relatively weak in the systems containing higher and branched chain alcohols for steric reasons (*13*–*15*). Also, the degree of deassociation of alcohol aggregates in these systems would be higher. In view of this, the positive contributions to the excess enthalpies associated with structure breaking of alcohols and furfural aggregates, which occurs as a consequence of their mixing, outweigh the negligibly small negative contribution arising from the interaction between alkanol and furfural molecules. A similar conclusion was drawn from the studies on the volumetric behavior of these binary mixtures (*16*).

Glossary

H_m^E	excess molar enthalpy, J mol^{-1}
x	mole fraction of furfural
A_i	constants in eq 1, J mol^{-1}
$\sigma(H_m^E)$	standard deviation of the least-squares fit, J mol^{-1}
$\bar{H}_i^E$	partial molar excess enthalpies, J mol^{-1}
P	pressure, bar
T	temperature, K
$H_{m\,0.5}^E$	excess molar enthalpy at equimolar concentration, J mol^{-1}

Registry No. Furfural, 98-01-1; methanol, 67-56-1; ethanol, 64-17-5; 1-propanol, 71-23-8; 2-propanol, 67-63-0; 1-butanol, 71-36-3; 2-butanol, 78-92-2.

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Received for review December 12, 1988. Accepted June 7, 1989.

Solubility of Ethane in *n*-Hexane at Pressures to 5.4 MPa and Temperatures from 311 to 394 K

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Solubility data are presented for ethane in *n*-hexane at temperatures from 311 to 394 K (100 to 250 °F) at pressures to 5.4 MPa (780 psia). These data are in significant disagreement with the earlier measurements of Zais and Silberberg. The new data can be described with average deviations of less than 0.001 mole fraction by the Soave–Redlich–Kwong or Peng–Robinson equations when two interaction parameters per isotherm are used in the equation.

Introduction

As part of our work on the solubilities of ethane in *n*-paraffin solvents (*1*, *2*), we observed that the literature data on the solubility of ethane in *n*-hexane (*3*) appears to be inconsistent with similar data for ethane in higher and lower carbon number *n*-paraffin solvents. This inconsistency became apparent during our investigations of generalized parameter equation-of-state (EOS) representations (*4*, *5*) of such systems. Oellrich et. al (*6*) have reported similar inconsistencies. As a result, we decided to perform additional measurements on ethane + *n*-hexane.

Experimental Details

The apparatus and procedures were identical with those described previously (*7*). Estimated uncertainties in experimental measurements are 0.1 K in temperature and less than 0.002 in mole fraction. The uncertainty in the measured bubble-point pressure depends on the steepness of the *p*–*x* relation and is on the order of 25 kPa (4 psia) in the present work.

The ethane employed in this work had a stated purity of 99.9+ mol % and was supplied by Matheson. The *n*-hexane was from Aldrich Chemical Company with a quoted purity of 99+ mol %. Both were used without further purification.

Table I. Solubility of Ethane in *n*-Hexane

mole fracn of ethane	pressure MPa	pressure psia	mole fracn of ethane	pressure MPa	pressure psia
310.9 K (37.8 °C, 100 °F)					
0.095	0.393	57.0	0.403	1.689	245.0
0.136	0.552	80.1	0.503	2.164	313.8
0.163	0.600	95.7	0.522	2.257	327.3
0.206	0.834	121.0	0.552	2.401	348.3
0.259	1.057	153.3	0.602	2.657	385.4
0.288	1.178	170.8	0.610	2.699	391.4
0.347	1.429	207.3	0.652	2.914	422.7
0.373	1.560	226.3			
338.7 K (65.6 °C, 150 °F)					
0.072	0.463	67.1	0.392	2.372	344.0
0.107	0.642	93.1	0.442	2.717	394.0
0.201	1.180	171.1	0.499	3.119	452.4
0.204	1.200	174.0	0.520	3.268	474.0
0.301	1.787	259.2	0.564	3.590	520.7
0.352	2.116	306.9			
366.5 K (93.3 °C, 200 °F)					
0.109	0.958	138.9	0.300	2.428	352.1
0.111	0.964	139.8	0.306	2.471	358.4
0.112	0.982	142.4	0.310	2.507	363.6
0.202	1.659	240.6	0.382	3.121	452.6
0.203	1.643	238.3	0.397	3.254	471.9
0.208	1.690	245.1			
394.3 K (121.1 °C, 250 °F)					
0.076	1.051	152.5	0.309	3.256	472.3
0.108	1.333	193.3	0.358	3.772	547.1
0.162	1.819	263.8	0.401	4.223	612.5
0.199	2.157	312.9	0.407	4.309	625.0
0.251	2.672	387.6	0.504	5.399	783.0
0.307	3.236	469.3			

Results

The experimental results appear in Table I. Comparison with the data of Zais and Silberberg appears in Figure 1. This comparison is shown in terms of deviations of their measured

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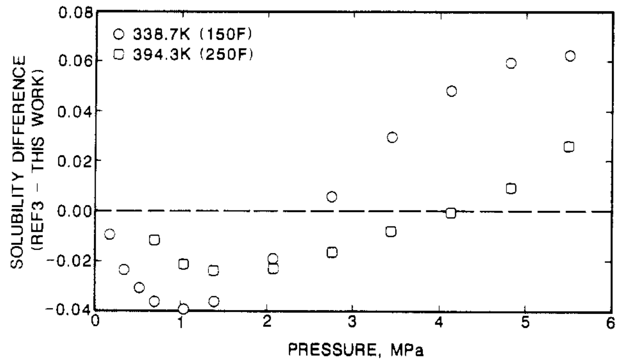

Figure 1. Comparison of ethane solubilities in *n*-hexane.

Table II. Soave and Peng–Robinson Equation of State Representations of Ethane Solubility in *n*-Hexane

temp, K (°F)	Soave param (P–R param)		error in ethane mole fracn[a]	
	C_{ij}	D_{ij}	rms	max
310.9 (100)	0.000 (0.005)	0.002 (0.000)	0.001	0.002
	0.001 (0.005)		0.001	0.002
338.7 (150)	0.003 (0.005)	−0.004 (−0.004)	0.001	0.002
	0.000 (0.002)		0.003	0.009
366.5 (200)	0.006 (0.005)	−0.007 (−0.005)	0.001	0.002
	0.000 (0.001)		0.001	0.002
394.3 (250)	0.025 (0.021)	−0.021 (−0.018)	0.001	0.002
	0.011 (0.009)		0.003	0.007
310.9, 338.7 366.5, 394.3	0.008 (0.010)	−0.008 (−0.008)	0.004	0.010
	0.003 (0.005)		0.004	0.013
	0.000	0.000	0.004	0.015

[a] Errors are essentially identical for the Soave and the Peng–Robinson equations of state.

solubilities from those of the present work. Figure 1 reveals substantial disagreement between the two data sets at 150 and 250 °F. These differences in mole fractions are larger than the combined expected uncertainties in the data (0.002 for this work; 0.008 and 0.015 at 150 and 250° F, respectively, as reported by Zais and Silberberg). Systematic variations between the two data sets are seen for both isotherms. At 100 and 200 °F, no previous data are available for comparison.

The ability of the Soave (*8*) or Peng–Robinson (*9*) EOS to represent our measured solubilities is documented in Table II. Results are shown for cases where one (C_{ij}) or two (C_{ij}, D_{ij}) interaction parameters are employed. These interaction parameters were determined by minimizing the sum of squares of deviations between the predicted and experimental bubble-point pressures.

Each equation is capable of describing the data with a root-mean-square error of 0.004 mole fraction when constant values of interaction parameters are used over the complete temperature range. When two parameters are fitted to each isotherm, root-mean-square errors are 0.001 or less; this illustrates both the ability of the EOS and the precision of our reported data. The interaction parameters show small, but systematic, variations with temperature. In contrast to the case for heavier paraffin solvents (*1*), the measurements for *n*-hexane are represented almost equally well by the Soave EOS without interaction parameters (last row in Table II).

Registry No. Ethane, 74-84-0; *n*-hexane, 110-54-3.

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Received for review September 6, 1988. Accepted June 13, 1989. Acknowledgment is made to the U.S. Department of Energy (DE-FG22-86PC90523) for financial support of this work.