6.488 90	20.5107	20.0757	25.2760
b_3/MPa	−1.508 09	0.278 706	−0.869 019	−0.837 653	−1.261 80
E_T/K	100	100	100	100	100
P_0/MPa	2.0	2.0	2.0	2.0	2.0
A_R/kg·m^{-3}	58.1042	1.157 59	77.4368	96.7465	126.980
B_R	0.243 629	0.034 607 7	0.281 528	0.315 002	0.359 812
C_R/K	530.778	543.086	514.538	504.901	493.772
D_R	0.200 445	0.084 809 8	0.250 033	0.288 386	0.351 817
RMSD/kg·m^{-3}	0.1711	0.1576	0.1581	0.1261	0.1210
RMSDr/%	0.0237	0.0206	0.0215	0.0182	0.0177
bias/kg·m^{-3}	0.0218	0.0232	0.0253	0.0244	0.0227

The mixtures were prepared from the degassed pure liquids by mass with an uncertainty in the mole fraction of ±0.0002. Therefore, the excess molar volume should be accurate to within ±0.02 cm^3·mol^{-1}.

Results and Discussion

In this work, the densities of five gravimetrically prepared diisopropyl ether (1) + 1-butanol (2) mixtures with $x_1 = 0.2001$, 0.3508, 0.5001, 0.6503, and 0.8000 (∼320 data points for each mixture) in the compressed liquid state were measured from 273 K to 473 K at 5 K intervals and from 0.3 MPa up to 35 MPa at 5 MPa intervals. The measurements covered a density range between (518 and 830) kg·m^{-3}. Densities of 1-butanol were measured in the same temperature range and at pressures up to 40 MPa (336 data points), which covers a density range between (621 and 848) kg·m^{-3}. The measured density values (mixtures and 1-butanol) are available as Supporting Information.

For each mixture and for the pure components, the measured densities were correlated with the three-dimensional $P\rho T$-correlating model TRIDEN.[1−3,5] In this model the Tait equation for isothermal compressed densities was combined with a modified Rackett equation for the liquid saturation densities and the Wagner vapor pressure equation in the "2.5,5" form, used as a reference state (ρ_0 and P_0), which is required for the Tait equation. Using these equations, it is possible to correlate the $P\rho T$ data in the whole liquid state up to the critical point, nearly within experimental error. For DIPE and 1-butanol the required parameters for the Wagner equation (eq 1) are taken from the *Dortmund Data Bank for Pure Component Properties*.[9] These parameters were fitted using experimental vapor pressure data from different sources.

$$\ln(P_0/\text{kPa}) = \ln(P_c/\text{kPa}) + \frac{A_W(1 - T_r) + B_W(1 - T_r)^{1.5} + C_W(1 - T_r)^{2.5} + D_W(1 - T_r)^5}{T_r} \quad (1)$$

At temperatures below the normal boiling point, the reference pressure is set to $P_0 = 0.1013$ MPa (for the pure components). The densities and correlation parameters for DIPE were already published.[5]

Table 2. Parameters for the TRIDEN Correlation Model for Diisopropyl Ether (DIPE) and 1-Butanol: Temperature Range, Pressure Range, Number of Data Points, Tait Parameters, Rackett Parameters, Wagner Parameters, Critical Temperature, Critical Pressure, Normal Boiling Point, Molar Mass, and Absolute (RMSD) and Relative (RMSDr) Root Mean Square Deviations, and the Mean Deviation (bias) as Statistical Values for the TRIDEN Fit

	DIPE	1-butanol
T_{min}/K	273.2	273
T_{max}/K	473.1	473
P_{min}/MPa	0.34	0.29
P_{max}/MPa	35	40
ρ_{min}/kg·m^{-3}	470.9	621.4
ρ_{max}/kg·m^{-3}	773.8	847.6
data points	328	336
C_T	0.082 860 8	0.081 878 1
b_0/MPa	317.385	554.181
b_1/MPa	−146.968	−283.562
b_2/MPa	21.7937	54.4330
b_3/MPa	−1.039 11	−3.955 24
E_T/K	100	100
A_R/kg·m^{-3}	52.1000	87.2765
B_R	0.232 377	0.297 345
C_R/K	505.577	533.383
D_R	0.253 450	0.222 845
RMSD/kg·m^{-3}	0.2421	0.2356
RMSDr/%	0.0353	0.0326
bias/kg·m^{-3}	0.0138	0.0168
A_W	−7.362 13	−8.029 81
B_W	1.918 67	0.804 066
C_W	−5.893 25	−5.569 40
D_W	12.1373	−6.106 76
T_c/K	500.0	562.9
P_c/kPa	2877.6	4417.8
T_b/K	341.5	390.8
M/g·mol^{-1}	102.18	74.12

To simplify the model and make it applicable for the correlation of mixtures, the Wagner vapor pressure equation was omitted. Therefore, a fixed reference pressure $P_0 = 2$ MPa for all temperatures was used for the mixtures. The reference densities ρ_0 at $P_0 = 2$ MPa were calculated from the compressed liquid density measurements and correlated with the modified Rackett equation (eq 2):

$$\rho_0 = A_R/B_R^{[1+(1-(T/C_R)^{D_R})]} \quad (2)$$

Table 3. Calculated Molar Excess Volumes V^E of Diisopropyl Ether (1) + 1-Butanol (2) Mixtures at Selected Temperatures and Pressures

		V^E/cm^3·mol^{-1}						
T/K	x_1	P/MPa = 0.1	P/MPa = 2.5	P/MPa = 5	P/MPa = 10	P/MPa = 20	P/MPa = 30	P/MPa = 35
273.15	0.2001	−0.6469	−0.6305	−0.6146	−0.5866	−0.5424	−0.5094	−0.4960
273.15	0.3508	−0.9604	−0.9366	−0.9135	−0.8730	−0.8095	−0.7623	−0.7431
273.15	0.5001	−1.0875	−1.0586	−1.0307	−0.9817	−0.9050	−0.8481	−0.8250
273.15	0.6503	−1.0842	−1.0530	−1.0227	−0.9697	−0.8866	−0.8250	−0.7999
273.15	0.8	−0.9266	−0.8991	−0.8723	−0.8254	−0.7519	−0.6974	−0.6752
298.15	0.2001	−0.7692	−0.7428	−0.7177	−0.6742	−0.6078	−0.5599	−0.5406
298.15	0.3508	−1.1464	−1.1068	−1.0691	−1.0043	−0.9057	−0.8348	−0.8065
298.15	0.5001	−1.2661	−1.2205	−1.1771	−1.1030	−0.9912	−0.9116	−0.8801
298.15	0.6503	−1.1994	−1.1541	−1.1110	−1.0376	−0.9280	−0.8510	−0.8207
298.15	0.8	−0.9654	−0.9283	−0.8928	−0.8325	−0.7430	−0.6803	−0.6558
323.15	0.2001	−0.9022	−0.8607	−0.8221	−0.7574	−0.6632	−0.5986	−0.5735
323.15	0.3508	−1.3381	−1.2751	−1.2167	−1.1193	−0.9784	−0.8821	−0.8447
323.15	0.5001	−1.4571	−1.3858	−1.3199	−1.2110	−1.0557	−0.9514	−0.9114
323.15	0.6503	−1.3340	−1.2663	−1.2038	−1.1014	−0.9577	−0.8634	−0.8277
323.15	0.8	−1.0172	−0.9651	−0.9165	−0.8375	−0.7280	−0.6569	−0.6304
373.15	0.2001		−1.1242	−1.0317	−0.8928	−0.7216	−0.6219	−0.5865
373.15	0.3508		−1.6135	−1.4752	−1.2700	−1.0204	−0.8768	−0.8262
373.15	0.5001		−1.7384	−1.5816	−1.3525	−1.0809	−0.9291	−0.8765
373.15	0.6503		−1.5419	−1.3959	−1.1865	−0.9457	−0.8160	−0.7722
373.15	0.8		−1.0747	−0.9699	−0.8224	−0.6577	−0.5718	−0.5434
423.15	0.2001		−1.5349	−1.2630	−0.9431	−0.6554	−0.5288	−0.4898
423.15	0.3508		−2.0946	−1.6992	−1.2484	−0.8606	−0.6968	−0.6472
423.15	0.5001		−2.2606	−1.8013	−1.2926	−0.8713	−0.7000	−0.6491
423.15	0.6503		−2.0030	−1.5651	−1.0945	−0.7198	−0.5730	−0.5304
423.15	0.8		−1.3094	−1.0013	−0.6838	−0.4444	−0.3552	−0.3300
473.15	0.2001		−3.2759	−1.8160	−0.9114	−0.4261	−0.2578	−0.2064
473.15	0.3508		−4.6619	−2.4204	−1.1164	−0.4531	−0.2258	−0.1558
473.15	0.5001		−5.0539	−2.4367	−1.0522	−0.4100	−0.2013	−0.1375
473.15	0.6503		−4.3579	−1.9050	−0.7590	−0.2968	−0.1630	−0.1235
473.15	0.8		−2.6855	−0.9950	−0.3252	−0.1101	−0.0638	−0.0519

For the Tait eq 3

$$\rho = \rho_0 / \left[1 - C_T \ln\left(\frac{B_T + P}{B_T + P_0}\right)\right] \tag{3}$$

the following temperature dependence is used for the parameter B_T:

$$B_T = b_0 + b_1\frac{T}{E} + b_2\left(\frac{T}{E}\right)^2 + b_3\left(\frac{T}{E}\right)^3 \tag{4}$$

The parameter C_T is a temperature independent constant.

To evaluate the correlations, the absolute (RMSD) and relative (RMSDr) root-mean-square deviations and the mean deviation (bias) are used as statistical values for the TRIDEN fits.

$$\mathrm{RMSD} = \sqrt{\frac{1}{n}\sum_n (\rho_{\mathrm{exp}} - \rho_{\mathrm{calc}})^2} \tag{5}$$

$$\mathrm{RMSDr} = 100\sqrt{\frac{1}{n}\sum_n \left(\frac{\rho_{\mathrm{exp}} - \rho_{\mathrm{calc}}}{\rho_{\mathrm{exp}}}\right)^2} \tag{6}$$

$$\mathrm{bias} = \frac{1}{n}\sum_n (\rho_{\mathrm{exp}} - \rho_{\mathrm{calc}}) \tag{7}$$

The TRIDEN parameters for the Tait equation, the Rackett equation, and the Wagner equation (only for the pure components), the temperature and pressure range covered, and additional statistical values are given in Table 1 for the mixtures and in Table 2 for the pure components DIPE and 1-butanol.

For an easy application of the correlations, a TRIDEN Excel Add-In was developed for the calculation of densities and derived properties (e.g., compressibilities) as a function of temperature and pressure.

The molar excess volume of a binary mixture can be calculated by

$$V^E = x_1 M_1\left(\frac{1}{\rho_{\mathrm{mix}}} - \frac{1}{\rho_1}\right) + x_2 M_2\left(\frac{1}{\rho_{\mathrm{mix}}} - \frac{1}{\rho_2}\right) \tag{8}$$

where x_i is the mole fraction of component i, ρ_i is the density of the pure component, ρ_{mix} is the density of the mixture, and M_i is the molar mass of component i.

For the correlation of isothermal–isobaric molar excess volumes, a Redlich–Kister polynomial

$$V^E = x_1 x_2 \sum_{i=0}^{n} A_i (2x_1 - 1)^i \tag{9}$$

is appropriate, where the adjustable A_i parameters are fitted by a least-squares method.

To calculate mixture densities or molar excess volumes as a function of temperature, pressure, and composition, a dynamic calculation function was integrated into the TRIDEN Excel Add-In. In the first step the excess volumes at a given temperature and pressure are calculated for the five compositions using eq 8 with the help of the densities calculated with the parameters given in Tables 1 and 2. In the next step these isothermal–isobaric molar excess volumes are correlated using eq 9, and in the last step, the V^E values are calculated for the desired composition. In this way, excess volumes and densities as functions of temperature, pressure, and composition can be calculated using only the TRIDEN fits for the mixture and the pure

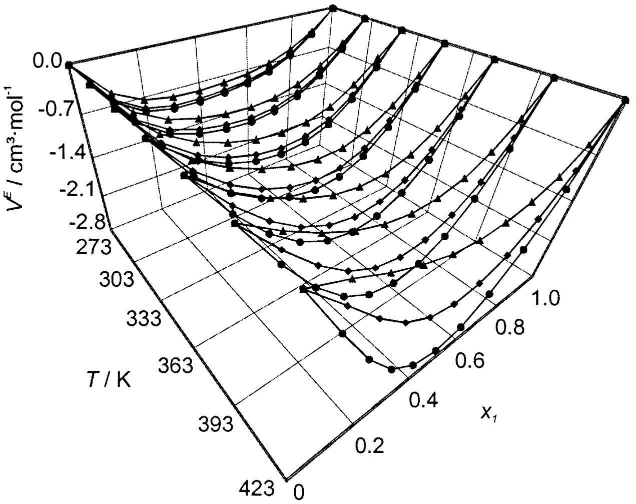

Figure 1. Excess molar volume of the binary mixture diisopropyl ether (DIPE) + 1-butanol at temperatures between 273 K and 423 K: ●, 1 MPa; ◆, 5 MPa; ▲, 20 MPa.

Table 4. Parameters A_i of Eq 9 for Molar Excess Volumes of Diisopropyl Ether (1) + 1-Butanol (2) Mixtures at Selected Temperatures and Pressures and Absolute Root Mean Square Deviations

T / K	P / MPa	A_0	A_1	A_2	A_3	RMSD / cm^3·mol^{-1}
273.15	0.1	−4.3517	0.7369	−1.5767	2.0094	0.1973
273.15	2.5	−4.2342	0.6825	−1.5137	1.9938	0.1902
273.15	5.0	−4.1225	0.6310	−1.4535	1.9797	0.1832
273.15	10.0	−3.9267	0.5408	−1.3472	1.9560	0.1705
273.15	20.0	−3.6198	0.3999	−1.1782	1.9233	0.1492
273.15	30.0	−3.3924	0.2956	−1.0504	1.9014	0.1321
273.15	35.0	−3.3001	0.2530	−0.9977	1.8933	0.1248
298.15	0.1	−5.0672	0.1946	−0.9921	2.3139	0.1235
298.15	2.5	−4.8819	0.1545	−0.9430	2.2593	0.1189
298.15	5.0	−4.7086	0.1189	−0.8976	2.2083	0.1145
298.15	10.0	−4.4119	0.0639	−0.8214	2.1172	0.1067
298.15	20.0	−3.9647	−0.0049	−0.7102	1.9729	0.0943
298.15	30.0	−3.6465	−0.0407	−0.6344	1.8598	0.0851
298.15	35.0	−3.5203	−0.0513	−0.6053	1.8117	0.0813
323.15	0.1	−5.8326	−0.2176	−0.4777	2.2930	0.0614
323.15	2.5	−5.5432	−0.2502	−0.4476	2.2098	0.0598
323.15	5.0	−5.2798	−0.2741	−0.4225	2.1321	0.0583
323.15	10.0	−4.8442	−0.2998	−0.3855	1.9956	0.0561
323.15	20.0	−4.2227	−0.3010	−0.3444	1.7769	0.0532
323.15	30.0	−3.8055	−0.2725	−0.3259	1.6047	0.0518
323.15	35.0	−3.6454	−0.2535	−0.3216	1.5309	0.0514
373.15	2.5	−6.9535	−0.5915	0.2312	0.9336	0.0075
373.15	5.0	−6.3267	−0.6481	0.2029	0.9134	0.0034
373.15	10.0	−5.4103	−0.6766	0.1425	0.8654	0.0038
373.15	20.0	−4.3236	−0.6054	0.0397	0.7617	0.0153
373.15	30.0	−3.7163	−0.4959	−0.0364	0.6569	0.0245
373.15	35.0	−3.5060	−0.4420	−0.0675	0.6078	0.0284
423.15	2.5	−9.0425	−0.4754	0.4323	−1.9337	0.0036
423.15	5.0	−7.2056	−0.8341	0.3640	−1.4631	0.0039
423.15	10.0	−5.1705	−1.0392	0.2423	−0.8599	0.0045
423.15	20.0	−3.4855	−0.9995	0.1364	−0.2728	0.0070
423.15	30.0	−2.8001	−0.9001	0.1050	−0.0088	0.0105
423.15	35.0	−2.5967	−0.8564	0.0982	0.0689	0.0123
473.15	2.5	−20.2161	−1.8746	4.4179	−3.3154	0.2832
473.15	5.0	−9.7476	−3.5786	2.6797	−1.9286	0.1821
473.15	10.0	−4.2093	−2.4625	0.9592	−1.6357	0.0856
473.15	20.0	−1.6402	−0.9755	−0.0996	−1.8608	0.0025
473.15	30.0	−0.8052	−0.2766	−0.5561	−2.0376	0.0493
473.15	35.0	−0.5501	−0.0473	−0.7157	−2.1042	0.0662

components. Other researchers often fit the Redlich−Kister parameters for every temperature and pressure. But then more than 300 fits with about 1200 parameters are required, without the possibility to interpolate in temperature and pressure.

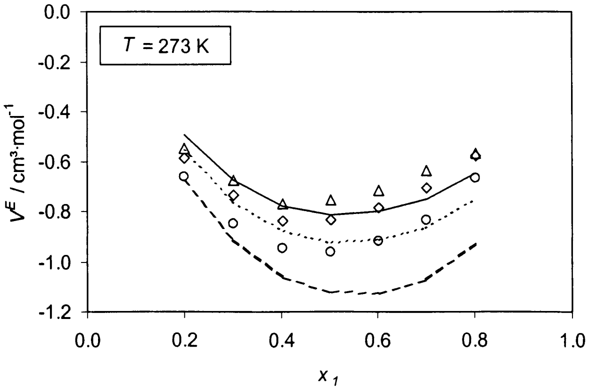

Figure 2. Excess volumes for diisopropyl ether (DIPE) (1) + 1-butanol (2) mixtures at 273 K together with literature values: ○, 0.1 MPa (ref 10); ◇, 20 MPa (ref 10); △, 40 MPa (ref 10); - - -, 0.1 MPa (this work); ···, 20 MPa (this work); —, 40 MPa (this work).

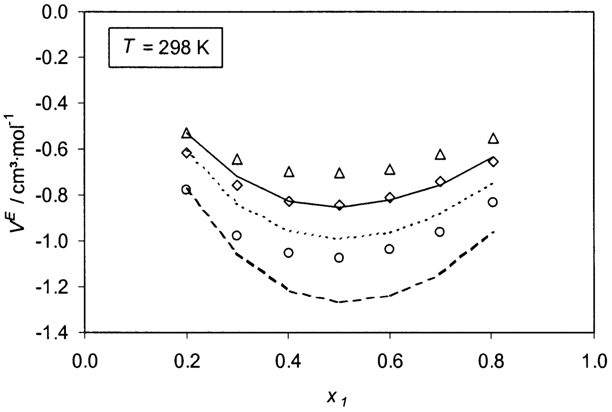

Figure 3. Excess volumes for diisopropyl ether (DIPE) (1) + 1-butanol (2) mixtures at 298 K together with literature values: ○, 0.1 MPa (ref 10); ◇, 20 MPa (ref 10); △, 40 MPa (ref 10); - - -, 0.1 MPa (this work); ···, 20 MPa (this work); —, 40 MPa (this work).

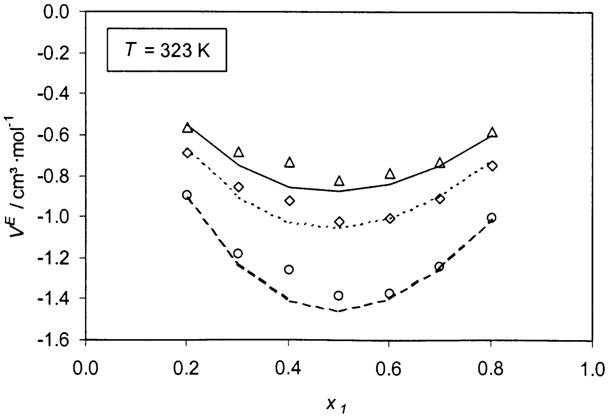

Figure 4. Excess volumes for diisopropyl ether (DIPE) (1) + 1-butanol (2) mixtures at 323 K together with literature values: ○, 0.1 MPa (ref 10); ◇, 20 MPa (ref 10); △, 40 MPa (ref 10); - - -, 0.1 MPa (this work); ···, 20 MPa (this work); —, 40 MPa (this work).

For selected temperatures and pressures, excess volumes were calculated. The calculated excess volumes and the parameters for eq 9 are given in Tables 3 and 4. The measurements covered the excess volume range between (−0.02 and −5) cm^3·mol^{-1}. A few excess volumes for the temperature range between 273 K and 423 K, at (1, 5, and 20) MPa, are presented in Figure 1.

For the system DIPE + 1-butanol, excess volumes were also published by Ulbig et al.[10] for (273, 298, and 323) K at (0.1, 20, 40, and 60) MPa. In Figures 2−4 the values of Ulbig et al. together with the calculated excess volumes of this work are shown. The calculations of the 40 MPa values are a slight extrapolation, but the TRIDEN model allows

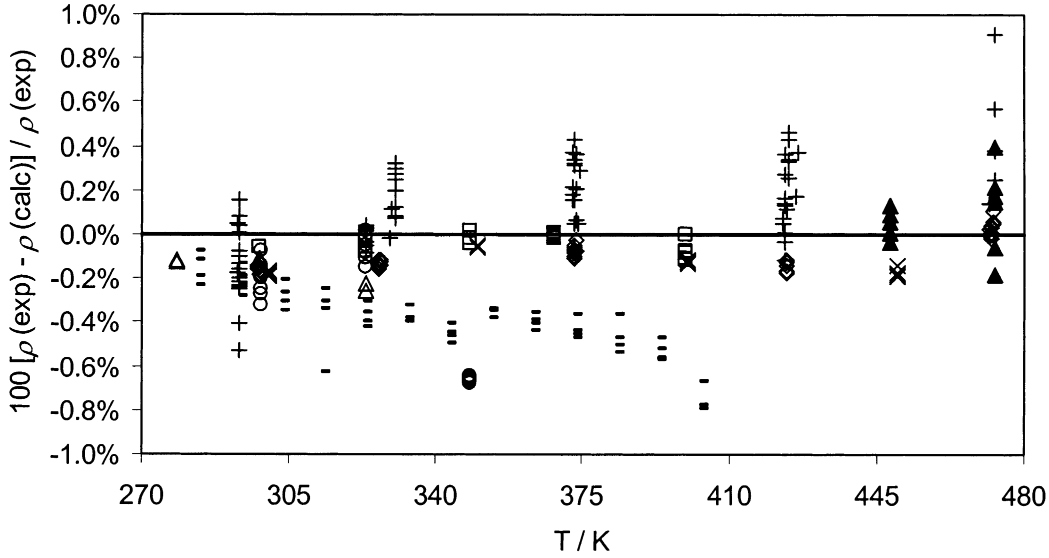

Figure 5. Relative deviations between published densities and the TRIDEN correlation for the experimental densities of 1-butanol: △, ref 10; −, ref 11; +, ref 12; □, ref 13; ▲, ref 14; ×, ref 15; ◇, ref 16; ○, ref 17.

very reliable extrapolations in pressure.[3] As can be seen qualitative agreement for all temperatures is obtained. Higher deviations are observed at 273 K and 298 K.

The accuracy of the density measurements is very important for the determination of excess volumes. Ulbig et al. estimated a maximum uncertainty of ±0.05 $kg \cdot m^{-3}$ for their vibrating tube density measurements and one of ±0.005 $cm^3 \cdot mol^{-1}$ for the determination of the excess volumes for the moderate temperature range between 273 K and 323 K. For a wide temperature range covered a higher uncertainty of ±0.2 $kg \cdot m^{-3}$ is obtained, and therefore, somewhat higher uncertainties for the determination of excess volumes are expected.

In Figure 5 the deviations between published densities[10−17] and the TRIDEN correlation of measured 1-butanol densities are shown. The range of ±1% is exceeded by some of the older data of Mamadov and Aliev[11] and of Golubev and Vagina[12] with deviations up to −2.2% (at 413 K) and +1.7% (at 473 K), respectively. Nevertheless, the measurements agree very well with the newer data of Gates et al.[13] and of Shakhverdiev et al.[14] Furthermore, the pure component densities of Ulbig et al.[10] for DIPE and 1-butanol are in agreement with the correlations with relative root mean square deviations of 0.17% for both.[5]

Summary

Density measurements in the compressed liquid state were performed for five diisopropyl ether (DIPE) + 1-butanol mixtures and for pure 1-butanol for temperatures between 273 K and 473 K and pressures up to 35 MPa using a high-temperature, high-pressure vibrating tube densimeter. All data were correlated with the TRIDEN model. Excess volumes were calculated and compared with literature values. With a few exceptions, the excess volumes show good agreement with the literature data for the temperature range covered. Also the densities of 1-butanol show very good agreement with literature data.

The high reliability of the measurement system was already demonstrated for pure component densities in the compressed liquid and supercritical states.[1−5] Therefore, the measurements on binary mixtures for the determination of excess volumes are a further step and a successful application of the technique described.

Supporting Information Available:

All measured density values for the five mixtures and for 1-butanol. This material is available free of charge via the Internet at http://pubs.acs.org.

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