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Densities, viscosities, and isobaric heat capacities of the system (1-butanol + cyclohexane) at high pressures

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ABSTRACT

The cyclohexane and the system of 1-butanol + cyclohexane have been characterized using densities, viscosities and isobaric heat capacities measurements. For that, the densities were measured in a high-pressure vibrating tube densimeter at five temperatures from (293.15 to 333.15) K and pressures up to 100 MPa. The measurements were correlated with the empirical Tamman–Tait equation.

Moreover, the isobaric heat capacities of the binary system were measured in a high-pressure automated flow calorimeter at T = (293.15 and 313.15) K and pressures up to 25 MPa for pure cyclohexane and in admixture with 1-butanol. The excess molar heat capacities were assessed for the mixture and a positive deviation from the ideality was obtained, except for a small part in the region rich in alkanol.

The viscosity measurements were carried out, at the calorimeter conditions, for correcting the experimental values of isobaric heat capacities due to friction along the tube. The viscosity was measured at atmospheric pressure in a Stabinger Anton Paar SVM 3000 viscometer in the temperature range of (293.15 to 333.15) K for cyclohexane and the mixtures. At high pressure, the viscosities were estimated using Lucas method.

1. Introduction

The increasing production and use of biofuels are a direct consequence of the European Commission and National legal acts, encouraging such production and the use of biofuels [1]. The knowledge of the thermophysical properties of these biofuels is of great importance scientifically and in particular for engineering purposes.

Numerous technologies for new generation of biofuels are being developed to produce more sustainable ones; they use different biocomponents like cellulosic ethanol, biobutanol and algae biofuels. The production of butanol from biomass and its utilization as fuel has the potential to reduce the petroleum consumption worldwide, as well as to significantly reduce the green house gas emissions and to achieve sustainability.

Recent work demonstrated that butanol can work in the internal combustion of engine designed to be use with gasoline without modification [2], but can also be blended with conventional fuel. This study focuses on the thermodynamic characterization of a new blend of 1-butanol and cyclohexane using volumetric and isobaric heat capacities measurements in order to continue the contribution to this international effort towards development and use of environmental sustainable fuels.

2. Experimental

2.1. Materials

1-Butanol and cyclohexane were purchased from Sigma–Aldrich, and all of the compounds were of the highest purity available, chromatography quality reagent (of series puriss. p.a.) with a purity >0.995 by gas chromatography, GC. They were used as provided and were also checked by gas chromatography using a HP 7890 gas chromatograph with a FID detector and checked using a Mettler Toledo C20 coulometric Karl Fischer titrator. Their mole fractions were higher than 0.997 and the quantity of water was lower than (180 and 70) ppm for each compound respectively, these characteristics are summarized in table 1.

2.2. Apparatus and procedure

Liquid mixtures were prepared by weighting with an estimated uncertainty in the mass fractions of $\pm 5 \cdot 10^{-4}$. A Sartorius CP 224 S balance was used with an accuracy of $\pm 1 \cdot 10^{-4}$ g. Before the

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TABLE 1
Material description.

Chemical name	Source	Mass fraction purity (GC)	Purification method	Water content
1-Butanol	Sigma–Aldrich	⩾0.997	None	⩽180 ppm
Cyclohexane	Sigma–Aldrich	⩾0.997	None	⩽70 ppm

measurements all the substances were degassed using a Branson 3210 ultrasound bath for at least 15 min at room temperature.

The densities were measured using an Anton Paar DMA HPM vibrating-tube densimeter described in detail previously [3]. This model is suitable for the high accurate determination of density in the range (0 to 3) $g \cdot cm^{-3}$, with a resolution of 10^{-5} $g \cdot cm^{-3}$.

TABLE 2
Experimental densities for cyclohexane at different pressures and temperatures.[a]

p/MPa	ρ/($g \cdot cm^{-3}$)				
	T/K				
	293.15	303.15	313.15	323.15	333.15
			Cyclohexane		
0.1	0.7784	0.7690	0.7597	0.7501	0.7403
1.0	0.7791	0.7698	0.7603	0.7508	0.7411
2.0	0.7799	0.7707	0.7612	0.7518	0.7422
5.0	0.7824	0.7733	0.7640	0.7548	0.7455
10.0	0.7863	0.7775	0.7684	0.7595	0.7505
15.0	0.7899	0.7813	0.7726	0.7639	0.7553
20.0	0.7934	0.7851	0.7766	0.7682	0.7597
30.0		0.7921	0.7841	0.7761	0.7681
40.0		0.7985	0.7909	0.7832	0.7756

[a] Standard uncertainties ($k = 1$): $u_r(p) = 2 \cdot 10^{-4}$ (Pa/Pa); $u(T) = 10$ mK, $u(\rho) = 0.35$ $kg \cdot m^{-3}$.

TABLE 3
Experimental densities for the mixtures {1-butanol (x) + cyclohexane (1-x)} at different mole fractions, pressures and temperatures.[a]

p/MPa	ρ/($g \cdot cm^{-3}$) T/K									
	293.15	303.15	313.15	323.15	333.15	293.15	303.15	313.15	323.15	333.15
			x = 0.1000					*x = 0.2000*		
0.1	0.7795	0.7701	0.7604	0.7506	0.7407	0.7814	0.7720	0.7625	0.7528	0.7430
1.0	0.7802	0.7708	0.7613	0.7516	0.7417	0.7820	0.7728	0.7633	0.7538	0.7440
2.0	0.7810	0.7717	0.7622	0.7526	0.7428	0.7829	0.7737	0.7643	0.7548	0.7451
5.0	0.7835	0.7744	0.7651	0.7556	0.7461	0.7853	0.7763	0.7671	0.7578	0.7483
10.0	0.7873	0.7785	0.7695	0.7603	0.7511	0.7892	0.7804	0.7715	0.7625	0.7533
15.0	0.7911	0.7824	0.7736	0.7648	0.7559	0.7928	0.7843	0.7756	0.7669	0.7580
20.0	0.7945	0.7862	0.7777	0.7690	0.7605	0.7963	0.7880	0.7795	0.7711	0.7625
30.0		0.7932	0.7851	0.7769	0.7689		0.7950	0.7870	0.7790	0.7708
40.0		0.7996	0.7919	0.7842	0.7765		0.8014	0.7937	0.7861	0.7783
50.0			0.7983	0.7908	0.7835			0.8001	0.7928	0.7852
60.0			0.8042	0.7972	0.7900			0.8060	0.7990	0.7917
70.0				0.8029	0.7961				0.8046	0.7977
80.0				0.8086	0.8019				0.8101	0.8033
90.0					0.8073					0.8087
100.0					0.8124					0.8138
			x = 0.3003					*x = 0.4005*		
0.1	0.7839	0.7746	0.7652	0.7556	0.7459	0.7866	0.7776	0.7684	0.7589	0.7494
1.0	0.7845	0.7753	0.7661	0.7566	0.7469	0.7873	0.7783	0.7692	0.7599	0.7503
2.0	0.7853	0.7762	0.7670	0.7576	0.7480	0.7881	0.7792	0.7701	0.7608	0.7514
5.0	0.7877	0.7788	0.7697	0.7605	0.7511	0.7905	0.7817	0.7728	0.7637	0.7545
10.0	0.7916	0.7829	0.7741	0.7652	0.7561	0.7943	0.7857	0.7771	0.7683	0.7594
15.0	0.7952	0.7867	0.7782	0.7696	0.7608	0.7978	0.7896	0.7812	0.7727	0.7640
20.0	0.7986	0.7904	0.7821	0.7737	0.7652	0.8013	0.7932	0.7850	0.7767	0.7684
30.0		0.7974	0.7894	0.7816	0.7734		0.8002	0.7923	0.7844	0.7764
40.0		0.8038	0.7962	0.7886	0.7808		0.8065	0.7990	0.7914	0.7838
50.0			0.8025	0.7951	0.7877			0.8051	0.7979	0.7906
60.0			0.8084	0.8014	0.7941			0.8109	0.8041	0.7970
70.0				0.8069	0.8000				0.8096	0.8029
80.0				0.8123	0.8057				0.8150	0.8084
90.0					0.8109					0.8137
100.0					0.8160					0.8187
			x = 0.4997					*x = 0.6001*		
0.1	0.7897	0.7809	0.7718	0.7626	0.7531	0.7931	0.7845	0.7757	0.7666	0.7574
1.0	0.7903	0.7816	0.7727	0.7635	0.7541	0.7937	0.7852	0.7765	0.7675	0.7584
2.0	0.7911	0.7825	0.7736	0.7645	0.7552	0.7945	0.7860	0.7774	0.7685	0.7594
5.0	0.7934	0.7850	0.7762	0.7673	0.7582	0.7969	0.7885	0.7800	0.7713	0.7624
10.0	0.7972	0.7889	0.7805	0.7718	0.7630	0.8005	0.7925	0.7841	0.7757	0.7671
15.0	0.8008	0.7927	0.7844	0.7761	0.7675	0.8040	0.7961	0.7880	0.7799	0.7715
20.0	0.8042	0.7963	0.7883	0.7801	0.7718	0.8074	0.7996	0.7918	0.7838	0.7757
30.0		0.8031	0.7954	0.7877	0.7798		0.8064	0.7989	0.7912	0.7836
40.0		0.8094	0.8020	0.7946	0.7870		0.8126	0.8053	0.7981	0.7907
50.0			0.8081	0.8010	0.7937			0.8114	0.8044	0.7972
60.0			0.8138	0.8070	0.8001			0.8170	0.8105	0.8034
70.0				0.8126	0.8058				0.8158	0.8092
80.0				0.8179	0.8113				0.8211	0.8146
90.0					0.8165					0.8198
100.0					0.8215					0.8247