J. Chem. Eng. Data **2006,** *51,* 1051−1055 **1051**

Isobaric Vapor−Liquid Equilibria for the Binary Mixtures of Styrene with Ethylbenzene, *o*-Xylene, *m*-Xylene, and *p*-Xylene

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Consistent vapor−liquid equilibria (VLE) data have been determined at (5 and 15) kPa for the binary systems styrene + ethylbenzene, + *o*-xylene, + *m*-xylene, and + *p*-xylene in the temperature range (324 to 359) K. The binary systems exhibit very slight deviations from ideal behavior, and no azeotrope is present. The VLE data were well-correlated by the Wilson, NRTL, and UNIQUAC equations.

Introduction

Mixtures of styrene with ethylbenzene and xylene isomers are frequently found in industrial processes, for instance, in the production of styrene by catalytic dehydrogenation of ethylbenzene. For correct design of separation processes, the knowledge of accurate vapor−liquid equilibria (VLE) data is essential. Additionally, the separation of these mixtures is further complicated due to similar boiling points of the components and the tendency of styrene to polymerize quickly. To minimize or even totally eliminate undesirable polymerization, the distillation of these mixtures is usually carried out at low temperatures and, therefore, low pressures. The pressure range used for industrial applications normally is between 5 kPa and 15 kPa.[1] The present work was undertaken to measure VLE data of the binary systems ethylbenzene (1) + styrene (2), *o*-xylene (1) + styrene (2), *m*-xylene (1) + styrene (2), and *p*-xylene (1) + styrene (2) at (5 and 15) kPa. For the system ethylbenzene + styrene, isobaric and isothermal VLE data have been reported in the literature. References 2 to 8 report isobaric VLE data, but not at (5 and 15) kPa; refs 9 to 11 report isothermal VLE data. References 12 and 13 are the only ones for the systems *o*-xylene + styrene and *m*-xylene + styrene, respectively. Both of them report isobaric VLE data at 60 mmHg. For the system *p*-xylene + styrene, no VLE data have been previously published.

Experimental Section

Chemicals. Styrene (99.5+ %) and *o*-xylene (99+ %) were purchased from Fluka Chemie, and ethylbenzene (99 %), *m*-xylene (99+ %; anhydrous), and *p*-xylene (99+ %, HPLC grade) were supplied by Aldrich. The reagents were used without further purification after chromatography failed to show any significant impurities. The densities of pure liquids were measured at 298.15 K using an Anton Paar DMA 55 densimeter. Temperature was controlled to ± 0.01 K with a thermostated bath. The uncertanties in density and refractive index measurements are ± 0.01 kg·m^{-3} and ± 0.0002, respectively. The experimental values of these properties are given in Table 1 together with those given in the literature.

Table 1. Density (d) and Refractive Index (n_D) of the Chemicals

	d (298.15 K)/kg·m^{-3}		n_D (298.15 K)	
component	expt	lit[a]	expt	lit[a]
styrene	902.30	901.40	1.5438	1.5440
ethylbenzene	862.74	862.57	1.4932	1.4932
o-xylene	875.99	875.63	1.5020	1.5030
m-xylene	859.80	859.86	1.4944	1.4946
p-xylene	856.55	856.70	1.4930	1.4933

[a] Ref 19.

Table 2. Experimental Vapor Pressure Data for Pure Components

styrene		ethylbenzene		*o*-xylene		*m*-xylene		*p*-xylene	
T/K	P/kPa	T/K	P/kPa	T/K	P/kPa	T/K	P/kPa	T/K	P/kPa
313.06	2.0	305.49	2.0	316.01	2.5	307.84	2.0	306.95	2.0
327.14	4.0	319.24	4.0	330.78	5.0	321.77	4.0	320.77	4.0
336.09	6.0	328.05	6.0	340.03	7.5	330.64	6.0	329.64	6.0
342.72	8.0	334.62	8.0	346.93	10.0	337.24	8.0	336.26	8.0
348.10	10.0	339.90	10.0	352.52	12.5	342.57	10.0	341.60	10.0
352.62	12.0	344.38	12.0	357.26	15.0	347.07	12.0	346.10	12.0
356.55	14.0	348.27	14.0	361.36	17.5	350.98	14.0	350.02	14.0
360.07	16.0	351.73	16.0	365.02	20.0	354.46	16.0	353.51	16.0
363.22	18.0	354.86	18.0	368.29	22.5	357.59	18.0	356.65	18.0
366.06	20.0	357.68	20.0	371.27	25.0	360.42	20.0	359.49	20.0
368.71	22.0	360.28	22.0	374.04	27.5	363.04	22.0	362.14	22.0
371.17	24.0	362.70	24.0	376.58	30.0	365.44	24.0	364.55	24.0
373.43	26.0	364.94	26.0			367.74	26.0	366.83	26.0
		367.06	28.0			369.85	28.0	368.96	28.0
		369.04	30.0			371.87	30.0	371.00	30.0

Apparatus and Procedure. An all-glass Fischer LABODEST vapor−liquid equilibrium apparatus model 602/D, manufactured by Fischer Labor und Verfahrenstechnik (Germany), was used in the equilibrium determinations. The equilibrium vessel was a dynamic recirculating still, equipped with a Cottrell circulation pump. The still is capable of handling pressures from (0.25 to 400) kPa and temperature up to 523 K. The Cottrell pump ensures that both liquid and vapor phases are in intimate contact during boiling and also in contact with the temperature-sensing element. The equilibrium temperature was measured with a digital Hart Scientific thermometer model 1502A and a Pt 100 probe Hart Scientific model 5622 calibrated at the Spanish Instituto Nacional de Técnica Aeroespacial. The uncertainty is estimated to be ± 0.02 K. For the pressure measurement, a digital manometer with an uncertainty of ± 0.05 kPa is used. The temperature probe was calibrated against the ice and steam points of distilled water. The manometers were calibrated using the vapor pressure of ultrapure water.

In each VLE experiment, the pressure was fixed and held constant by using a vacuum pump, and the heating and shaking

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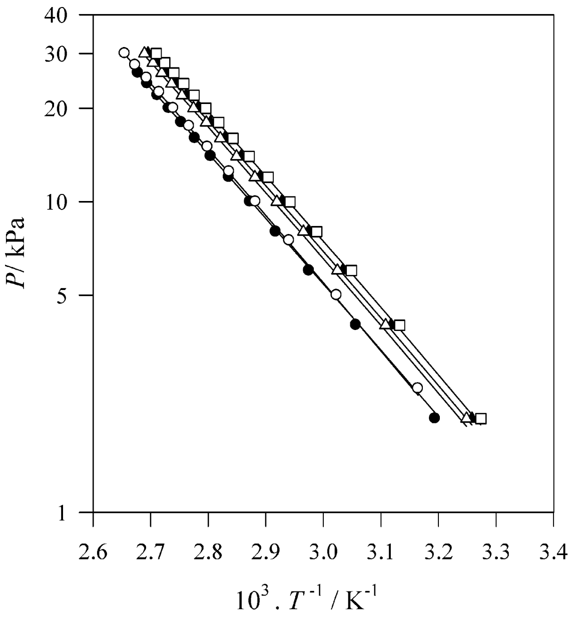

Figure 1. Vapor pressures: ●, styrene; ○, *o*-xylene; △, *m*-xylene; ▲, *p*-xylene; and □, ethylbenzene; —, Antoine correlations with parameters from ref 14.

Table 3. Calculated Antoine Coefficients in Equation 1

compound	A_i	B_i	C_i	100 ΔP^a
styrene	14.9081	3897.57	−38.89	0.06
ethylbenzene	14.1588	3397.18	−53.35	0.18
o-xylene	14.8797	3897.50	−37.04	0.11
m-xylene	14.7837	3790.23	−38.89	0.05
p-xylene	14.7186	3757.21	−38.99	0.06

[a] Average percentage deviation in vapor pressure: $\Delta P = 1/N\sum_i^N |P_i^{\mathrm{expt}} - P_i^{\mathrm{cal}}|/P_i^{\mathrm{expt}}$ (N, number of data points).

Table 4. Experimental Vapor−Liquid Equilibrium Data for Ethylbenzene (1) + Styrene (2)

P = 5.0 kPa			P = 15.0 kPa		
T/K	x_1	y_1	T/K	x_1	y_1
330.93	0.078	0.113	357.84	0.039	0.055
330.50	0.139	0.202	357.50	0.081	0.113
329.85	0.192	0.264	357.12	0.121	0.165
329.50	0.229	0.306	356.67	0.171	0.224
329.27	0.244	0.325	356.30	0.211	0.278
328.90	0.290	0.377	355.79	0.256	0.329
328.49	0.351	0.443	355.29	0.312	0.392
328.07	0.412	0.508	354.75	0.368	0.454
327.50	0.471	0.568	354.46	0.412	0.499
326.89	0.534	0.627	354.02	0.460	0.544
326.42	0.594	0.683	353.60	0.513	0.590
326.04	0.655	0.732	353.09	0.573	0.646
325.61	0.713	0.784	352.62	0.623	0.692
325.18	0.773	0.832	352.19	0.679	0.741
324.55	0.891	0.920	351.67	0.755	0.807
324.38	0.939	0.957	351.21	0.841	0.877
			350.90	0.886	0.915
			350.48	0.938	0.952
			350.21	0.978	0.984

Table 5. Experimental Vapor−Liquid Equilibrium Data for *o*-Xylene (1) + Styrene (2)

P = 5.0 kPa			P = 15.0 kPa		
T/K	x_1	y_1	T/K	x_1	y_1
331.85	0.047	0.050	358.31	0.048	0.051
331.80	0.091	0.097	358.27	0.092	0.095
331.73	0.141	0.149	358.23	0.138	0.141
331.66	0.192	0.203	358.18	0.186	0.191
331.60	0.246	0.259	358.14	0.230	0.238
331.52	0.307	0.322	358.09	0.275	0.285
331.45	0.364	0.378	358.04	0.321	0.332
331.38	0.412	0.427	357.99	0.371	0.380
331.31	0.478	0.495	357.93	0.431	0.440
331.26	0.502	0.517	357.88	0.473	0.491
331.20	0.552	0.566	357.82	0.532	0.537
331.15	0.598	0.614	357.75	0.582	0.590
331.10	0.649	0.662	357.69	0.635	0.640
331.05	0.697	0.710	357.62	0.688	0.696
330.98	0.742	0.753	357.56	0.744	0.750
330.94	0.789	0.798	357.48	0.803	0.812
330.90	0.838	0.846	357.40	0.864	0.869
330.83	0.901	0.905	357.31	0.926	0.929
330.79	0.948	0.950	357.25	0.970	0.971

Table 6. Experimental Vapor−Liquid Equilibrium Data for *m*-Xylene (1) + Styrene (2)

P = 5.0 kPa			P = 15.0 kPa		
T/K	x_1	y_1	T/K	x_1	y_1
331.87	0.015	0.019	357.74	0.086	0.106
331.68	0.042	0.055	357.65	0.114	0.135
331.43	0.089	0.115	357.39	0.156	0.189
331.09	0.138	0.174	357.11	0.200	0.232
330.77	0.190	0.234	356.88	0.238	0.272
330.48	0.243	0.298	356.59	0.285	0.334
330.20	0.295	0.354	356.32	0.331	0.385
329.90	0.348	0.413	356.02	0.381	0.435
329.62	0.392	0.460	355.76	0.428	0.486
329.46	0.420	0.487	355.51	0.477	0.534
329.25	0.461	0.529	355.21	0.527	0.578
328.98	0.511	0.576	354.92	0.575	0.630
328.71	0.567	0.629	354.65	0.623	0.674
328.49	0.610	0.671	354.39	0.678	0.718
328.16	0.669	0.722	354.12	0.725	0.765
327.88	0.724	0.772	353.83	0.775	0.812
327.63	0.779	0.820	353.70	0.808	0.836
327.31	0.843	0.874	353.34	0.879	0.895
327.09	0.896	0.917	353.06	0.933	0.945
326.79	0.957	0.966	352.85	0.968	0.974
326.69	0.978	0.983			

systems of the liquid mixture were turned on. The system was kept at the boiling point at least for 30 min to ensure that the steady state was reached. Then, samples of liquid and condensate were taken for analysis. The sample extractions were carried out with special syringes that allowed withdrawal of small volume samples (0.1 μL). At least two analyses were made for each sample.

Analysis. Concentration of the liquid and condensed phases were determined using a Hewlett-Packard 5890 series II gas chromatograph (GC), after calibration with gravimetrically prepared standard solutions. A flame ionization detector was used together with a 60 m, 0.20 mm i.d. capillary column SUPELCOWAX 10. Column, injector, and detector temperatures were (393, 498, and 523) K, respectively. Very good peak separation was achieved under these conditions, and calibration analyses were carried out to convert the peak area ratio to the mass composition of the sample. The uncertainty in the mole fraction was usually less than 0.001. Periodically, the refractive index of a liquid sample was also measured with the purpose of ensuring that polymerization of styrene was negligible.

Results and Discussion

The pure component vapor pressures were determined experimentally in the adequate range temperature for VLE calculations, using the same equipment as that for obtaining the VLE data. The pertinent results appear in Table 2 and Figure 1. The measured vapor pressures were correlated using the Antoine equation:

$$\ln(P_i^0/\mathrm{kPa}) = A_i - \frac{B_i}{(T/\mathrm{K}) + C_i} \qquad (1)$$

whose parameters A_i, B_i, and C_i are reported in Table 3 and were fitted by a nonlinear optimization method to minimize the

Table 7. Experimental Vapor−Liquid Equilibrium Data for *p*-Xylene (1) + Styrene (2)

$P = 5.0$ kPa			$P = 15.0$ kPa		
T/K	x_1	y_1	T/K	x_1	y_1
331.96	0.017	0.024	357.88	0.047	0.063
331.68	0.045	0.063	357.50	0.103	0.134
331.37	0.088	0.119	357.21	0.147	0.188
331.13	0.130	0.171	356.74	0.211	0.260
330.87	0.177	0.231	356.33	0.268	0.326
330.58	0.220	0.282	356.00	0.318	0.378
330.26	0.261	0.328	355.66	0.370	0.433
329.88	0.307	0.382	355.38	0.419	0.478
329.54	0.355	0.431	355.15	0.447	0.513
329.21	0.406	0.484	354.78	0.510	0.575
328.88	0.451	0.532	354.45	0.556	0.621
328.55	0.511	0.588	354.05	0.611	0.672
328.13	0.569	0.643	353.79	0.655	0.712
327.89	0.621	0.690	353.43	0.713	0.763
327.44	0.674	0.736	353.12	0.765	0.808
327.10	0.725	0.781	352.70	0.829	0.862
326.80	0.780	0.826	352.39	0.894	0.915
326.59	0.828	0.866	352.04	0.949	0.960
326.25	0.886	0.913			
325.95	0.942	0.957			
325.80	0.977	0.983			

Table 8. Consistency Test Statistics for the Binary Systems

system	P/kPa	100 AADy^a	AADP^b/kPa
ethylbenzene (1) + styrene (2)	5.0	0.37	0.020
	15.0	0.26	0.029
o-xylene (1) + styrene (2)	5.0	0.13	0.005
	15.0	0.20	0.010
m-xylene (1) + styrene (2)	5.0	0.33	0.003
	15.0	0.29	0.015
p-xylene (1) + styrene (2)	5.0	0.43	0.014
	15.0	0.29	0.023

[a] Average absolute deviation in vapor phase composition: $\mathrm{AAD}y = 1/N\sum_{i=1}^{N}|y_1^{\mathrm{expt}} - y_1^{\mathrm{cal}}|_i$ (N, number of data points). [b] Average absolute deviation in pressure: $\mathrm{AAD}P = 1/N\sum_{i=1}^{N}|P_i^{\mathrm{expt}} - P_i^{\mathrm{cal}}|$.

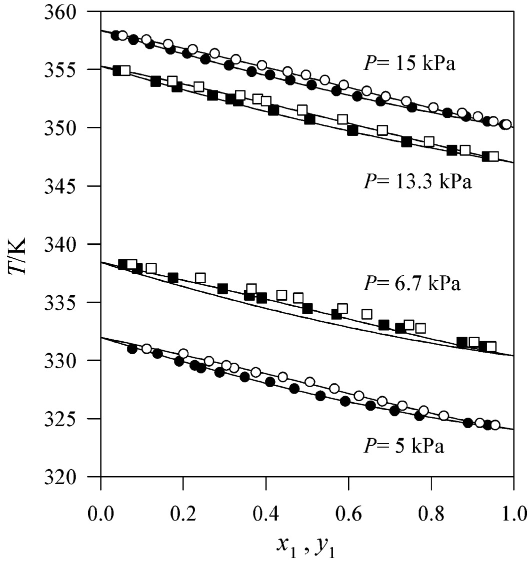

Figure 2. Boiling temperature diagram for the system ethylbenzene (1) + styrene (2) at 5.0 kPa and 15.0 kPa: ●, ○, experimental data reported in this work; ■, □, experimental data of Chaiyavech and Van Winkle;[2] —, smoothed data using the Wilson model with the parameters given in Table 9 and eq 3.

average percentage deviation in vapor pressure (ΔP). Figure 1 shows a comparison of data obtained and Antoine correlation with parameters taken from ref 14. It can be observed that the parameters of ref 14 give a fair correlation of the experimental vapor pressures reported in this work for styrene ($\Delta P = 1.10$ %), ethylbenzene ($\Delta P = 1.29$ %), *o*-xylene ($\Delta P = 1.51$ %), *m*-xylene ($\Delta P = 2.36$ %), and *p*-xylene ($\Delta P = 1.54$ %).

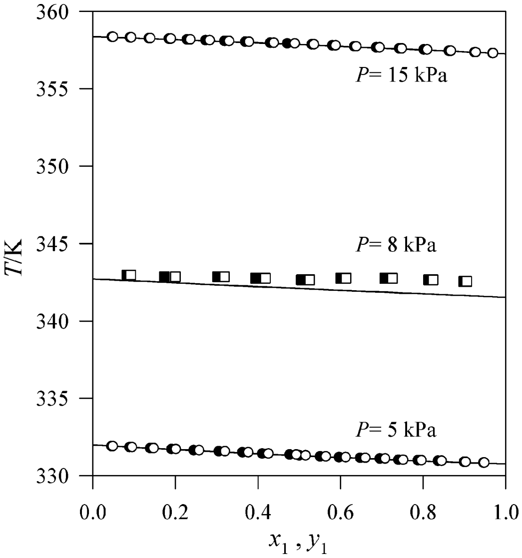

Figure 3. Boiling temperature diagram for the system *o*-xylene (1) + styrene (2) at 5.0 kPa and 15.0 kPa: ●, ○, experimental data reported in this work; ■, □, experimental data of Kormina et al.;[12] —, smoothed data using the Wilson model with the parameters given in Table 9 and eq 3.

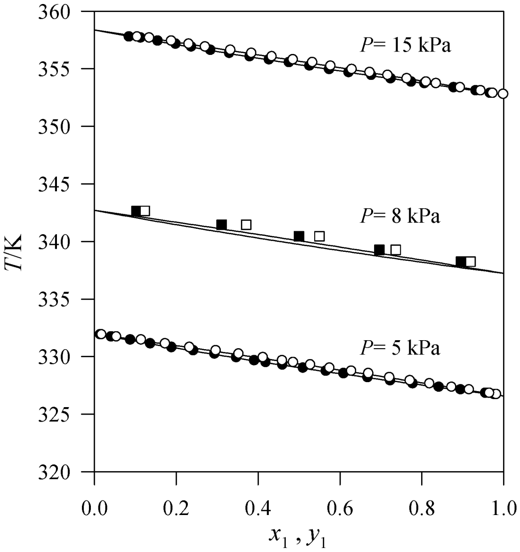

Figure 4. Boiling temperature diagram for the system *m*-xylene (1) + styrene (2) at 5.0 kPa and 15.0 kPa: ●, ○, experimental data reported in this work; ■, □, experimental data of Kormina et al.;[13] —, smoothed data using the Wilson model with the parameters given in Table 9 and eq 3.

The experimental VLE data for the four binary systems at $P = (5$ and $15)$ kPa are reported in Tables 4 to 7 and in Figures 2 to 5. According to the obtained results, the studied binary systems form almost ideal solutions and no azeotropes were found. The VLE data reported in Tables 4 to 7 were found to be thermodynamically consistent by the point-to-point method of Van Ness et al.[15] as modified by Fredenslund et al.[16] using a one-parameter Legendre polynomial. The vapor phase was assumed to be ideal. Pertinent consistency details and statistics are presented in Table 8. The VLE data were also correlated with Wilson, NRTL, and UNIQUAC equations. The parameters of these models were obtained by minimizing the following objective function (OF):

$$\mathrm{OF} = \sum_{i=1}^{N} 100 \times \left(\left| \frac{P_i^{\mathrm{expt}} - P_1^{\mathrm{calc}}}{P_i^{\mathrm{expt}}} \right| + \left| y_i^{\mathrm{expt}} - y_1^{\mathrm{calc}} \right| \right) \qquad (2)$$

Table 9. Parameters and Correlation Statistics for Different G^E Models

model	A^0_{12}/J·mol^{-1}	A^1_{12}/J·mol^{-1}·K^{-1}	A^0_{21}/J·mol^{-1}	A^1_{21}/J·mol^{-1}·K^{-1}	α_{12}	100 AADy[a]	100 ΔP[b]
			Ethylbenzene (1) + Styrene (2)				
Wilson[c]	−3724.14	6.77	8456.63	−19.01		0.27	0.29
NRTL	17409.76	−43.01	−11056.90	26.18	0.2	0.27	0.30
UNIQUAC[d]	1597.55	−1.85	−692.94	−0.25		0.26	0.30
			o-Xylene (1) + Styrene (2)				
Wilson[c]	376.18	4.37	357.31	−9.80		0.16	0.05
NRTL	297.99	−9.98	411.10	−1.03	0.2	0.16	0.05
UNIQUAC[d]	129.27	−0.08	103.85	−0.57		0.16	0.04
			m-Xylene (1) + Styrene (2)				
Wilson[c]	70.65	−2.33	94.66	−1.21		0.31	0.07
NRTL	1951.48	−4.58	−1283.04	−8.00	0.2	0.30	0.09
UNIQUAC[d]	−288.13	−1.33	392.79	1.40		0.29	0.07
			p-Xylene (1) + Styrene (2)				
Wilson[c]	−1835.44	−5.23	2517.83	1.16		0.30	0.23
NRTL	24965.88	−66.47	−19238.24	50.83	0.2	0.32	0.21
UNIQUAC[d]	−973.64	0.44	−973.64	−0.30		0.30	0.19

[a] Average absolute deviation in vapor phase composition. [b] Average percentage deviation in pressure. [c] Liquid volumes have been estimated from the Rackett equation.[20] [d] Volume and surface parameters from ref 14.

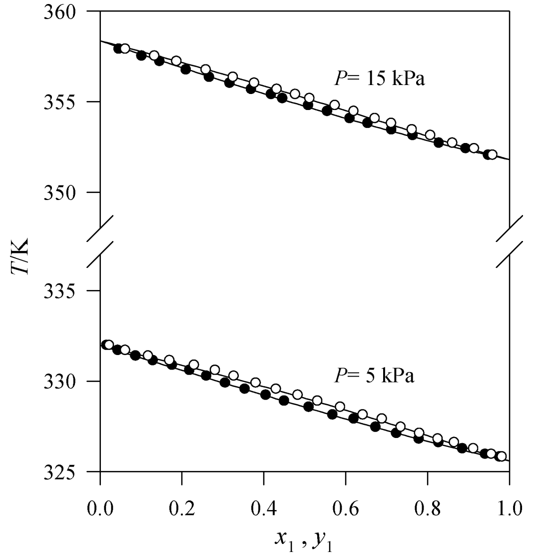

Figure 5. Boiling temperature diagram for the system *p*-xylene (1) + styrene (2) at 5.0 kPa and 15.0 kPa: ●, ○, experimental data reported in this work; —, smoothed data using the Wilson model with the parameters given in Table 9 and eq 3.

and are reported in Table 9, together with the pertinent statistics of VLE interpolation. Simultaneous correlation of experimental data at (5 and 15) kPa was carried out for each system, and for that reason, to take into account the dependence of the excess energy on temperature, the parameters for all these equation (A_{ij}, A_{ji}) were considered to be linear function of the temperature:[17,18]

$$A_{ij} = A^0_{ij} + A^1_{ij}T \tag{3}$$

An inspection of the results shows that all three models gave a reasonable fit of the binary systems and that no significant differences were observed between models. Figures 2 to 4 show a graphical comparison between isobaric experimental VLE data reported in the literature and the data calculated at the pertinent pressure conditions using the Wilson model with the parameters obtained in this work. As it has been mentioned previously, refs 2 to 8 report isobaric VLE data for the system ethylbenzene + styrene, but only the data determined by Chaiyavech and Van Winkle[2] at (6.7 and 13.3) kPa have been represented in Figure 2 because the rest of the literature data are thermodynamically inconsistent by the point-to-point method[15,16] as pointed out in ref 14. Also, the literature data[12,13] for the systems *o*-xylene + styrene and *m*-xylene + styrene are thermodynamically inconsistent according with ref 14, but the graphical comparison has been made with these data in Figures 3 and 4, respectively, because there are no more references for these systems. From these comparisons, it can be observed that the Wilson model with the parameters obtained in this work gives a fair description of the literature data.

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Received for review December 15, 2005. Accepted February 16, 2006. This work has been financed by MCT, Spain (Project PPQ2000-1335).

JE050523S