# Vapor-Liquid Equilibrium for Binary Systems 2-Butanone with 2-Butanol, 1-Pentanol, and Isoamyl Alcohol

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**Vapor-liquid equilibrium data at atmospheric pressure for the systems 2-butanone–2-butanol, 2-butanone–1-pentanol, and 2-butanone–isoamyl alcohol were determined in an improved Othmer still. The binary mixtures were analyzed by refractive index measurements. Activity coefficients have been calculated.**

Vapor-liquid equilibrium data are of especial interest for alcohol–ketone systems because these systems exhibit nonideality due to association through hydrogen bonding (*6*) and also because of their excellent solvent properties and the need to establish the conditions for their separation by distillation. In this study, vapor-liquid equilibrium data have been determined for the systems 2-butanone–1-pentanol and 2-butanone–isoamyl alcohol at atmospheric pressure. Data have also been redetermined for the 2-butanone–2-butanol system (*1*) at atmospheric pressure, since previous data were obtained using several innovative modifications of a Colburn-type still.

## EXPERIMENTAL

**Purity of Liquids.** Analytical reagent-grade liquids were used. The 2-butanone, isoamyl alcohol, and 1-pentanol were obtained from Matheson, Coleman and Bell, and the 2-butanol was obtained from Eastman Kodak Co. All reagents were further purified and dried following standard procedures (*11*) and were fractionally distilled several times. The physical properties of the liquids used are listed with literature data in Table I.

Table I. Physical Properties of Pure Liquids

| | Normal bp, °C | | Ref. index, $n^{25}D$ | |
|---|---|---|---|---|
| Liquid | Exptl | Lit. (*11*) | Exptl | Lit. |
| 2-Butanone | 79.5 | 79.50 | 1.3761 | 1.37612 (*11*) |
| 2-Butanol | 99.5 | 99.529 | 1.3946 | 1.39495 (*10*) |
| 1-Pentanol | 138.0 | 138.06 | 1.4075 | 1.40796 (*11*) |
| Isoamyl alcohol | 132.0 | 132.00 | 1.4041 | 1.4046 (*5*) |

Table II. Smoothed Analytical Data for Binary Systems at 25°C

| Mole fraction, 2-butanone (*1*), $x_i$ | Refractive index at 25°C, $n^{25}D$, for 2-butanone (*1*) with second component (*2*) | | |
|---|---|---|---|
| | 2-Butanol (*2*) | 1-Pentanol (*2*) | Isoamyl alcohol (*2*) |
| 0.000 | 1.3946 | 1.4075 | 1.4041 |
| 0.100 | 1.3923 | 1.4048 | 1.4016 |
| 0.200 | 1.3901 | 1.4020 | 1.3992 |
| 0.300 | 1.3881 | 1.3991 | 1.3967 |
| 0.400 | 1.3861 | 1.3962 | 1.3941 |
| 0.500 | 1.3842 | 1.3932 | 1.3913 |
| 0.600 | 1.3825 | 1.3901 | 1.3885 |
| 0.700 | 1.3809 | 1.3868 | 1.3854 |
| 0.800 | 1.3793 | 1.3833 | 1.3822 |
| 0.900 | 1.3777 | 1.3798 | 1.3790 |
| 1.000 | 1.3761 | 1.3761 | 1.3761 |

**Analytical Method.** Refractive index measurements were used to analyze vapor and liquid samples from the still. An Abbe refractometer controlled at 25° ± 0.2°C was used. Measurements were estimated to be reproducible to within ±0.0001. Calibration data are shown in Table II. The maximum deviation of experimental data points from a smooth curve is ±0.005 mole fraction.

**Apparatus and Procedures.** Equilibrium data were obtained using an improved Othmer still (*7*). Temperature measurements were made to within ±0.1°C, using mercury-in-glass thermometers. Observed temperatures were corrected to 760 torr (*8*); however, since atmospheric pressure recorded during experimental work showed only small deviations from 760 torr, pressure effects on the equilibrium data were negligible and no correction was made. The overall reliability of data is estimated to be ±0.005 mole fraction. Measurements on the methanol–water system agreed with previously reported data on this system (*4*) to within ±0.005 mole fraction.

## RESULTS

**Calculation of Activity Coefficients.** Activity coefficients were calculated, assuming ideal vapor behavior, for experimental equilibrium points using the equation

$$\gamma_i = \frac{y_i P}{x_i p_i^0}$$

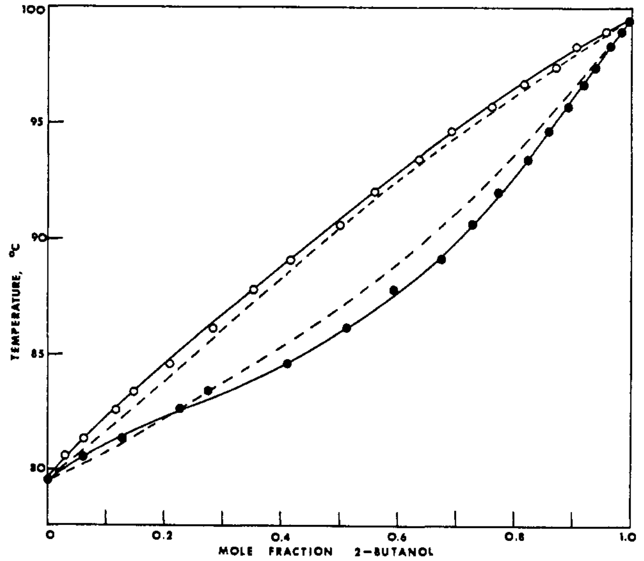

Figure 1. Boiling point–composition curve for 2-butanone–2-butanol system

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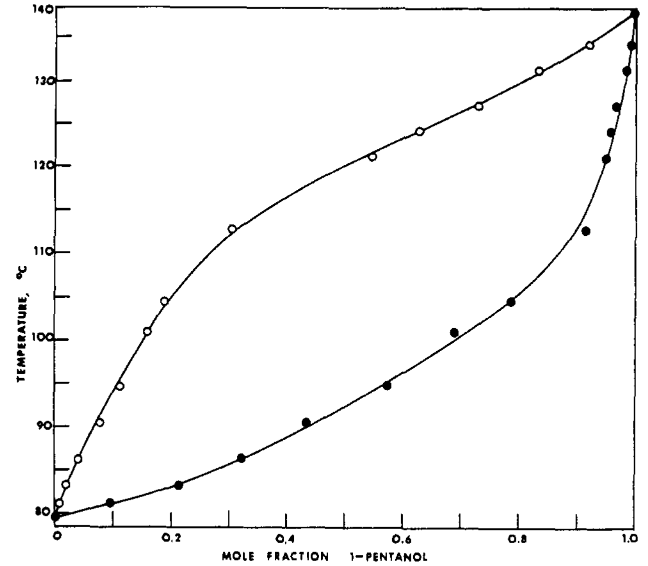

Figure 2. Boiling point–composition curve for 2-butanone–1-pentanol system

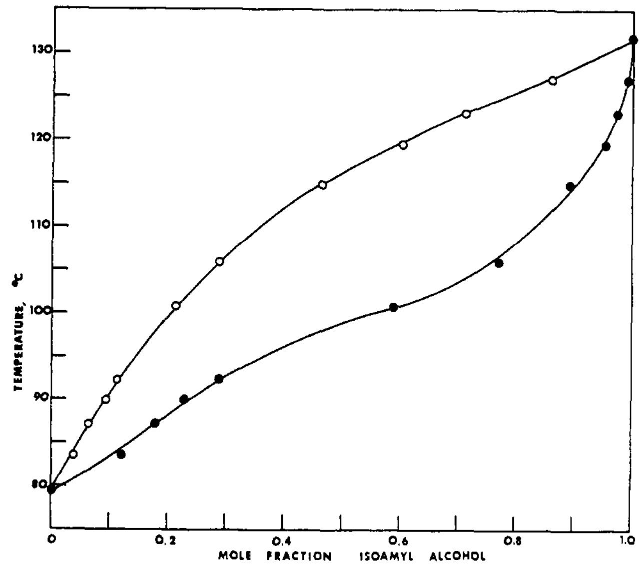

Figure 3. Boiling point–composition curve for 2-butanone–isoamyl alcohol system

Table III. Vapor-Liquid Equilibrium Data at 1-Atm Pressure

| Bp, °C | $x_1$ | $y_1$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|
| System 2-Butanone–2-Butanol | | | | |
| 80.5 | 0.945 | 0.970 | 1.001 | 1.305 |
| 82.6 | 0.774 | 0.882 | 1.045 | 1.130 |
| 83.4 | 0.725 | 0.852 | 1.048 | 1.121 |
| 84.6 | 0.588 | 0.791 | 1.130 | 0.997 |
| 86.2 | 0.485 | 0.715 | 1.209 | 1.006 |
| 87.8 | 0.405 | 0.646 | 1.241 | 1.005 |
| 90.6 | 0.270 | 0.497 | 1.322 | 1.024 |
| 92.0 | 0.225 | 0.439 | 1.342 | 1.011 |
| 93.5 | 0.175 | 0.364 | 1.370 | 1.005 |
| 94.7 | 0.138 | 0.305 | 1.407 | 0.996 |
| 95.7 | 0.108 | 0.238 | 1.361 | 1.011 |
| 96.7 | 0.080 | 0.182 | 1.368 | 1.005 |
| 98.3 | 0.036 | 0.092 | 1.468 | 0.994 |
| 99.0 | 0.016 | 0.042 | 1.479 | 0.996 |
| System 2-Butanone–1-Pentanol | | | | |
| 81.1 | 0.903 | 0.992 | 1.053 | 1.195 |
| 86.2 | 0.678 | 0.956 | 1.155 | 1.502 |
| 90.4 | 0.565 | 0.922 | 1.176 | 1.587 |
| 94.8 | 0.425 | 0.889 | 1.328 | 1.369 |
| 101.0 | 0.310 | 0.842 | 1.447 | 1.193 |
| 104.4 | 0.217 | 0.814 | 1.822 | 1.051 |
| 121.4 | 0.049 | 0.455 | 2.920 | 1.160 |
| 124.2 | 0.045 | 0.373 | 2.434 | 1.174 |
| 127.0 | 0.035 | 0.268 | 2.107 | 1.202 |
| 131.2 | 0.015 | 0.167 | 2.781 | 1.123 |
| 134.2 | 0.009 | 0.075 | 1.945 | 1.094 |
| System 2-Butanone–Isoamyl Alcohol | | | | |
| 83.5 | 0.880 | 0.963 | 0.961 | 2.036 |
| 87.1 | 0.820 | 0.938 | 0.911 | 1.901 |
| 89.9 | 0.771 | 0.905 | 0.860 | 2.023 |
| 92.3 | 0.712 | 0.890 | 0.853 | 1.668 |
| 100.7 | 0.410 | 0.789 | 1.034 | 1.109 |
| 105.9 | 0.227 | 0.711 | 1.461 | 0.932 |
| 114.9 | 0.107 | 0.535 | 1.831 | 0.904 |
| 119.5 | 0.045 | 0.397 | 2.909 | 0.930 |
| 123.1 | 0.027 | 0.289 | 3.231 | 0.945 |
| 127.1 | 0.005 | 0.139 | 7.633 | 0.971 |

The vapor pressures of 2-butanol and 1-pentanol were estimated from the integrated form of the Clausius-Clapeyron equation assuming the previously determined (*2*, *3*) heats of vaporization of 12.00 and 13.60 kcal mol$^{-1}$, respectively, were constant over the temperature range used. The constants of integration were evaluated from the boiling points at 1-atm pressure. The equations used were:

$$\log p^0(\text{atm}) = 7.035 - 2622/T$$
(2-butanol)

$$\log p^0(\text{atm}) = 7.226 - 2972/T$$
(1-pentanol)

Vapor pressures for 2-butanone were obtained using previously evaluated (*11*) Antoine equation constants, and for isoamyl alcohol were obtained from a smooth plot of the previously determined values (*9*). Experimental results are shown in Figures 1, 2, and 3 and tabulated in Table III.

## NOMENCLATURE

$P$ = total pressure, torr
$p_i^0$ = vapor pressure of pure component $i$, torr
$x_i$ = mole fraction of component $i$ in liquid phase
$y_i$ = mole fraction of component $i$ in vapor phase
$\gamma_i$ = liquid phase activity coefficient of component $i$

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