Available online at www.sciencedirect.com
ScienceDirect
J. Chem. Thermodynamics 40 (2008) 671–676
JCT
www.elsevier.com/locate/jct

Excess molar volumes of (octane + benzene, or toluene, or 1,3-xylene, or 1,3,5-trimethylbenzene) at temperatures between (298.15 and 328.15) K

L. Morávková, J. Linek *

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

Received 4 October 2007; received in revised form 30 October 2007; accepted 30 October 2007
Available online 7 November 2007

Abstract

The densities of (octane + benzene, or toluene, or 1,3-xylene, or 1,3,5-trimethylbenzene) were measured at temperatures (298.15, 308.15, 318.15, and 328.15) K by means of a vibrating-tube densimeter. The excess molar volumes V_m^E calculated from the density data provide the temperature dependence of V_m^E in the temperature range of (298 to 328) K. The V_m^E results were correlated using the fourth-order Redlich–Kister equation, with the maximum likelihood principle being applied for the determination of the adjustable parameters. It was found that the values of V_m^E are not very much dependent on temperature and in all cases decrease with the number of methyl groups on benzene ring of the alkylbenzene.

Keywords: Octane; Benzene; Toluene; 1,3-Xylene; 1,3,5-Trimethylbenzene; Binary mixture; Density; Excess volume; Temperature dependence

1. Introduction

Research activities of our laboratory comprise, among others, the systematic measurement of volumetric properties of different groups of organic compounds. Our new 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] and (cyclohexane + nonane) at elevated temperatures and pressures [2], the system (octane + aromate) have been studied.

The densities and excess volumes of the investigated liquids and their mixtures are required, for instance, for relating excess enthalpy and excess Gibbs free 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 at atmospheric pressure with the low-pressure densimeter will be used as reference density values for determining the parameters of the Tait correlation equation because the values of densities measured with the high-pressure densimeter cell are not sufficiently accurate for this purpose.

2. Experimental

2.1. Materials

The octane and the alkylbenzenes used in the experiments were the following products from Fluka: octane, puriss., A.R., g.c. mass fraction ⩾0.995; benzene, A.R., g.c. mass fraction ⩾0.997; toluene, CHROMASOLV, g.c. mass fraction ⩾0.999; 1,3-xylene, puriss. p.a., g.c. mass fraction >0.99; 1,3,5-trimethylbenzene (1,3,5-TMBZ), puriss., g.c. mass fraction 0.99. They were used without further purification and were dried and stored over 0.4 nm molecular sieves. In order to check the purity of the substances, their density and refractive index values were determined at $T = 298.15$ K and compared with the

* Corresponding author. Tel.: +420 220390270; fax: +420 2 209 20661.
E-mail addresses: moravkova@icpf.cas.cz (L. Morávková), linek@icpf.cas.cz (J. Linek).

0021-9614/$ - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.jct.2007.10.010

literature data [3] with the agreement being, in general, good (table 1). The contents of the substances were also determined by gas chromatography (HP Ser.II. model 5890 chromatograph with capillary column type 1909 1Z-413E and f.i.d., column temperature 413.3 K, helium flow rate $4.2 \cdot 10^{-4}\ cm^3 \cdot s^{-1}$).

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

Component	$\rho/(g \cdot cm^{-3})$			n_D			w
	Experimental	Literature	Reference	Experimental	Literature	Reference	
Octane	0.69862	0.69862	[3]	1.3950	1.39505	[3]	0.9991
Benzene	0.87363	0.8737	[3]	1.4979	1.49792	[3]	0.9996
Toluene	0.86229	0.8623	[3]	1.4941	1.49414	[3]	0.9995
1,3-Xylene	0.85985	0.86009	[3]	1.4945	1.49464	[3]	0.9957
1,3,5-TMBZ	0.86113	0.86111	[3]	1.4967	1.49684	[3]	0.9927

TABLE 2
Densities ρ and excess molar volumes V_m^E for (octane + benzene) at mole fraction x of octane and temperature T

T/K: 298.15			308.15			318.15			328.15		
x	$\rho/(g \cdot cm^{-3})$	$V_m^E/(cm^3 \cdot mol^{-1})$	x	$\rho/(g \cdot cm^{-3})$	$V_m^E/(cm^3 \cdot mol^{-1})$	x	$\rho/(g \cdot cm^{-3})$	$V_m^E/(cm^3 \cdot mol^{-1})$	x	$\rho/(g \cdot cm^{-3})$	$V_m^E/(cm^3 \cdot mol^{-1})$
0.00000	0.87362	0.000	0.00000	0.86301	0.000	0.00000	0.85216	0.000	0.00000	0.84149	0.000
0.06831	0.85082	0.234	0.06734	0.84085	0.217	0.06734	0.83041	0.231	0.06734	0.82009	0.234
0.13579	0.83114	0.409	0.13348	0.82180	0.389	0.13348	0.81170	0.402	0.13348	0.80167	0.411
0.20415	0.81351	0.542	0.19895	0.80498	0.530	0.19323	0.79652	0.534	0.19323	0.78683	0.532
0.26163	0.80023	0.622	0.25624	0.79181	0.613	0.25106	0.78328	0.629	0.25106	0.77379	0.628
0.33215	0.78549	0.692	0.32830	0.77691	0.682	0.32892	0.76743	0.696	0.32892	0.75815	0.704
0.39125	0.77433	0.722	0.38880	0.76556	0.719	0.39372	0.75554	0.734	0.39372	0.74647	0.739
0.45813	0.76282	0.732	0.46819	0.75218	0.725	0.46810	0.74319	0.748	0.46810	0.73435	0.746
0.53879	0.75032	0.703	0.52842	0.74295	0.711	0.53024	0.73380	0.738	0.53024	0.72513	0.731
0.60539	0.74095	0.660	0.59710	0.73335	0.661	0.58656	0.72602	0.694	0.58656	0.71746	0.691
0.66404	0.73337	0.597	0.65918	0.72532	0.606	0.67090	0.71536	0.606	0.67090	0.70693	0.608
0.71158	0.72759	0.539	0.72484	0.71754	0.517	0.72484	0.70907	0.538	0.72484	0.70075	0.539
0.79787	0.71791	0.411	0.81557	0.70774	0.361	0.81557	0.69939	0.389	0.81557	0.69120	0.392
0.86825	0.71070	0.283	0.88516	0.70086	0.226	0.88516	0.69261	0.255	0.88516	0.68452	0.257
0.92640	0.70515	0.166	0.95146	0.69477	0.082	0.95146	0.68661	0.113	0.95146	0.67862	0.112
1.00000	0.69860	0.000	1.00000	0.69044	0.000	1.00000	0.68247	0.000	1.00000	0.67454	0.000

TABLE 3
Densities ρ and excess molar volumes V_m^E for (octane + toluene) at mole fraction x of octane and temperature T

T/K: 298.15			308.15			318.15			328.15		
x	$\rho/(g \cdot cm^{-3})$	$V_m^E/(cm^3 \cdot mol^{-1})$	x	$\rho/(g \cdot cm^{-3})$	$V_m^E/(cm^3 \cdot mol^{-1})$	x	$\rho/(g \cdot cm^{-3})$	$V_m^E/(cm^3 \cdot mol^{-1})$	x	$\rho/(g \cdot cm^{-3})$	$V_m^E/(cm^3 \cdot mol^{-1})$
0.00000	0.86229	0.000	0.00000	0.85286	0.000	0.00000	0.84360	0.000	0.00000	0.83429	0.000
0.06540	0.84589	0.074	0.06540	0.83660	0.073	0.06750	0.82695	0.078	0.06750	0.81777	0.079
0.12831	0.83123	0.133	0.12831	0.82206	0.129	0.12290	0.81422	0.129	0.12290	0.80512	0.135
0.19794	0.81617	0.180	0.19794	0.80710	0.179	0.20523	0.79669	0.188	0.20523	0.78773	0.194
0.25241	0.80513	0.211	0.25241	0.79614	0.211	0.26130	0.78556	0.223	0.26130	0.77668	0.233
0.31201	0.79374	0.235	0.31201	0.78482	0.236	0.31424	0.77567	0.242	0.31424	0.76687	0.253
0.39305	0.77927	0.256	0.39305	0.77046	0.259	0.39798	0.76100	0.266	0.39798	0.75232	0.277
0.45440	0.76905	0.262	0.45440	0.76031	0.266	0.45533	0.75161	0.273	0.45533	0.74301	0.285
0.54085	0.75559	0.259	0.54085	0.74693	0.268	0.53876	0.73882	0.269	0.53876	0.73032	0.284
0.60290	0.74656	0.246	0.60290	0.73798	0.252	0.60781	0.72894	0.256	0.60781	0.72055	0.267
0.67173	0.73709	0.224	0.67173	0.72858	0.232	0.66791	0.72081	0.236	0.66791	0.71248	0.249
0.72018	0.73075	0.203	0.72018	0.72230	0.209	0.72620	0.71332	0.208	0.72620	0.70506	0.220
0.80637	0.72008	0.155	0.80637	0.71170	0.163	0.79849	0.70451	0.167	0.79849	0.69633	0.179
0.87266	0.71236	0.109	0.87266	0.70405	0.115	0.86301	0.69707	0.124	0.86301	0.68897	0.131
0.93118	0.70588	0.062	0.93118	0.69762	0.067	0.91435	0.69143	0.081	0.91435	0.68339	0.084
1.00000	0.69861	0.000	1.00000	0.69044	0.000	1.00000	0.68249	0.000	1.00000	0.67455	0.000