J. Chem. Thermodynamics 42 (2010) 920–925

Contents lists available at ScienceDirect

J. Chem. Thermodynamics

journal homepage: www.elsevier.com/locate/jct

Volumetric behaviour of the ternary liquid system composed of methyl *tert*-butyl ether, toluene, and isooctane at temperatures from (298.15 to 328.15) K: Experimental data and correlation

L. Morávková, Z. Wagner, Z. Sedláková, J. Linek *

E. Hála Laboratory of Thermodynamics, Institute of Chemical Process Fundamentals of the ASCR, v.v.i., 165 02 Prague 6, Czech Republic

ARTICLE INFO

Article history:
Received 9 February 2010
Received in revised form 2 March 2010
Accepted 3 March 2010
Available online 7 March 2010

Keywords:
Toluene
Isooctane
MTBE
Ternary mixture
Density
Speed of sound
Excess volume
Adiabatic compressibility
Ternary data fitting

ABSTRACT

The densities and speeds of sound of (methyl *tert*-butyl ether {MTBE} + toluene + isooctane) were measured at four temperatures over the range (298.15 to 328.15) K and the respective values of excess volumes V_m^E and adiabatic compressibility κ_S were calculated. The V_m^E and κ_S values for the ternary and corresponding binaries were fitted to the Redlich–Kister equation considering various numbers of ternary constants. The necessary number of ternary constants needed to describe the system is discussed.

1. Introduction

Research activities of our laboratory comprise, among others, the systematic measurement of volumetric properties of different groups of organic compounds. Our present project is devoted to the systematic study of liquid systems modelling liquid engine fuels. After measuring (cyclohexane + alkane) at normal pressure and temperature 298.15 K [1], (cyclohexane + nonane) at temperatures from (298.15 to 328.15) K and at pressures up to 40 MPa [2] (octane + benzene, or +toluene, or +1,3-xylene, or +1,3,5-trimethylbenzene) at temperatures between (298.15 and 328.15) K [3], and (octane + benzene) at temperatures from (298.15 to 328.15) K and at pressures up to 40 MPa [4], the binary [5] and ternary systems containing methyl *tert*-butyl ether (MTBE) have been studied with the aim to decide what and how many ternary constants, in addition to the binary constants, are needed to fit the ternary data to Redlich–Kister equation within the error of experimental results. This measurement is also of practical importance with respect to use of MTBE as the liquid fuel antiknock additive.

The thorough literature search showed that there exist no ternary data for this system. However, to be able to do the test, we needed a most accurate and mutually consistent binary (and ternary) data. Not finding such data sets, we decided to measure the title binary systems [5] as the first step followed by the ternary data measurements described in this work.

The densities and excess volumes of the investigated liquids and their mixtures are required, for instance, for relating excess enthalpy and excess Gibbs energy values. From a practical point of view, the data are useful for the design of mixing, storage, and process equipment. Last but not least, the data measured reflect interactions between the molecules of the mixtures studied and can serve for testing the theories of the liquid state.

2. Experimental

2.1. Materials

The chemicals used in the experiments were the following products from Fluka: MTBE (methyl *tert*-butyl ether, methyl 1,1-dimethylethyl ether), puriss., g.c. mass fraction purity ⩾ 0.95, toluene, RdH, for chromatography, g.c. mass fraction purity ⩾ 0.995, isooctane (2,2,4-trimethylpentane), RdH puriss. p.a., g.c. mass fraction purity ⩾ 0.995. The substances were used without further

---

* Corresponding author. Tel.: +420 2 203 90111; fax: +420 2 209 20661.
E-mail address: linek@icpf.cas.cz (J. Linek).

0021-9614/$ - see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.jct.2010.03.005

TABLE 1
Densities ρ and refractive index values n_D at T = 298.15 K of the pure components, and their comparison with literature; w is the mass fraction purity as determined by g.l.c.

Component	$\rho/(\text{g}\cdot\text{cm}^{-3})$			n_D			w
	Experimental	Literature	Reference	Experimental	Literature	Reference	
Toluene	0.86219	0.8623	[5]	1.4941	1.49414	[5]	0.9995
Isooctane	0.68779	0.68781	[5]	1.38905	1.38898	[5]	0.9996
MTBE	0.73527	0.7353	[6]	1.36648	1.3664	[6]	0.9989

TABLE 2
Experimental values of density ρ, calculated excess molar volume V_m^E, speed of sound u and adiabatic compressibility κ_S for (x_1 MTBE + x_2 toluene + x_3 isooctane) at temperature T and atmospheric pressure; $x_3 = 1 - x_1 - x_2$.

x_2/x_3	x_1	x_2	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$V_m^E/(\text{cm}^3\cdot\text{mol}^{-1})$	$u/(\text{m}\cdot\text{s}^{-1})$	$10^4\ \kappa_S/\text{MPa}^{-1}$
			T = 298.15 K			
2.89955	0.00000	0.74356	0.80092	0.059	1221.3	8.37
	0.10802	0.66325	0.79450	−0.033	1202.9	8.70
	0.20785	0.58902	0.78838	−0.093	1185.6	9.02
	0.29143	0.52687	0.78322	−0.142	1171.0	9.31
	0.40526	0.44223	0.77594	−0.174	1150.4	9.74
	0.51104	0.36357	0.76909	−0.194	1131.1	10.16
	0.60317	0.29507	0.76298	−0.194	1113.9	10.56
	0.71135	0.21463	0.75566	−0.174	1093.3	11.07
	0.80398	0.14575	0.74923	−0.134	1075.2	11.54
	0.89857	0.07542	0.74259	−0.083	1056.7	12.06
	1.00000		0.73527	0.000	1036.4	12.66
0.98020	0.00000	0.49500	0.75464	0.101	1162.0	9.81
	0.08989	0.45050	0.75318	0.078	1151.8	10.01
	0.20511	0.39347	0.75123	0.053	1138.5	10.27
	0.29634	0.34831	0.74964	0.033	1127.8	10.49
	0.40704	0.29352	0.74762	0.017	1114.4	10.77
	0.50068	0.24716	0.74587	0.002	1102.8	11.02
	0.59580	0.20008	0.74400	−0.007	1090.8	11.30
	0.70796	0.14456	0.74173	−0.014	1076.2	11.64
	0.81463	0.09176	0.73947	−0.017	1062.2	11.99
	0.90603	0.04651	0.73743	−0.009	1049.5	12.31
	1.00000		0.73527	0.000	1036.4	12.66
0.33926	0.00000	0.25332	0.71851	0.101	1118.2	11.13
	0.09951	0.22811	0.71967	0.131	1110.2	11.27
	0.19178	0.20474	0.72081	0.152	1102.9	11.40
	0.29594	0.17835	0.72219	0.171	1094.5	11.56
	0.40045	0.15188	0.72372	0.175	1085.9	11.72
	0.49923	0.12686	0.72525	0.173	1077.9	11.87
	0.60622	0.09975	0.72707	0.158	1069.1	12.03
	0.69768	0.07658	0.72877	0.133	1061.6	12.18
	0.80983	0.04817	0.73097	0.100	1052.2	12.36
	0.89825	0.02578	0.73288	0.059	1044.8	12.50
	1.00000		0.73527	0.000	1036.4	12.66
			308.15 K			
2.89955	0.00000	0.74356	0.79200	0.048	1179.2	9.08
	0.10802	0.66325	0.78542	−0.050	1160.4	9.45
	0.20785	0.58902	0.77917	−0.118	1142.8	9.83
	0.29143	0.52687	0.77389	−0.172	1127.9	10.16
	0.40526	0.44223	0.76644	−0.205	1106.9	10.65
	0.51104	0.36357	0.75942	−0.226	1087.2	11.14
	0.60317	0.29507	0.75314	−0.220	1069.5	11.61
	0.71135	0.21463	0.74565	−0.198	1048.7	12.19
	0.80398	0.14575	0.73905	−0.151	1030.3	12.75
	0.89857	0.07542	0.73222	−0.091	1011.4	13.35
	1.00000		0.72472	0.000	990.8	14.06
0.98020	0.00000	0.49500	0.74600	0.087	1120.2	10.68
	0.08989	0.45050	0.74440	0.062	1109.7	10.91
	0.20511	0.39347	0.74227	0.033	1096.0	11.21
	0.29634	0.34831	0.74052	0.014	1084.9	11.47
	0.40704	0.29352	0.73830	−0.002	1071.1	11.81
	0.50068	0.24716	0.73637	−0.014	1059.1	12.11
	0.59580	0.20008	0.73432	−0.021	1046.8	12.43
	0.70796	0.14456	0.73180	−0.023	1031.7	12.84
	0.81463	0.09176	0.72930	−0.018	1017.2	13.25
	0.90603	0.04651	0.72707	−0.009	1006.1	13.59
	1.00000		0.72472	0.000	990.8	14.06
0.33926	0.00000	0.25332	0.71010	0.085	1076.6	12.15
	0.09951	0.22811	0.71108	0.119	1068.2	12.32
	0.19178	0.20474	0.71206	0.142	1060.5	12.49

(*continued on next page*)