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Vapor−Liquid Equilibria in the 2-Methylcyclohexanol + 2-Methylcyclohexyl Ethanoate System at 101.325 kPa

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Vapor−liquid equilibrium data were measured using the Świętosławski ebulliometric still in the binary 2-methylcyclohexanol + 2-methylcyclohexyl ethanoate system at a constant pressure of (101.325 ± 0.070) kPa. The saturated vapor pressures were also measured for samples of mole fraction purity of 99.97 % 2-methylcyclohexanol and 99.98 % 2-methylcyclohexyl ethanoate over wide temperature ranges by comparative ebulliometry. The experimental data were correlated using the maximum-likelihood method, and overall measures of data reproducibility are given. The results are compared with literature data. VLE experimental data were tested for thermodynamic consistency by means of several different consistency tests and were demonstrated to be consistent.

Introduction

In this work, the results of measurements on the saturated vapor pressures of 2-methylcyclohexanol and 2-methylcyclohexyl ethanoate and vapor−liquid equilibria (VLE) for the system 2-methylcyclohexanol + 2-methylcyclohexyl ethanoate are reported.

Experimental Section

Chemicals. Samples of 2-methylcyclohexanol and 2-methylcyclohexyl ethanoate, of technical quality, were supplied by Alwernia S.A. Chemical Company (Alwernia, Poland). Each of the components was a mixture of cis (*Z*) and trans (*E*) isomers. Since the properties of both isomers are very similar (cf., e.g., Figure 1), no attempt was made to separate them. However, further purification was applied to remove other impurities. Samples were dried over 4 Å type molecular sieves and distilled on 40-TP laboratory column. The middle boiling fraction within a 5 mK range was collected. Impurities were determined chromatographically. Water content was checked using Fischer's reagent and was on the limit of detectability. Physical properties of the substances used together with their purity are listed in Table 1.

Vapor Pressure. Saturated vapor pressure was measured over a temperature range of (361.23 to 439.57) K for 2-methylcyclohexanol and of (368.01 to 458.00) K for 2-methylcyclohexyl ethanoate, respectively. The comparative ebulliometric technique comprising a dynamic twin ebulliometer assembly was used as described elsewhere.[1] Temperature was measured on an ITS-90 scale with a platinum resistance thermometer (Leeds & Northrup, model 8163-C) operated in conjunction with a Mueller bridge (Leeds & Northrup, type G-2) and an electronic null detector (Leeds & Northrup, model 9834). To provide replicate data, each equilibrium point was measured six times. The maximum uncertainty in the temperature measurement and the associated pressure inconstancy were estimated at ± 5 mK and ± 7 Pa, respectively. Tables 2 (for 2-methylcyclohexanol) and 3 (for 2-methylcyclohexyl ethanoate) list the observed (T_i, P_i) data pairs with their estimated precision measures (σ_{T_i}, σ_{P_i}).

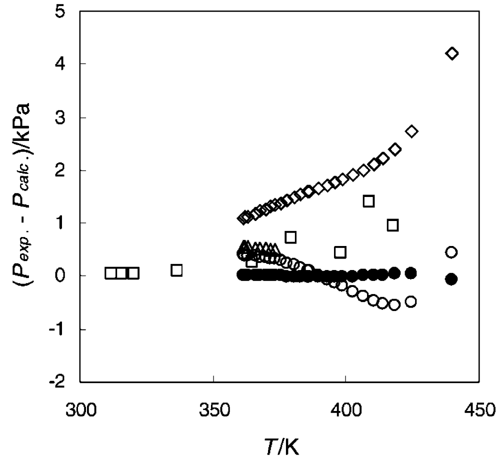

Figure 1. 2-Methylcyclohexanol. Deviations between the experimental saturated vapor pressures and the values calculated with eq 1 vs temperature: ●, this work; □, Goodwin and Newsham;[4] Δ, calculated from the Antoine parameters reported by Riddick et al.;[5] ◊ (cis), calculated from the saturated vapor pressure equation taken from the KBD Data Base;[6] ○ (trans), calculated from the saturated vapor pressure equation taken from the KBD Data Base.[6]

Vapor−Liquid Equilibria. The comparative technique involving the Świętosławski-type dynamic twin ebulliometer assembly mounted and operated as described previously[1] was used. Temperature was measured on an ITS-90 scale with a platinum resistance thermometer (Leeds & Northrup, model 8163-C) operated in conjunction with a Mueller bridge (Leeds & Northrup, type G-2) and an electronic null detector (Leeds & Northrup, model 9834). Details on the measuring technique were reported by Choliński et al.[2] The equilibrium pressure in the assembly was measured via the boiling temperature of high-purity water[3] used as the reference substance in a barometric ebulliometer operated simultaneously with the proper still. Liquid-phase and vapor condensate samples were analyzed using calibration curves constructed from n_D versus x_1 data measured with a precision Pulfrich refractometer at (293.15 ± 0.01) K. The estimated precision of the equilibrium mixture composition

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Table 1. Purity, Normal Boiling Temperatures (T_{nb}) and Refractive Indices (n_D^{20}) of Pure Components

substance	purity mol %	T_{nb}/K, this work	n_D^{20} mixture of isomers, this work	n_D^{20} *cis* isomer, lit.	n_D^{20} *trans* isomer, lit.
2-methycyclohexanol	99.92	439.85	1.46313	1.4620	1.4596
2-methylcyclohexyl ethanoate	99.94	458.51	1.43896	1.4376	1.4353

Table 2. Experimental Temperatures (T), Orthobaric Pressures (P), Precision Measures (σ_T and σ_P), Calculated Residuals, ΔT (= $T_{exp} - T_{calc}$) and ΔP (= $P_{exp} - P_{calc}$), and Overall Measures of Data-Point Reproduction (κ_i^s) of 2-Methylcyclohexanol

T/K	σ_T/K	ΔT/K	P/kPa	σ_P/kPa	ΔP/kPa	κ_i^s
361.23	0.010	−0.023	5.394	0.003	0.008	−0.97
361.23	0.010	−0.023	5.394	0.003	0.008	−0.97
362.23	0.008	−0.021	5.668	0.003	0.010	−1.20
363.13	0.010	−0.021	5.919	0.003	0.007	−0.84
365.70	0.009	−0.015	6.693	0.002	0.002	−0.56
367.68	0.008	−0.004	7.345	0.002	0.001	−0.15
369.92	0.002	0.000	8.152	0.003	0.002	−0.16
371.63	0.004	−0.002	8.817	0.002	0.002	−0.27
373.16	0.007	−0.002	9.448	0.003	0.001	−0.12
375.31	0.003	−0.002	10.399	0.002	0.002	−0.30
377.78	0.002	0.001	11.578	0.003	−0.005	0.50
380.39	0.006	0.019	12.943	0.002	−0.004	1.01
383.11	0.006	0.010	14.517	0.003	−0.004	0.61
385.95	0.008	0.006	16.323	0.004	−0.002	0.27
386.10	0.007	0.015	16.418	0.002	−0.002	0.63
389.56	0.005	0.009	18.864	0.004	−0.008	0.77
393.07	0.006	0.003	21.648	0.010	−0.009	0.29
395.88	0.002	0.004	24.104	0.003	−0.009	1.02
398.52	0.004	0.014	26.604	0.003	−0.008	1.25
402.67	0.004	0.001	30.990	0.006	−0.002	0.11
406.67	0.004	0.000	35.730	0.002	0.000	−0.03
410.73	0.007	−0.001	41.114	0.006	0.000	−0.04
414.00	0.001	0.000	45.898	0.005	−0.004	0.25
418.26	0.003	−0.025	52.847	0.002	0.006	−2.48
424.63	0.003	−0.016	64.662	0.004	0.015	−1.84
439.57	0.003	0.018	100.473	0.004	−0.011	1.85

Table 3. Experimental Temperatures (T), Orthobaric Pressures (P), Precision Measures (σ_T and σ_P), Calculated Residuals, ΔT (= $T_{exp} - T_{calc}$) and ΔP (= $P_{exp} - P_{calc}$), and Overall Measures of Data-Point Reproduction (κ_i^s) of 2-Methylcyclohexyl Ethanoate

T/K	σ_T/K	ΔT/K	P/kPa	σ_P/kPa	ΔP/kPa	κ_i^s
368.01	0.027	0.058	5.320	0.003	−0.003	0.98
369.86	0.005	0.004	5.758	0.004	−0.010	1.05
371.87	0.009	0.024	6.261	0.002	−0.005	1.42
373.83	0.006	0.003	6.787	0.006	−0.009	0.66
376.56	0.005	−0.002	7.594	0.004	0.003	−0.37
379.93	0.003	0.000	8.675	0.003	0.001	−0.06
383.36	0.006	−0.006	9.912	0.002	0.002	−0.51
386.65	0.013	0.013	11.216	0.005	−0.004	0.53
391.27	0.006	0.002	13.318	0.001	0.000	0.16
393.39	0.004	0.002	14.379	0.004	−0.003	0.36
394.15	0.003	0.001	14.773	0.005	−0.007	0.62
398.42	0.004	−0.013	17.204	0.002	0.005	−1.68
401.60	0.002	−0.001	19.193	0.003	0.003	−0.45
403.30	0.007	−0.003	20.341	0.007	0.005	−0.35
405.73	0.002	−0.004	22.082	0.003	0.012	−1.86
410.71	0.005	−0.007	26.013	0.005	0.008	−0.90
415.57	0.006	−0.011	30.387	0.004	0.005	−0.88
418.74	0.002	0.000	33.542	0.008	0.007	−0.34
421.20	0.003	0.011	36.157	0.001	−0.001	1.61
423.84	0.004	0.008	39.173	0.002	−0.002	0.89
426.54	0.005	0.012	42.453	0.004	−0.006	1.15
429.41	0.003	0.000	46.213	0.004	0.000	0.02
433.20	0.002	0.002	51.551	0.001	0.000	0.48
440.40	0.004	−0.005	63.092	0.008	0.012	−0.77
458.00	0.008	−0.030	100.130	0.003	0.002	−1.54

Table 4. Experimental Liquid- and Vapor-Phase Mole Fractions (x_1 and y_1), Boiling Temperatures (T), Calculated Residuals, Δx_1 (= $x_{1,exp} - x_{1,calc}$), Δy_1 (= $y_{1,exp} - y_{1,calc}$), ΔT (= $T_{exp} - T_{calc}$), and ΔP (= $P_{exp} - P_{calc}$), and Measures of Data-Point Reproduction (κ_i^s) of 2-Methylcyclohexanol (1) + 2-Methylcyclohexyl Ethanoate (2) System at P/kPa = (101.325 ± 0.070)

x_1	Δx_1	y_1	Δy_1	T/K	ΔT/K	ΔP/kPa	κ_i^s
0.0158	0.0000	0.0299	0.0053	458.16	0.00	−0.14	1.14
0.0462	−0.0001	0.0770	0.0060	457.39	0.01	−0.02	0.64
0.0934	0.0015	0.1408	0.0027	456.40	0.03	−0.15	1.52
0.1535	0.0009	0.2213	−0.0014	454.97	0.02	−0.07	0.78
0.2110	0.0009	0.2953	−0.0028	453.70	0.02	−0.07	0.82
0.2532	0.0007	0.3438	−0.0069	452.77	0.01	−0.04	0.86
0.3840	−0.0003	0.4956	−0.0044	450.01	−0.01	0.05	0.66
0.4811	−0.0018	0.6034	0.0049	448.04	−0.04	0.18	1.92
0.5332	−0.0012	0.6418	−0.0043	447.11	−0.04	0.16	1.63
0.6539	−0.0002	0.7467	−0.0010	445.12	−0.01	0.03	0.30
0.6824	0.0001	0.7649	−0.0052	444.67	0.00	0.00	0.53
0.7313	0.0007	0.8120	0.0046	443.96	0.03	−0.11	1.15
0.8046	0.0005	0.8670	0.0050	442.79	0.02	−0.08	0.95
0.8670	0.0010	0.9101	0.0039	441.91	0.04	−0.17	1.64
0.9157	0.0001	0.9456	0.0045	441.09	0.01	−0.03	0.55
0.9592	0.0003	0.9745	0.0032	440.48	0.01	−0.06	0.61
0.9864	0.0000	0.9910	0.0005	440.11	0.00	−0.13	0.91

measurements was assumed to be ± 0.001 mole fraction. The estimated uncertainties in equilibrium temperature and pressure were ± 0.02 K and ± 0.070 kPa. These estimates were evaluated during the MML calculations, as described below. From these calculations, it follows that the more correct uncertainty in vapor-phase composition should be ± 0.005 mole fraction. The equilibrium vapor and liquid compositions and the boiling points at a constant pressure (101.325 ± 0.070) kPa are given in Table 4 and are presented in Figure 3.

Results and Discussion

To obtain the fits of the saturated vapor pressures to the Antoine equation

for 2-methylcyclohexanol

$$\ln(P/\text{kPa}) = 13.61807 - \frac{2876.62}{T/\text{K} - 120.214} \qquad (1)$$

for 2-methylcyclohexyl ethanoate

$$\ln(P/\text{kPa}) = 14.33384 - \frac{3780.88}{T/\text{K} - 69.346} \qquad (2)$$

the maximum likelihood method was used as described in more detail elsewhere.[1,3] Tables 2 (for 2-methylcyclohexanol) and 3 (for 2-methylcyclohexyl ethanoate) list the deviations (ΔT_i, ΔP_i) between the observed and calculated variables. The ΔT_i and ΔP_i values allow us to check whether the values obtained for error variances are appropriate by assessing whether or not the variations in these fall properly within their (computed) confidence intervals. Since neither ΔT_i nor ΔP_i alone is adequately representative as an overall measure of reproduction for an individual data point, we suggested[1]

$$\kappa_i^s = \text{sgn}(\Delta T_i)\kappa_i/\hat{\sigma} \qquad (3)$$

where for the present case

$$\kappa_i = [(\Delta P_i/\sigma_{P_i})^2 + (\Delta T_i/\sigma_{T_i})^2]^{1/2} \qquad (4)$$

as an overall measure of data-point reproduction, where κ_i is the distance between the ith observed and estimated data points in the (P, T) space and σ_T and σ_P are adopted as length units.

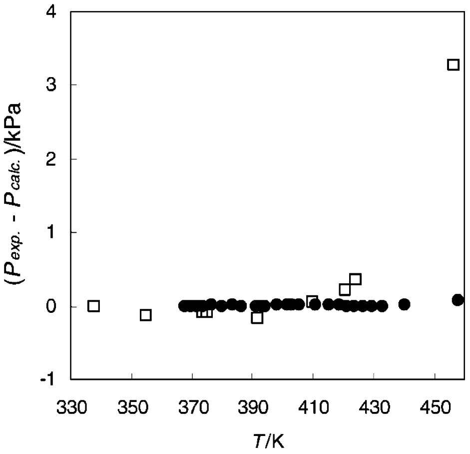

Figure 2. 2-Methylcyclohexyl ethanoate. Deviations between the experimental saturated vapor pressures and the values calculated with eq 2 vs temperature: ●, this work; □, Goodwin and Newsham.[4]

The κ_i^s values are seen (eq 3) to be scaled with respect to $\hat{\sigma}$ (i.e., to the standard deviation of κ_i given by the formula):

$$\hat{\sigma} = [\sum_{i=1}^{n} \kappa_i^2/(n-3)]^{1/2} \tag{5}$$

where n is the number of experimental points. The sign of ΔT_i has been attributed to κ_i to have the experimental point located "below" or "above" the response curve. When systematical errors are absent, sign of κ_i^s should be randomly distributed, and absolute values should be about unity; large κ_i values ($\gg 1$) may indicate outliers. Easy measure of the randomness of κ_i^s is number of sign changes test. If two neighboring κ_i^s have opposite signs, then one speaks of a sign change. Total number of sign changes should be roughly equal to $n/2 \pm (n/2)^{1/2}$ (limits at 68 % probability level). The corresponding values are 5 (9 to 15) for 2-methylcyclohexanol and 5 (9 to 15) for 2-methylcyclohexyl ethanoate, where values in parentheses are limits calculated at 68 % probability level.

The calculated deviations (Tables 2 and 3) in observed temperature (ΔT) and pressure (ΔP) show a consistently statistical pattern and, especially as regards temperature, they do not rise in the vicinity to the normal boiling point. This shows that the substance is thermally stable and shows no signs of decomposition as the temperature is increased. Indirectly, this fact is also a confirmation of the high purity of the sample used for the measurements.

Saturated vapor pressures for 2-methylcyclohexanol and 2-methylcyclohexyl ethanoate can be compared with corresponding literature data.[4−6] Deviations between the experimental data, both the newly measured and taken from literature, and the values calculated with relevant equations with parameters fitted to the new data versus temperature are presented in Figures 1 and 2. The equilibrium vapor and liquid compositions and the boiling points at 101.325 kPa are given in Table 3.

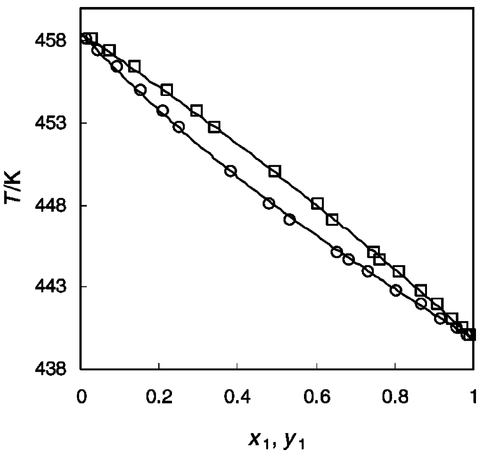

Figure 3. 2-Cyclohexanol (1) + 2-methylcyclohexyl ethanoate (2) system at P/kPa = 101.325. Circles and squares correspond to liquid and vapor phases, respectively. Lines were calculated with the Wilson parameters fitted to the experimental data.

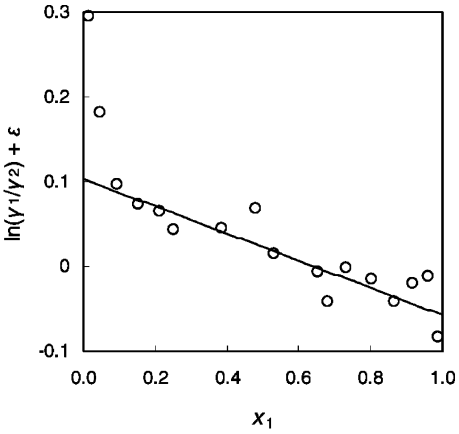

Figure 4. Thermodynamic consistency test for the 2-cyclohexanol (1) + 2-methylcyclohexyl ethanoate (2) system at P/kPa = 101.325. Note that two first points were neglected. The scatter of this points results primarily from unfavorable error propagation of liquid phase and vapor phase compositions.

The thermodynamic consistency of the data was verified using the area and the point-to-point and point tests. To perform an area test, the ln $\gamma_1/\gamma_2 + \epsilon$ values has been calculated. Values of ϵ, for isobaric data equal to $-H^E/RT^2(dT/dx_1)_\sigma$, were calculated with enthalpy of mixing (H^E) represented by a regular formula with the estimated value of A/J·mol^{-1} equal to 2300. Vapor phase nonideality was accounted for using a truncated virial equation of state with second virial coefficients calculated according to Tsonopoulos.[7] Molar liquid volumes were calculated using the Yen and Woods procedure.[7] The plot of the ln $\gamma_1/\gamma_2 + \epsilon$ values versus liquid mole fraction x_1 is presented in Figure 4. The ln $\gamma_1/\gamma_2 + \epsilon$ values versus liquid mole fraction x_1 were represented by the 2/2 polynomial[8] with the rmsd(ln $\gamma_1/\gamma_2 + \epsilon$) = 0.0167 and the total number of sign changes equal to 7 (5, 10), where values in parentheses are limits calculated at 68 % probability level. The Redlich−Kister area test[9] is passed with the absolute area deficit equal to 0.0084 (<0.01 − critical value for acceptable data[8]). The area test according to Herington[10,11] is passed with the area relative difference equal to 0.052 (<0.1 − critical value for consistent data).

Two point-to-point tests were used, that proposed by McDermott and Ellis and further modified by Wisniak and Tamir[12] and that of Samuels and Ulrichson.[13] Our data passed both above tests. In calculations uncertainties in all the measurables were used as reported above with value for vapor phase as modified after the MML calculations.

Seven point tests were used. The y values test as proposed by Van Ness et al.[14] and Christiansen and Fredenslund[15] was used in two versions; using the simple Barker's method and using the MML method without and with experimental vapor-phase compositions. Experimental data passed both tests. For the Barker's method $\delta(y_1) = 0.0046 < 0.001 + 0.005$ (= $s(x_1) + s(y_1)$) with the total number of sign changes equal to 4 (6, 10) with limits calculated at 68 % probability level. Similar results are obtained using the MML method.

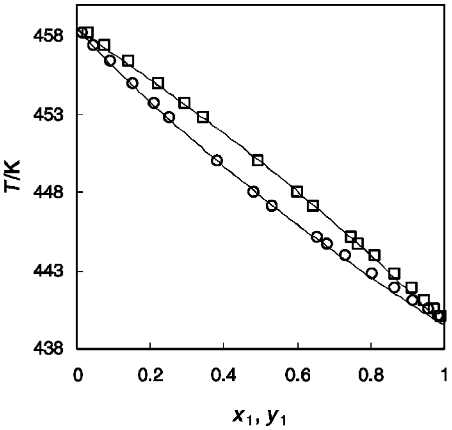

Figure 5. Thermodynamic consistency test for the 2-cyclohexanol (1) + 2-methylcyclohexyl ethanoate (2) system at P/kPa = 101.325. Results of the extended, pressure dependent area test (numerical integration of the Gibbs−Duhem equation with ln $\gamma_1/\gamma_2 + \epsilon$ values represented by the approximating curve from Figure 4).

Direct tests of Oracz[16] and Van Ness[17] were used. According to Van Ness qualification, data with $\delta = 0.063$ have quality index equal to 3, which means they are (fairly) good. Using criteria proposed by Oracz, where direct test values are compared with error propagation boundaries, only two points are slightly outside of the boundaries estimated with the uncertainties in variables reported above. This indicates good quality of data.

Application of the Kojima et al.[18] point test results in $\delta = 0.0085$ (<0.05 − consistent data). The critical value equal to 0.05 was adopted after the Kojima's recommendation. The infinite dilution activity coefficient test according to Kojima et al.[18] was not passed for both test values I_1 and I_2; $I_1 = 0.98 > 0.30$ and $I_2 = 1.06 > 0.30$, where critical test values are according to Kojima et al.[18]

The extended pressure dependent area test according to Oracz[8] results in $100\delta P/P = 0.418$ (<0.5 − good data[8]). Curve presented in Figure 4, represented by the 2/2 polynomial[8] as stated above, was used in numerical integration according to procedure outlined in ref 8. The resulting phase boundaries are presented in Figure 5.

For the LW test according to Wisniak,[19] most of points passed the test having test values lower than 3. Three points have test values slightly higher than 3, and another three (extreme) points deviate more than 5. Values of molar enthalpies of vaporization at the boiling temperature needed for the test calculations were estimated from saturated vapor pressure versus temperature relations given by eqs 1 and 2.

The x values test according to Eubank et al.[20] was also used. According to the criteria proposed by the authors, all points are at least acceptable whereas more than half of them are of good quality. The rmsd(x_1) = 0.008 (<0.01 for good data[20]).

Most of above methods (the area, point-to-point, Kojima's, and direct tests) can be regarded as byproducts of the extended pressure dependent area test[8] and were encapsulated into a single procedure. Results of all above consistency test applied to our data, except for the infinite dilution activity coefficients test according to Kojima et al.,[18] indicate at least acceptable quality of our data, and most of them indicate that data are of good quality.

Models based on the local composition models were used for correlation of the experimental data: Wilson, modified Wilson, NRTL, and UNIQUAC (cf., e.g., ref 7). Coefficients of these equations were obtained by a modified Barker's method. As mentioned above, vapor phase nonideality was accounted for using a truncated virial equation of state with second virial coefficients calculated according to Tsonopoulos.[7] Molar liquid volumes were calculated using the Yen and Woods procedure.[7] Results indicate that all above equations represent experimental data with sufficient and near the same accuracy. Thus the experimental data were reduced by means of the multiresponse maximum likelihood method (cf., e.g., ref 7) with the modified Wilson equation. The objective function used was

$$\mathrm{OF} = \sum_{i=1}^{N} [(\Delta x_{1,i}/\sigma_x)^2 + (\Delta y_{1,i}/\sigma_y)^2 + (\Delta P_i/\sigma_P)^2 + (\Delta T_i/\sigma_T)^2]/(4n - n_\mathrm{p}) \quad (6)$$

where ΔZ_i is the deviation between the observed and calculated variable z for the ith experimental point, σ_Z is the estimated uncertainty in the variable z, n is the number of experimental points, and n_p is the number of adjustable parameters in the model used.

The modified Wilson equation was used in the form

$$\frac{G^\mathrm{E}}{RT} = -x_1 \ln(x_1 + \Lambda_{12}x_2) - x_2 \ln(x_2 + \Lambda_{21}x_1) \quad (7)$$

with

$$\Lambda_{ij} = \exp\left(-\frac{a_{ij}}{T}\right) \quad (8)$$

where a_{ij} is the adjustable binary interaction parameter.

Table 4 reports the deviations (Δx_1, Δy_1, ΔT_i, ΔP_i) between the observed and calculated variables. The values of these deviations allow to check whether the values adopted for error variances are appropriate, by assessing whether or not the variations in these fall properly within their (computed) confidence intervals. Since neither among these deviations alone is adequately representative as an overall measure of reproduction for an individual data point, we suggest using

$$\kappa_i = \sqrt{[(\Delta x_{1,i}/\sigma_x)^2 + (\Delta y_{1,i}/\sigma_y)^2 + (\Delta P_i/\sigma_P)^2 + (\Delta T_i/\sigma_T)^2]/4} \quad (9)$$

as an overall measure of data-point reproduction. When systematical errors are absent κ_i values should be about unity; large κ_i values ($\gg 1$) may indicate outliers. The measures of data-point reproduction, κ_i, are reported in Table 4. Contrary to the saturated vapor pressures no sign of any deviation can be attributed to κ_i. The distribution of deviations together with their signs must be investigated for all measured variables. Deviations must be reasonably within declared uncertainties and must represent reasonable scatter of signs. As previously, the number of sign changes test can be applied. The resulting values are 4, 4, 2, and 2 for liquid and vapor compositions, temperature, and pressure, correspondingly. The expected boundary values are (6, 10) at the 68 % confidence level. Thus all above values are too low. From other hand, the deviations are enough small, and the overall relative deviation is equal to 0.939. This result is very satisfactory.

Parameters a_{ij} of eq 7 together with their standard errors $\sigma(a_{ij})$ and correlation coefficient q are reported in Table 5. Goodwin and Newsham[4] reported VLE data measured at (6.67, 13.33, and 39.46) kPa with an uncertainty of ± 0.01 kPa. Although the ratio of isomers can be different in both cases it can be expected that due to the similarity of behavior of both isomers data measured by Goodwin and Newsham and reported

Table 5. Parameters a_{ij} of Equation 7 with Their Standard Errors $\sigma(a_{ij})$ and Correlation Coefficient q for the 2-Methylcyclohexanol (1) + 2-Methylcyclohexyl Ethanoate (2) System at P/kPa = (101.325 ± 0.070)

	ij	
	12	21
a_{ij}/K	212.84	−102.226
$\sigma(a_{ij}$/K)	30.2	20.9
q	−0.9987	

in this work can be simultaneously represented with the same $G^E(T, x)$ dependence. To this end the modified Wilson equation and the Barker's method was used. To avoid discrepancy in saturated vapor pressures, in simultaneous VLE data reduction Antoine equations with parameters fitted to the original saturated vapor pressure data were used for corresponding data sets. The agreement between experimental and correlated values is satisfactory, the overall standard deviation in pressure is $\sigma(P/\text{kPa}) = 0.278$.

Literature Cited

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