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DENSITIES AND APPARENT MOLAR VOLUME OF BENZIMIDAZOLE IN PURE & BINARY SOLVENT MIXTURES OF N-PROPANOL + WATER

***Sachin S. Kale**

Department of Chemistry, A.C.S. College, Navapur, Dist – Nandurbar, Maharashtra, India.

***Corresponding Author: Sachin S. Kale**

Department of Chemistry, A.C.S. College, Navapur, Dist – Nandurbar, Maharashtra, India.

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ABSTRACT

Benzimidazole is an important pharmacophore in medicinal chemistry. Benzimidazoles are having a many therapeutic uses like antibacterial, antifungal, analgesics, antitumor, antiparasitic, antihistamine, and antiviral. Using bicapillary pycnometer densities of Benzimidazole in n-propanol with water were measured over the entire composition range at temperatures from 293.15 to 313.15 K. Densities of the saturated solution of benzimidazole in a pure and binary mixture of solvents were measured at mentioned temperature. This density data was used to calculate apparent molar volume. The apparent molar volume (ϕv) values for all solutions in pure solvents or in mixed solvent increases with the increase of temperature. The density of benzimidazole in pure water solution decreases slightly with the increase in temperature but for pure n-propanol solution it increases with increase in temperature.

KEYWORDS: Benzimidazole, n-propanol, Density, Apparent molar volume.

INTRODUCTION

Because of their various biological activity and clinical applications benzimidazole derivatives square measure of wide interest, with relevance their restrictive activity and their favorable property magnitude relation they're remarkably effective compounds. In drug discovery benzimidazole ring displays a crucial heterocyclic pharmacophore. These compounds possess totally different substituent's within the benzimidazole structure square measure related to a large vary of biological activities as well as anti-bacterial, anti-cancer, anti-viral, medicine, anti-oxidant, anti-fungal, anti-helmintic, antihistaminic, nucleon pump substance, anticoagulant properties and anti-hypertensive.[1-3]

U. Domanska and M.K. Kozlowska[4] studied solubilities, density, partition coefficient and surface tension for imidazoles + n-decane/ octan-1-ol/ water, temperature range used for measurements were from 270 K to melting temperature of the compound. S.

Baluja and F. Karia[5] studied density, sound velocity and viscosity of 1H-benzimidazole and 2-methyl benzimidazole derivative in chloroform and methanol solution. The measurement was carried out at 298.15 K over a whole range of concentration.

Benzimidazole is a very important compound for synthesis of pharmaceuticals and physical properties such as density need to be studied systematically. Therefore it is planned to measure the density of benzimidazole in pure water, n-propanol, and in mixed solvents water + n-propanol at temperatures ranges from 293.15 to 313.15 K.

MATERIALS AND METHOD

MATERIALS: Benzimidazole was provided by Spectrochem with purity 99%, n-Propanol was provided by spectrochem with purity 99.8%.

METHOD: In the present work a bicapillary pycnometer having 15 c.c. bulk volumes was used for measurement of density. Chromic acid was used to clean the capillary of the pycnometer. Then pycnometer was further washed with distilled water and acetone and it was dried with hot air blower. Then it was accurately weighed on Scale-Tec balance having a sensitivity of 1 x 10^{-4} mg. For calibration of the pycnometer triple distilled water was used. About 15 - 20 ml of water was taken in a beaker and is filled to the limb 'P' of the pycnometer. During filling of water to the pycnometer, air bubble was avoided. Water filled up to mark 'R' in limb 'Q' by capillary action. Pycnometer was weighed again.

In the glass-sided thermostat, pycnometer was mounted vertically. Thermostat temperature was controlled within 0.01^0 C. The height of water i.e. h_1 and h_2 in limb 'P and Q' were measured at all experimental temperatures (293.15 to 313.15) K by using a travelling microscope. From the known densities of water at a various

temperature and the weights of the water taken in the pycnometer, corresponding volumes of water were calculated. The height (h_1+h_2) versus volume of water plot yields a straight line. The slope and intercept values are obtained by using least square method which is used for calculating the density of liquids.[6,7]

From thermostat, pycnometer was removed. It is cleaned as per procedure mentioned above. After this experimental liquid was filled in the pycnometer and it is mounted vertically in the thermostat. For finding the total height (h_1+h_2) at different temperatures for experimental liquids, the same procedure was repeated. From their total height, the corresponding volume of liquids under investigation was obtained from the calibration curve and the corresponding densities thus determined.

The repetition of measurements of density for each experimental liquid was carried out three to four times and the average result was calculated.[8-18]

RESULT AND DISCUSSION

Tables 1 show molalities (m), densities (ρ) and apparent molar volumes (Φv) of benzimidazole for various initial mole fractions (x_C^0) of n-propanol in water at temperatures (293.15 to 313.15) K. Figures 1 show plot of densities versus temperature (T/K), for benzimidazole + water + n-propanol with the initial mole fraction of n-propanol.

Apparent molar volume (Φv) is calculated by using equation (1). From tables 1, it is observed that Φv values are positive for benzimidazole pure solvents, water, n-propanol solutions and binary mixtures of water with n-propanol solutions at 293.15 to 313.15 K. The apparent molar volume (Φv) values for all solutions in pure solvents or in mixed solvent increases with the increase of temperature. The density of benzimidazole in pure water solution decreases slightly with the increase in temperature but for pure n-propanol solution it increases with increase in temperature.

Table 1: Molalities (m), densities (ρ) and apparent molar volumes (Φv) of benzimidazole for various mole fractions, (x_C^0), of n-propanol at temperatures (293.15 to 313.15) K.

T/K	x_C^0	m /mol.kg^{-1}	$\rho \cdot 10^{-3}$ kg·m^{-3}	$\Phi v.10^6$/m^3.mol^{-1}
293.15	0.0000	0.0402	0.9988	87.0558
	0.0322	0.0654	0.9850	88.3111
	0.0697	0.2232	0.9741	96.2596
	0.1139	0.5655	0.9617	100.1578
	0.1666	0.9700	0.9514	97.1973
	0.2306	1.4113	0.9418	96.9183
	0.3102	1.8473	0.9334	95.9026
	0.4116	2.2834	0.9234	97.0818
	0.5453	2.5416	0.9112	96.4422
	0.7296	2.5095	0.8929	95.4631
	1.0000	2.1521	0.8629	96.5979
295.15	0.0000	0.0414	0.9980	94.1287
	0.0322	0.0690	0.9841	94.5498
	0.0697	0.2447	0.9737	96.1398
	0.1139	0.6042	0.9613	99.9928
	0.1666	1.0344	0.9512	97.6049
	0.2306	1.4978	0.9421	97.1808
	0.3102	1.9365	0.9340	95.8840
	0.4116	2.3981	0.9243	97.0795
	0.5453	2.6799	0.9124	96.6935
	0.7296	2.6102	0.8932	95.8183
	1.0000	2.2061	0.8603	98.4345
298.15	0.0000	0.0443	0.9973	95.7449
	0.0322	0.0812	0.9833	97.1852
	0.0697	0.2825	0.9725	98.3521
	0.1139	0.6781	0.9609	100.2211
	0.1666	1.1395	0.9512	97.8206
	0.2306	1.6302	0.9428	97.3320
	0.3102	2.1074	0.9342	96.8738
	0.4116	2.5620	0.9253	97.2259
	0.5453	2.8493	0.9132	97.0027
	0.7296	2.7728	0.8940	96.1650
	1.0000	2.3680	0.8611	99.0214

300.15	0.0000	0.0481	0.9969	95.2409
	0.0322	0.0870	0.9829	96.3592
	0.0697	0.3129	0.9717	99.7418
	0.1139	0.7275	0.9604	100.6578
	0.1666	1.2188	0.9516	97.9564
	0.2306	1.7236	0.9436	97.1220
	0.3102	2.2216	0.9354	96.6751
	0.4116	2.7137	0.9258	97.8282
	0.5453	2.9797	0.9143	97.1006
	0.7296	2.8940	0.8951	96.2753
	1.0000	2.4227	0.8612	98.7392
303.15	0.0000	0.0546	0.9962	96.4315
	0.0322	0.1009	0.9820	97.6486
	0.0697	0.3590	0.9709	100.1566
	0.1139	0.8221	0.9603	100.7293
	0.1666	1.3418	0.9515	98.5647
	0.2306	1.8918	0.9439	97.9471
	0.3102	2.4182	0.9365	97.2243
	0.4116	2.9143	0.9276	97.8136
	0.5453	3.1815	0.9158	97.2064
	0.7296	3.0484	0.8960	96.2816
	1.0000	2.5448	0.8621	98.5588
305.15	0.0000	0.0583	0.9956	98.0354
	0.0322	0.1168	0.9813	99.8996
	0.0697	0.3937	0.9704	100.5929
	0.1139	0.8775	0.9604	100.3467
	0.1666	1.4327	0.9518	98.7308
	0.2306	2.0062	0.9448	98.0209
	0.3102	2.5685	0.9377	97.4546
	0.4116	3.0813	0.9289	98.0679
	0.5453	3.3241	0.9170	97.2771
	0.7296	3.1694	0.8967	96.5085
	1.0000	2.6422	0.8627	98.6168
308.15	0.0000	0.0647	0.9946	99.5388
	0.0322	0.1339	0.9805	99.7763
	0.0697	0.4525	0.9697	100.9842
	0.1139	0.9850	0.9601	101.1762
	0.1666	1.5874	0.9508	100.5391
	0.2306	2.1908	0.9455	98.6335
	0.3102	2.7868	0.9393	97.7013
	0.4116	3.3209	0.9311	98.1387
	0.5453	3.5502	0.9181	97.8033
	0.7296	3.3758	0.8979	96.9719
	1.0000	2.7217	0.8638	97.5942
310.15	0.0000	0.0713	0.9942	97.2494
	0.0322	0.1441	0.9862	97.3360
	0.0697	0.3944	0.9686	97.6952
	0.1139	1.0559	0.9599	101.3908
	0.1666	1.6795	0.9498	101.6696
	0.2306	2.3338	0.9466	98.7669
	0.3102	2.9475	0.9401	98.1520
	0.4116	3.4860	0.9315	98.6354
	0.5453	3.7016	0.9195	97.7354
	0.7296	3.5588	0.8988	97.6209
	1.0000	2.8490	0.8648	97.8551
313.15	0.0000	0.0779	0.9931	99.4037
	0.0322	0.1663	0.9789	99.9039
	0.0697	0.5662	0.9689	100.9980

	0.1139	1.1828	0.9610	100.5730
	0.1666	1.8619	0.9504	102.3140
	0.2306	2.5648	0.9484	98.9450
	0.3102	3.2338	0.9423	98.5699
	0.4116	3.7850	0.9340	98.8994
	0.5453	3.9729	0.9210	98.3098
	0.7296	3.7106	0.9001	97.2700
	1.0000	2.9876	0.8660	97.6037

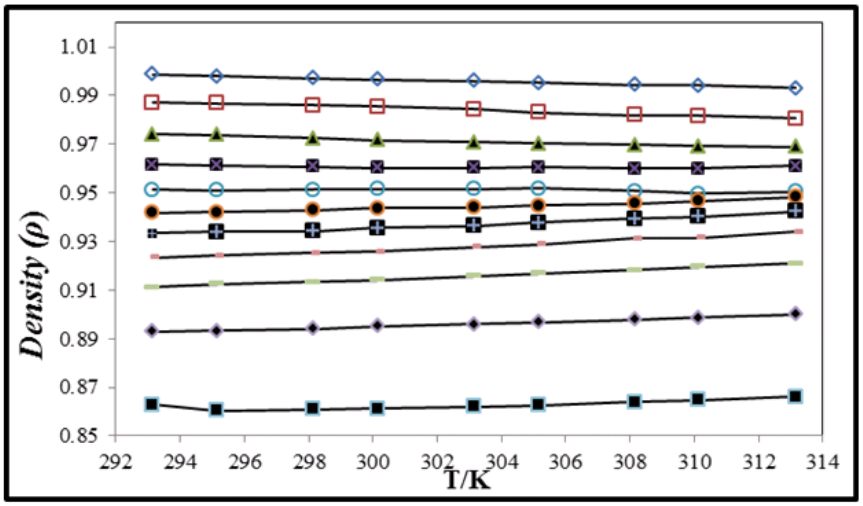

Figure 1: Plot of density versus temperature (T/K) for benzimidazole + water + n-propanol system with initial mole fraction.

The density of a liquid or liquid mixture is calculated as the mass per unit volume and is generally expressed in CGS as $g.cm^{-3}$ or more appropriately in SI as $kg.m^{-3}$.

Apparent molar volume[19] can be calculated by using following equation (1).

$$\Phi v = \frac{1}{m}\left[\frac{1000+mM}{\rho} - \frac{1000}{\rho_0}\right] \ldots (1)$$

Where, m = Molality, M = Molecular weight of solute, ρ_0 = Density of pure water or solvent system, ρ = Density of solution.

CONCLUSION

Densities of the saturated solution of benzimidazole in a pure and binary mixture of solvents were measured at 293.15 to 313.15 K. This density data was used to calculate apparent molar volume. The apparent molar volume (Φv) values for all solutions in pure solvents or in mixed solvent increases with the increase of temperature. The density of benzimidazole in pure water solution decreases slightly with the increase in temperature but for pure n-propanol solution it increases with increase in temperature.

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