



Thermophysical properties of 1,2,4-trimethylbenzene in admixtures with 1-butanol or 2-butanol at high pressures



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ABSTRACT

The systems of 1-butanol or 2-butanol + 1,2,4-trimethylbenzene were characterized measuring densities and isobaric heat capacities at high pressures. Densities of 2-butanol and 1,2,4-trimethylbenzene and the binary systems 1-butanol or 2-butanol + 1,2,4-trimethylbenzene were measured at the ranges $p = (0.1\text{--}140)$ MPa and $T = (273.15\text{--}333.15)$ K. For these measurements, a high-pressure vibrating tube densimeter was used and data were successfully correlated with the empirical Tammann-Tait equation. In order to complete the characterization, isobaric heat capacities were measured over the range of $(0.1\text{--}25)$ MPa at two different temperatures (293.15 and 313.15) K for the same pure compounds and binary mixtures. These measurements were performed in a high-pressure automated flow calorimeter. Excess molar heat capacities were evaluated for the mixtures and a positive deviation from the ideality was obtained for both systems.

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1. Introduction

In order to implement new biofuels to the automotive market, it is important to characterize some mixtures as reference values. From an industrial point of view, oxygenated compounds from renewable sources can be used as additives of new generation fuels. Knowing thermodynamic behavior of new fuels will allow us to model and correlate properties as well as predict more complex mixtures' behavior.

Second-generation biofuels are able to use lands unsuitable for food crop production and to provide more efficient engineering processes. This can be considered as environmentally sustainable fuel production through a wide range of renewable raw materials, generating a non-harmful impact on the environment.

Bio-butanol (known as second generation biofuel) has the potential to play an important role in a sustainable manner because it can be produced from a variety of waste biomass. According to Szwaja and Naber [1] butanol can directly replace gasoline, either as a pure fuel or a blender, thanks to similar thermophysical properties with it. Due to its non-corrosive nature and its immiscibility with conventional fossil fuel, as mentioned by Cheng [2], the bio-butanol has many advantages such as a higher heating value than ethanol, it can be biologically produced from materials such as corn, grasses, leaves and crop residues, lower

vapor pressure compared with gasoline and ethanol or it can be used in existing engines in the pure form or mixed in any ratio with gasoline.

Based on these facts, it is clearly shown that butanol is a better alternative than ethanol as a biofuel because of its thermophysical properties.

This paper is part of a PhD thesis focused on thermophysical characterization of environmentally sustainable biofuels with mixtures of conventional reference hydrocarbons by several experimental techniques [3–6]. It reports the thermodynamic study of 1,2,4-trimethylbenzene plus 1-butanol or 2-butanol mixtures, using density and isobaric heat capacity measurements. There are not data for these mixtures in the literature, so that, it continues the contribution to the international effort towards the development and use of environmentally sustainable fuels.

2. Experimental

2.1. Materials

1,2,4-Trimethylbenzene, 1-butanol and 2-butanol were purchased from Fluka. All the compounds were of the highest purity available, chromatography quality reagent with a purity >0.997 (checked by gas chromatography, GC). The compounds were checked using a Mettler Toledo C20 coulometric Karl Fischer titrator, obtaining a quantity of water lower than 250 ppm. So, all the

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Table 1
Material description.

Chemical name	Source	Mass fraction purity (GC) ^a	Water content (mass %)	Purification method
1-Butanol	Sigma-Aldrich	≥0.999	0.020	None
2-Butanol ^b	Sigma-Aldrich	≥0.997	0.024	None
1,2,4-Trimethylbenzene	Aldrich-Chemistry	≥0.997	<0.020	None

^a From the supplier.^b Racemic mixture.

components were used as provided. The material description is summarized in Table 1.

2.2. Apparatus and procedure

Liquid mixtures were prepared by weighing. A Sartorius CP 224 S balance was used, with a precision of $\pm 1 \cdot 10^{-4}$ g, resulting in an estimated standard uncertainty in mole fractions of $\pm 2.5 \cdot 10^{-4}$. All the substances were degassed using a Branson 3210 ultrasonic bath, before the measurements, at room temperature for at least 15 min.

Densities were measured using an Anton Paar DMA HPM vibrating-tube densimeter. This model is suitable for the high accurate determination of density in the range (0–3000) kg·m⁻³, with a resolution of 10⁻² kg·m⁻³.

Experimental procedure for volumetric measurements is automated, except for filling and cleaning operations. The main part of the system is a commercial Anton Paar HPM vibrating-tube densimeter, but the experimental arrangement requires the construction and set-up of several pieces of equipment and peripherals. Experimental assembly was presented in previous papers [4,7]. Calibration was performed following the method developed by Lagourette et al. [8]. Firstly, fluid density, ρ , is related to vibration period, τ :

$$\rho(T, p) = A(T)\tau^2(T, p) - B(T, p) \quad (1)$$

where $A(T)$ and $B(T, p)$ are two characteristic parameters of the apparatus which can be determined by a calibration procedure at

Table 2
Experimental densities, ρ /(kg·m⁻³), of 1,2,4-trimethylbenzene and 2-butanol at different pressures and temperatures.^a

p /MPa	ρ /(kg·m ⁻³)						
	T /K						
	273.15	283.15	293.15	303.15	313.15	323.15	333.15
	<i>1,2,4-Trimethylbenzene</i>						
0.1	891.7	883.3	875.1	867.0	859.0	851.3	843.6
1.0	892.3	883.9	875.7	867.6	859.7	852.0	844.4
2.0	892.9	884.5	876.3	868.3	860.4	852.7	845.2
5.0	894.6	886.3	878.2	870.3	862.6	855.0	847.6
10.0	897.4	889.3	881.4	873.6	866.0	858.6	851.4
15.0	900.2	892.2	884.4	876.8	869.3	862.1	855.1
20.0	902.8	895.0	887.3	879.8	872.6	865.5	858.6
30.0	908.0	900.3	892.9	885.7	878.7	871.9	865.3
40.0	912.9	905.4	898.2	891.2	884.5	877.9	871.6
50.0	917.5	910.2	903.2	896.4	889.9	883.5	877.4
60.0	921.9	914.8	908.0	901.4	895.0	888.9	883.0
70.0	926.2	919.3	912.6	906.1	899.9	894.0	888.2
80.0	930.3	923.5	916.9	910.6	904.6	898.8	893.2
90.0	934.2	927.5	921.1	914.9	909.0	903.4	898.0
100.0	938.0	931.4	925.1	919.1	913.3	907.8	902.5
110.0	941.7	935.2	929.0	923.1	917.4	912.0	906.9
120.0	945.2	938.9	932.8	927.0	921.4	916.1	911.1
130.0	948.6	942.4	936.4	930.7	925.2	920.0	915.1
140.0	952.0	945.8	939.9	934.3	928.9	923.8	919.0
	<i>2-Butanol</i>						
0.1	822.3		806.3		789.4		770.7
1.0	822.7		807.0		790.1		771.6
2.0	823.4		807.8		791.0		772.6
5.0	825.4		810.0		793.5		775.5
10.0	828.7		813.6		797.5		780.1
15.0	831.8		817.0		801.4		784.4
20.0	834.7		820.2		805.1		788.6
30.0	840.4		826.5		811.9		796.2
40.0	845.7		832.3		818.3		803.2
50.0	850.7		837.7		824.1		809.6
60.0	855.4		842.8		829.6		815.7
70.0	859.9		847.7		835.0		821.4
80.0	864.3		852.3		839.9		826.7
90.0	868.4		856.7		844.6		831.8
100.0	872.4		860.9		849.0		836.6
110.0	876.3		865.0		853.3		841.2
120.0	879.9		868.8		857.5		845.5
130.0	883.5		872.7		861.5		849.8
140.0	887.2		876.3		865.4		853.9

^a Standard uncertainties ($k = 1$): $u_r(p) = 2 \cdot 10^{-4}$; $u_r(T) = 10$ mK; $u_r(\rho) = 0.35$ kg·m⁻³.

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