# Densities and Excess Molar Volumes of the Ternary Mixture 2-Butanol + Chloroform + Benzene and Binary Mixtures 2-Butanol + Chloroform, or + Benzene over the Temperature Range (288.15 to 313.15) K

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Densities $\rho$ and excess molar volumes $V^E$ of the 2-butanol + chloroform + benzene ternary mixtures and two binaries, 2-butanol + chloroform and 2-butanol + benzene, have been determined. Experimental $\rho$ measurements have been performed at six temperatures, (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K, and atmospheric pressure with an Anton Paar DNA 5000 digital vibrating tube densimeter. Excess molar volumes $V^E$ were correlated by the Redlich−Kister equation for binary mixtures and the Nagata−Tamura equation for ternary mixtures.

## Introduction

This paper is a continuation of our research of the volumetric properties of binaries and multicomponent mixtures containing alcohols (methanol, ethanol, propanol, and butanol) with chloroform and/or benzene, which have great importance in various industries.[1–5]

In this article, density $\rho$ measurements of the ternary system of 2-butanol + chloroform + benzene and the 2-butanol + chloroform and 2-butanol + benzene binary constituents at temperatures (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K and atmospheric pressure are presented. The related property, excess molar volume $V^E$, was calculated from the measured $\rho$ data.

The Redlich−Kister[6] equation was used for binary, while the Nagata and Tamura[7] equation was used for ternary $V^E$ data correlation.

To the best of our knowledge, literature data are not available for the investigated ternary system, as well as for the 2-butanol + chloroform binary system. The $\rho$ and $V^E$ literature data for the 2-butanol + benzene binary mixture cover only temperatures (303.15[8] and 308.15[9]) K.

## Experimental Section

***Chemicals.*** 2-Butanol (Merck) was supplied with a purity of > 99.0 mass % (p.a.), chloroform (stabilized with amylene) by Riedel-de Haën with a purity of 99.8 mass %, and benzene by Aldrich with a purity of 99.9 mass % (HPLC). Table 1 lists the measured densities of 2-butanol, chloroform, and benzene, which agree to within ± 0.07 kg·m$^{-3}$ with most of the corresponding literature values.[10–13]

***Measurements.*** Densities $\rho$ of the ternary and binary mixtures and corresponding pure substances were measured by means of an Anton Paar DMA 5000 digital vibrating U-tube densimeter (with automatic viscosity correction) having a stated accuracy ± 5·10$^{-3}$ kg·m$^{-3}$. The temperature in the cell was regulated to ± 0.001 K with a built-in solid-state thermostat. The temperature in the cell was measured by means of two integrated Pt 100 platinum thermometers, and temperature stability was better then ± 0.002 K. Calibration of the apparatus was performed daily using ambient air and ultrapure water. To minimize evaporation of the volatile solvents and to avoid the errors in composition, all mixtures were prepared by mass using the cell and the procedure described previously.[14,15] Presently, a Mettler AG 204 balance with a precision of 1·10$^{-4}$ g was used. The uncertainty of the mole fraction calculation was less than ± 1·10$^{-4}$. All molar quantities were based on the IUPAC relative atomic mass table. The experimental uncertainty in the density is about ± 1·10$^{-2}$ kg·m$^{-3}$, while the average uncertainty in excess molar volume is estimated to be ± 3·10$^{-9}$ m$^3$·mol$^{-1}$.

**Table 1. Densities $\rho$ of the Pure Components at 298.15 K and Atmospheric Pressure**

| | $\rho$·10$^{-3}$/(kg·m$^{-3}$) | |
|---|---|---|
| component | exptl | lit. |
| 2-butanol | 0.80247 | 0.8026[a], 0.80244[b] |
| chloroform | 1.47915 | 1.47970[a], 1.47919[c] |
| benzene | 0.87358 | 0.87360[a], 0.87365[d] |

[a] Riddick et al.[10] [b] Hales and Ellender.[11] [c] Francesconi et al.[12] [d] Tanaka and Yokoyama.[13]

## Results and Discussion

The excess molar volumes $V^E$ were calculated from the equation

$$V^E = \sum_{i=1}^{n} x_i M_i [(1/\rho) - (1/\rho_i)] \quad (1)$$

where $n$ is the number of components; $x_i$ is the mole fraction of component $i$ in the mixture; $M_i$ is its molecular weight; and $\rho$ and $\rho_i$ are the measured densities of the mixture and the pure component $i$, respectively.

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**Table 2. Densities $\rho$ and Excess Molar Volumes $V^E$ for 2-Butanol (1) + Chloroform (2) and 2-Butanol (1) + Benzene (2) from $T$ = (288.15 to 313.15 K) and Atmospheric Pressure**

| $x_1$ | $\rho \cdot 10^{-3}$ / kg·m$^{-3}$ | $V^E \cdot 10^6$ / m$^3$·mol$^{-1}$ | $x_1$ | $\rho \cdot 10^{-3}$ / kg·m$^{-3}$ | $V^E \cdot 10^6$ / m$^3$·mol$^{-1}$ | $x_1$ | $\rho \cdot 10^{-3}$ / kg·m$^{-3}$ | $V^E \cdot 10^6$ / m$^3$·mol$^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| 2-Butanol (1) + Chloroform (2) | | | | | | | | |
| $T$ = 288.15 K | | | | | | | | |
| 0.0000 | 1.49808 | 0.000 | 0.3507 | 1.23033 | 0.321 | 0.7008 | 0.99587 | 0.104 |
| 0.0514 | 1.45549 | 0.129 | 0.3995 | 1.19611 | 0.309 | 0.7446 | 0.96817 | 0.061 |
| 0.1045 | 1.41317 | 0.214 | 0.4502 | 1.16111 | 0.289 | 0.7984 | 0.93440 | 0.022 |
| 0.1518 | 1.37662 | 0.257 | 0.4978 | 1.12873 | 0.267 | 0.8507 | 0.90192 | −0.009 |
| 0.1962 | 1.34292 | 0.290 | 0.5460 | 1.09647 | 0.236 | 0.9000 | 0.87162 | −0.031 |
| 0.2512 | 1.30206 | 0.314 | 0.6008 | 1.06039 | 0.192 | 0.9486 | 0.84191 | −0.029 |
| 0.2998 | 1.26664 | 0.326 | 0.6498 | 1.02863 | 0.144 | 1.0000 | 0.81064 | 0.000 |
| $T$ = 293.15 K | | | | | | | | |
| 0.0000 | 1.48864 | 0.000 | 0.3507 | 1.22274 | 0.355 | 0.7008 | 0.99015 | 0.140 |
| 0.0514 | 1.44633 | 0.136 | 0.3995 | 1.18878 | 0.344 | 0.7446 | 0.96268 | 0.095 |
| 0.1045 | 1.40426 | 0.228 | 0.4502 | 1.15406 | 0.326 | 0.7984 | 0.92920 | 0.052 |
| 0.1518 | 1.36794 | 0.277 | 0.4978 | 1.12194 | 0.305 | 0.8507 | 0.89700 | 0.017 |
| 0.1962 | 1.33449 | 0.314 | 0.5460 | 1.08993 | 0.274 | 0.9000 | 0.86699 | −0.012 |
| 0.2512 | 1.29392 | 0.342 | 0.6008 | 1.05414 | 0.229 | 0.9486 | 0.83756 | −0.019 |
| 0.2998 | 1.25877 | 0.357 | 0.6498 | 1.02264 | 0.181 | 1.0000 | 0.80659 | 0.000 |
| $T$ = 298.15 K | | | | | | | | |
| 0.0000 | 1.47915 | 0.000 | 0.3507 | 1.21509 | 0.388 | 0.7008 | 0.98437 | 0.176 |
| 0.0514 | 1.43712 | 0.142 | 0.3995 | 1.18140 | 0.379 | 0.7446 | 0.95713 | 0.129 |
| 0.1045 | 1.39531 | 0.241 | 0.4502 | 1.14695 | 0.362 | 0.7984 | 0.92393 | 0.083 |
| 0.1518 | 1.35922 | 0.297 | 0.4978 | 1.11508 | 0.342 | 0.8507 | 0.89202 | 0.043 |
| 0.1962 | 1.32601 | 0.337 | 0.5460 | 1.08334 | 0.312 | 0.9000 | 0.86229 | 0.007 |
| 0.2512 | 1.28573 | 0.370 | 0.6008 | 1.04783 | 0.267 | 0.9486 | 0.83314 | −0.009 |
| 0.2998 | 1.25084 | 0.388 | 0.6498 | 1.01659 | 0.219 | 1.0000 | 0.80247 | 0.000 |
| $T$ = 303.15 K | | | | | | | | |
| 0.0000 | 1.46961 | 0.000 | 0.3507 | 1.20739 | 0.420 | 0.7008 | 0.97852 | 0.211 |
| 0.0514 | 1.42786 | 0.149 | 0.3995 | 1.17396 | 0.413 | 0.7446 | 0.95151 | 0.162 |
| 0.1045 | 1.38631 | 0.255 | 0.4502 | 1.13978 | 0.398 | 0.7984 | 0.91860 | 0.112 |
| 0.1518 | 1.35044 | 0.317 | 0.4978 | 1.10817 | 0.379 | 0.8507 | 0.88697 | 0.067 |
| 0.1962 | 1.31748 | 0.360 | 0.5460 | 1.07668 | 0.349 | 0.9000 | 0.85751 | 0.025 |
| 0.2512 | 1.27749 | 0.398 | 0.6008 | 1.04147 | 0.304 | 0.9486 | 0.82864 | 0.002 |
| 0.2998 | 1.24286 | 0.419 | 0.6498 | 1.01048 | 0.255 | 1.0000 | 0.79827 | 0.000 |
| $T$ = 308.15 K | | | | | | | | |
| 0.0000 | 1.46003 | 0.000 | 0.3507 | 1.19964 | 0.452 | 0.7008 | 0.97261 | 0.244 |
| 0.0514 | 1.41855 | 0.155 | 0.3995 | 1.16647 | 0.447 | 0.7446 | 0.94582 | 0.193 |
| 0.1045 | 1.37726 | 0.268 | 0.4502 | 1.13256 | 0.434 | 0.7984 | 0.91319 | 0.140 |
| 0.1518 | 1.34117 | 0.364 | 0.4978 | 1.10120 | 0.415 | 0.8507 | 0.88184 | 0.091 |
| 0.1962 | 1.30889 | 0.383 | 0.5460 | 1.06996 | 0.385 | 0.9000 | 0.85265 | 0.043 |
| 0.2512 | 1.26919 | 0.425 | 0.6008 | 1.03503 | 0.340 | 0.9486 | 0.82405 | 0.011 |
| 0.2998 | 1.23482 | 0.449 | 0.6498 | 1.00430 | 0.289 | 1.0000 | 0.79397 | 0.000 |
| $T$ = 313.15 K | | | | | | | | |
| 0.0000 | 1.45041 | 0.000 | 0.3507 | 1.19186 | 0.482 | 0.7008 | 0.96665 | 0.274 |
| 0.0514 | 1.40922 | 0.160 | 0.3995 | 1.15894 | 0.478 | 0.7446 | 0.94007 | 0.223 |
| 0.1045 | 1.36820 | 0.280 | 0.4502 | 1.12528 | 0.467 | 0.7984 | 0.90774 | 0.165 |
| 0.1518 | 1.33278 | 0.354 | 0.4978 | 1.09420 | 0.447 | 0.8507 | 0.87665 | 0.112 |
| 0.1962 | 1.30027 | 0.405 | 0.5460 | 1.06321 | 0.418 | 0.9000 | 0.84772 | 0.059 |
| 0.2512 | 1.26086 | 0.451 | 0.6008 | 1.02855 | 0.373 | 0.9486 | 0.81939 | 0.020 |
| 0.2998 | 1.22674 | 0.479 | 0.6498 | 0.99807 | 0.321 | 1.0000 | 0.78959 | 0.000 |
| 2-Butanol (1) + Benzene (2) | | | | | | | | |
| $T$ = 288.15 K | | | | | | | | |
| 0.0000 | 0.88425 | 0.000 | 0.3995 | 0.85021 | 0.424 | 0.8020 | 0.82297 | 0.203 |
| 0.0511 | 0.87901 | 0.136 | 0.4509 | 0.84644 | 0.422 | 0.8501 | 0.81996 | 0.154 |
| 0.0995 | 0.87460 | 0.212 | 0.5003 | 0.84293 | 0.411 | 0.9003 | 0.81684 | 0.101 |
| 0.1508 | 0.87004 | 0.284 | 0.5498 | 0.83948 | 0.393 | 0.9206 | 0.81557 | 0.081 |
| 0.2013 | 0.86576 | 0.335 | 0.5953 | 0.83641 | 0.368 | 0.9479 | 0.81392 | 0.048 |
| 0.2482 | 0.86191 | 0.371 | 0.6487 | 0.83284 | 0.334 | 1.0000 | 0.81064 | 0.000 |
| 0.2999 | 0.85780 | 0.399 | 0.7006 | 0.82946 | 0.294 | | | |
| 0.3486 | 0.85403 | 0.416 | 0.7493 | 0.82632 | 0.252 | | | |
| $T$ = 293.15 K | | | | | | | | |
| 0.0000 | 0.87892 | 0.000 | 0.3995 | 0.84520 | 0.452 | 0.8020 | 0.81851 | 0.225 |
| 0.0511 | 0.87367 | 0.146 | 0.4509 | 0.84148 | 0.452 | 0.8501 | 0.81560 | 0.171 |
| 0.0995 | 0.86929 | 0.227 | 0.5003 | 0.83802 | 0.443 | 0.9003 | 0.81258 | 0.113 |
| 0.1508 | 0.86477 | 0.303 | 0.5498 | 0.83464 | 0.424 | 0.9206 | 0.81136 | 0.090 |
| 0.2013 | 0.86054 | 0.356 | 0.5953 | 0.83162 | 0.398 | 0.9479 | 0.80976 | 0.054 |
| 0.2482 | 0.85674 | 0.394 | 0.6487 | 0.82813 | 0.363 | 1.0000 | 0.80659 | 0.000 |
| 0.2999 | 0.85269 | 0.424 | 0.7006 | 0.82483 | 0.321 | | | |
| 0.3486 | 0.84896 | 0.443 | 0.7493 | 0.82178 | 0.276 | | | |
| $T$ = 298.15 K | | | | | | | | |
| 0.0000 | 0.87358 | 0.000 | 0.3995 | 0.84014 | 0.482 | 0.8020 | 0.81400 | 0.247 |
| 0.0511 | 0.86833 | 0.155 | 0.4509 | 0.83649 | 0.484 | 0.8501 | 0.81117 | 0.189 |
| 0.0995 | 0.86396 | 0.242 | 0.5003 | 0.83308 | 0.475 | 0.9003 | 0.80825 | 0.126 |
| 0.1508 | 0.85948 | 0.322 | 0.5498 | 0.82975 | 0.456 | 0.9206 | 0.80707 | 0.101 |
| 0.2013 | 0.85530 | 0.378 | 0.5953 | 0.82679 | 0.430 | 0.9479 | 0.80485 | 0.047 |
| 0.2482 | 0.85154 | 0.419 | 0.6487 | 0.82337 | 0.394 | 1.0000 | 0.80247 | 0.000 |
| 0.2999 | 0.84754 | 0.450 | 0.7006 | 0.82015 | 0.349 | | | |
| 0.3486 | 0.84386 | 0.472 | 0.7493 | 0.81717 | 0.302 | | | |

**Table 2 Continued**

| $x_1$ | $\rho \cdot 10^{-3}$ / kg·m$^{-3}$ | $V^E \cdot 10^6$ / m$^3$·mol$^{-1}$ | $x_1$ | $\rho \cdot 10^{-3}$ / kg·m$^{-3}$ | $V^E \cdot 10^6$ / m$^3$·mol$^{-1}$ | $x_1$ | $\rho \cdot 10^{-3}$ / kg·m$^{-3}$ | $V^E \cdot 10^6$ / m$^3$·mol$^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| | | | | $T = 303.15$ K | | | | |
| 0.0000 | 0.86823 | 0.000 | 0.3995 | 0.83505 | 0.513 | 0.8020 | 0.80941 | 0.270 |
| 0.0511 | 0.86298 | 0.164 | 0.4509 | 0.83144 | 0.516 | 0.8501 | 0.80666 | 0.208 |
| 0.0995 | 0.85862 | 0.258 | 0.5003 | 0.82808 | 0.507 | 0.9003 | 0.80384 | 0.139 |
| 0.1508 | 0.85417 | 0.342 | 0.5498 | 0.82482 | 0.489 | 0.9206 | 0.80270 | 0.111 |
| 0.2013 | 0.85002 | 0.401 | 0.5953 | 0.82191 | 0.462 | 0.9479 | 0.80121 | 0.069 |
| 0.2482 | 0.84630 | 0.444 | 0.6487 | 0.81856 | 0.425 | 1.0000 | 0.79827 | 0.000 |
| 0.2999 | 0.84235 | 0.478 | 0.7006 | 0.81540 | 0.378 | | | |
| 0.3486 | 0.83872 | 0.501 | 0.7493 | 0.81250 | 0.329 | | | |
| | | | | $T = 308.15$ K | | | | |
| 0.0000 | 0.86287 | 0.000 | 0.3995 | 0.82992 | 0.543 | 0.8020 | 0.80474 | 0.293 |
| 0.0511 | 0.85761 | 0.173 | 0.4509 | 0.82635 | 0.548 | 0.8501 | 0.80207 | 0.227 |
| 0.0995 | 0.85325 | 0.274 | 0.5003 | 0.82304 | 0.539 | 0.9003 | 0.79934 | 0.153 |
| 0.1508 | 0.84883 | 0.362 | 0.5498 | 0.81982 | 0.522 | 0.9206 | 0.79825 | 0.122 |
| 0.2013 | 0.84472 | 0.425 | 0.5953 | 0.81696 | 0.495 | 0.9479 | 0.79618 | 0.059 |
| 0.2482 | 0.84103 | 0.471 | 0.6487 | 0.81368 | 0.456 | 1.0000 | 0.79397 | 0.000 |
| 0.2999 | 0.83713 | 0.506 | 0.7006 | 0.81059 | 0.407 | | | |
| 0.3486 | 0.83354 | 0.530 | 0.7493 | 0.80775 | 0.356 | | | |
| | | | | $T = 313.15$ K | | | | |
| 0.0000 | 0.85750 | 0.000 | 0.3995 | 0.82476 | 0.572 | 0.8020 | 0.80001 | 0.315 |
| 0.0511 | 0.85224 | 0.181 | 0.4509 | 0.82121 | 0.580 | 0.8501 | 0.79740 | 0.247 |
| 0.0995 | 0.84789 | 0.287 | 0.5003 | 0.81796 | 0.571 | 0.9003 | 0.79477 | 0.166 |
| 0.1508 | 0.84348 | 0.381 | 0.5498 | 0.81480 | 0.553 | 0.9206 | 0.79372 | 0.131 |
| 0.2013 | 0.83939 | 0.448 | 0.5953 | 0.81196 | 0.528 | 0.9479 | 0.79173 | 0.063 |
| 0.2482 | 0.83575 | 0.496 | 0.6487 | 0.80875 | 0.486 | 1.0000 | 0.78959 | 0.000 |
| 0.2999 | 0.83188 | 0.532 | 0.7006 | 0.80573 | 0.434 | | | |
| 0.3486 | 0.82834 | 0.558 | 0.7493 | 0.80295 | 0.381 | | | |

**Table 3. Densities $\rho$ and Excess Molar Volumes $V^E$ for 2-Butanol (1) + Chloroform (2) + Benzene (3) from $T = (288.15$ to $313.15)$ K and Atmospheric Pressure**

| $x_1$ | $x_2$ | $\rho \cdot 10^{-3}$ / kg·m$^{-3}$ | $V^E \cdot 10^6$ / m$^3$·mol$^{-1}$ | $x_1$ | $x_2$ | $\rho \cdot 10^{-3}$ / kg·m$^{-3}$ | $V^E \cdot 10^6$ / m$^3$·mol$^{-1}$ | $x_1$ | $x_2$ | $\rho \cdot 10^{-3}$ / kg·m$^{-3}$ | $V^E \cdot 10^6$ / m$^3$·mol$^{-1}$ | $x_1$ | $x_2$ | $\rho \cdot 10^{-3}$ / kg·m$^{-3}$ | $V^E \cdot 10^6$ / m$^3$·mol$^{-1}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | $T = 288.15$ K | | | | | | | | $T = 303.15$ K | | | | | |
| 0.0893 | 0.1023 | 0.93155 | 0.272 | 0.5393 | 0.1003 | 0.89512 | 0.343 | 0.0893 | 0.1023 | 0.91458 | 0.303 | 0.5393 | 0.1003 | 0.87945 | 0.431 |
| 0.0776 | 0.2164 | 0.99674 | 0.311 | 0.4785 | 0.2021 | 0.95612 | 0.350 | 0.0776 | 0.2164 | 0.97863 | 0.327 | 0.4785 | 0.2021 | 0.93917 | 0.437 |
| 0.0707 | 0.2988 | 1.04478 | 0.323 | 0.4192 | 0.3000 | 1.01594 | 0.384 | 0.0707 | 0.2988 | 1.02579 | 0.332 | 0.4192 | 0.3000 | 0.99770 | 0.468 |
| 0.0592 | 0.4006 | 1.10586 | 0.315 | 0.3617 | 0.3993 | 1.07819 | 0.387 | 0.0592 | 0.4006 | 1.08572 | 0.316 | 0.3617 | 0.3993 | 1.05860 | 0.468 |
| 0.0489 | 0.5008 | 1.16729 | 0.298 | 0.2988 | 0.4987 | 1.14274 | 0.371 | 0.0489 | 0.5008 | 1.14597 | 0.293 | 0.2988 | 0.4987 | 1.12173 | 0.446 |
| 0.0409 | 0.6001 | 1.22940 | 0.274 | 0.2415 | 0.5993 | 1.20894 | 0.369 | 0.0409 | 0.6001 | 1.20682 | 0.268 | 0.2415 | 0.5993 | 1.18649 | 0.437 |
| 0.0318 | 0.6986 | 1.29292 | 0.222 | 0.1819 | 0.6937 | 1.27377 | 0.327 | 0.0318 | 0.6986 | 1.26898 | 0.218 | 0.1819 | 0.6937 | 1.24993 | 0.383 |
| 0.0211 | 0.7895 | 1.35337 | 0.154 | 0.1218 | 0.7944 | 1.34459 | 0.269 | 0.0211 | 0.7895 | 1.32817 | 0.148 | 0.1218 | 0.7944 | 1.31924 | 0.312 |
| 0.1793 | 0.0998 | 0.92223 | 0.359 | 0.0615 | 0.8960 | 1.41883 | 0.163 | 0.1793 | 0.0998 | 0.90548 | 0.412 | 0.0615 | 0.8960 | 1.39199 | 0.184 |
| 0.1589 | 0.1999 | 0.97986 | 0.388 | 0.7190 | 0.1002 | 0.88393 | 0.102 | 0.1589 | 0.1999 | 0.96204 | 0.431 | 0.7190 | 0.1002 | 0.86803 | 0.280 |
| 0.1410 | 0.3031 | 1.04053 | 0.395 | 0.6412 | 0.1996 | 0.94324 | 0.234 | 0.1410 | 0.3031 | 1.02157 | 0.429 | 0.6412 | 0.1996 | 0.92686 | 0.327 |
| 0.1207 | 0.3985 | 1.09848 | 0.377 | 0.5596 | 0.3001 | 1.00599 | 0.262 | 0.1207 | 0.3985 | 1.07839 | 0.403 | 0.5596 | 0.3001 | 0.98817 | 0.360 |
| 0.0994 | 0.5001 | 1.16169 | 0.344 | 0.4795 | 0.4012 | 1.07023 | 0.315 | 0.0994 | 0.5001 | 1.14035 | 0.363 | 0.4795 | 0.4012 | 1.05098 | 0.410 |
| 0.0798 | 0.6005 | 1.22534 | 0.320 | 0.3981 | 0.4995 | 1.13505 | 0.328 | 0.0798 | 0.6005 | 1.20272 | 0.334 | 0.3981 | 0.4995 | 1.11419 | 0.428 |
| 0.0620 | 0.6968 | 1.28821 | 0.261 | 0.3200 | 0.6006 | 1.20287 | 0.347 | 0.0620 | 0.6968 | 1.26430 | 0.270 | 0.3200 | 0.6006 | 1.18054 | 0.436 |
| 0.0388 | 0.8009 | 1.35845 | 0.186 | 0.2374 | 0.7020 | 1.27334 | 0.352 | 0.0388 | 0.8009 | 1.33309 | 0.189 | 0.2374 | 0.7020 | 1.24958 | 0.419 |
| 0.0191 | 0.9009 | 1.42748 | 0.107 | 0.1563 | 0.8031 | 1.34652 | 0.284 | 0.0191 | 0.9009 | 1.40060 | 0.108 | 0.1563 | 0.8031 | 1.32105 | 0.341 |
| 0.3452 | 0.1017 | 0.91008 | 0.400 | 0.0806 | 0.8970 | 1.41716 | 0.183 | 0.3452 | 0.1017 | 0.89376 | 0.477 | 0.0806 | 0.8970 | 1.39028 | 0.214 |
| 0.3190 | 0.1999 | 0.96686 | 0.408 | 0.8103 | 0.1000 | 0.87708 | 0.094 | 0.3190 | 0.1999 | 0.94945 | 0.478 | 0.8103 | 0.1000 | 0.86253 | 0.166 |
| 0.2808 | 0.2987 | 1.02614 | 0.419 | 0.7182 | 0.2020 | 0.93981 | 0.119 | 0.2808 | 0.2987 | 1.00753 | 0.483 | 0.7182 | 0.2020 | 0.92371 | 0.211 |
| 0.2379 | 0.3933 | 1.08489 | 0.413 | 0.6298 | 0.2995 | 1.00062 | 0.205 | 0.2379 | 0.3933 | 1.06506 | 0.470 | 0.6298 | 0.2995 | 0.98304 | 0.307 |
| 0.1893 | 0.5052 | 1.15607 | 0.393 | 0.5383 | 0.4010 | 1.06601 | 0.247 | 0.1893 | 0.5052 | 1.13477 | 0.442 | 0.5383 | 0.4010 | 1.04687 | 0.352 |
| 0.1583 | 0.5986 | 1.21620 | 0.368 | 0.4497 | 0.4984 | 1.13013 | 0.309 | 0.1583 | 0.5986 | 1.19365 | 0.411 | 0.4497 | 0.4984 | 1.10950 | 0.412 |
| 0.1187 | 0.6980 | 1.28290 | 0.300 | 0.3602 | 0.6008 | 1.19972 | 0.319 | 0.1187 | 0.6980 | 1.25894 | 0.334 | 0.3602 | 0.6008 | 1.17748 | 0.416 |
| 0.0788 | 0.7992 | 1.35245 | 0.240 | 0.2698 | 0.6978 | 1.26789 | 0.330 | 0.0788 | 0.7992 | 1.32706 | 0.264 | 0.2698 | 0.6978 | 1.24409 | 0.415 |
| 0.0387 | 0.9007 | 1.42487 | 0.131 | 0.1753 | 0.8042 | 1.34514 | 0.293 | 0.0387 | 0.9007 | 1.39798 | 0.142 | 0.1753 | 0.8042 | 1.31980 | 0.349 |
| | | $T = 293.15$ K | | | | | | | | $T = 308.15$ K | | | | | |
| 0.0893 | 0.1023 | 0.92592 | 0.282 | 0.5393 | 0.1003 | 0.88995 | 0.372 | 0.0893 | 0.1023 | 0.90888 | 0.314 | 0.5393 | 0.1003 | 0.87412 | 0.461 |
| 0.0776 | 0.2164 | 0.99073 | 0.316 | 0.4785 | 0.2021 | 0.95053 | 0.378 | 0.0776 | 0.2164 | 0.97255 | 0.333 | 0.4785 | 0.2021 | 0.93340 | 0.466 |
| 0.0707 | 0.2988 | 1.03848 | 0.326 | 0.4192 | 0.3000 | 1.00991 | 0.412 | 0.0707 | 0.2988 | 1.01941 | 0.335 | 0.4192 | 0.3000 | 0.99150 | 0.497 |
| 0.0592 | 0.4006 | 1.09917 | 0.315 | 0.3617 | 0.3993 | 1.07171 | 0.414 | 0.0592 | 0.4006 | 1.07895 | 0.316 | 0.3617 | 0.3993 | 1.05196 | 0.495 |
| 0.0489 | 0.5008 | 1.16022 | 0.296 | 0.2988 | 0.4987 | 1.13578 | 0.396 | 0.0489 | 0.5008 | 1.13879 | 0.292 | 0.2988 | 0.4987 | 1.11461 | 0.472 |
| 0.0409 | 0.6001 | 1.22191 | 0.272 | 0.2415 | 0.5993 | 1.20152 | 0.391 | 0.0409 | 0.6001 | 1.19921 | 0.267 | 0.2415 | 0.5993 | 1.17890 | 0.461 |
| 0.0318 | 0.6986 | 1.28495 | 0.222 | 0.1819 | 0.6937 | 1.26588 | 0.345 | 0.0318 | 0.6986 | 1.26092 | 0.216 | 0.1819 | 0.6937 | 1.24187 | 0.403 |
| 0.0211 | 0.7895 | 1.34501 | 0.152 | 0.1218 | 0.7944 | 1.33619 | 0.284 | 0.0211 | 0.7895 | 1.31967 | 0.146 | 0.1218 | 0.7944 | 1.31070 | 0.326 |
| 0.1793 | 0.0998 | 0.91668 | 0.376 | 0.0615 | 0.8960 | 1.40994 | 0.170 | 0.1793 | 0.0998 | 0.89982 | 0.431 | 0.0615 | 0.8960 | 1.38294 | 0.192 |
| 0.1589 | 0.1999 | 0.97396 | 0.402 | 0.7190 | 0.1002 | 0.87870 | 0.160 | 0.1589 | 0.1999 | 0.95604 | 0.446 | 0.7190 | 0.1002 | 0.86281 | 0.317 |
| 0.1410 | 0.3031 | 1.03425 | 0.406 | 0.6412 | 0.1996 | 0.93784 | 0.265 | 0.1410 | 0.3031 | 1.01518 | 0.440 | 0.6412 | 0.1996 | 0.92128 | 0.358 |
| 0.1207 | 0.3985 | 1.09182 | 0.385 | 0.5596 | 0.3001 | 1.00010 | 0.294 | 0.1207 | 0.3985 | 1.07162 | 0.412 | 0.5596 | 0.3001 | 0.98211 | 0.391 |
| 0.0994 | 0.5001 | 1.15462 | 0.350 | 0.4795 | 0.4012 | 1.06387 | 0.346 | 0.0994 | 0.5001 | 1.13316 | 0.370 | 0.4795 | 0.4012 | 1.04442 | 0.442 |
| 0.0798 | 0.6005 | 1.21784 | 0.325 | 0.3981 | 0.4995 | 1.12815 | 0.362 | 0.0798 | 0.6005 | 1.19510 | 0.339 | 0.3981 | 0.4995 | 1.10714 | 0.460 |
| 0.0620 | 0.6968 | 1.28028 | 0.264 | 0.3200 | 0.6006 | 1.19548 | 0.376 | 0.0620 | 0.6968 | 1.25624 | 0.273 | 0.3200 | 0.6006 | 1.17298 | 0.465 |
| 0.0388 | 0.8009 | 1.35005 | 0.187 | 0.2374 | 0.7020 | 1.26550 | 0.372 | 0.0388 | 0.8009 | 1.32453 | 0.190 | 0.2374 | 0.7020 | 1.24150 | 0.444 |
| 0.0191 | 0.9009 | 1.41857 | 0.107 | 0.1563 | 0.8031 | 1.33808 | 0.303 | 0.0191 | 0.9009 | 1.39154 | 0.108 | 0.1563 | 0.8031 | 1.31246 | 0.360 |
| 0.3452 | 0.1017 | 0.90468 | 0.425 | 0.0806 | 0.8970 | 1.40824 | 0.194 | 0.3452 | 0.1017 | 0.88823 | 0.504 | 0.0806 | 0.8970 | 1.38122 | 0.224 |
| 0.3190 | 0.1999 | 0.96110 | 0.430 | 0.8103 | 0.1000 | 0.87230 | 0.117 | 0.3190 | 0.1999 | 0.94355 | 0.502 | 0.8103 | 0.1000 | 0.85753 | 0.189 |
| 0.2808 | 0.2987 | 1.01998 | 0.439 | 0.7182 | 0.2020 | 0.93451 | 0.150 | 0.2808 | 0.2987 | 1.00124 | 0.504 | 0.7182 | 0.2020 | 0.91820 | 0.240 |

**Table 3 Continued**

| $x_1$ | $x_2$ | $\rho\cdot10^{-3}$ / kg·m$^{-3}$ | $V^E\cdot10^6$ / m$^3$·mol$^{-1}$ | $x_1$ | $x_2$ | $\rho\cdot10^{-3}$ / kg·m$^{-3}$ | $V^E\cdot10^6$ / m$^3$·mol$^{-1}$ | $x_1$ | $x_2$ | $\rho\cdot10^{-3}$ / kg·m$^{-3}$ | $V^E\cdot10^6$ / m$^3$·mol$^{-1}$ | $x_1$ | $x_2$ | $\rho\cdot10^{-3}$ / kg·m$^{-3}$ | $V^E\cdot10^6$ / m$^3$·mol$^{-1}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.2379 | 0.3933 | 1.07833 | 0.431 | 0.6298 | 0.2995 | 0.99482 | 0.239 | 0.2379 | 0.3933 | 1.05835 | 0.491 | 0.6298 | 0.2995 | 0.97705 | 0.340 |
| 0.1893 | 0.5052 | 1.14902 | 0.409 | 0.5383 | 0.4010 | 1.05969 | 0.282 | 0.1893 | 0.5052 | 1.12757 | 0.459 | 0.5383 | 0.4010 | 1.04037 | 0.387 |
| 0.1583 | 0.5986 | 1.20872 | 0.382 | 0.4497 | 0.4984 | 1.12331 | 0.343 | 0.1583 | 0.5986 | 1.18604 | 0.425 | 0.4497 | 0.4984 | 1.10249 | 0.446 |
| 0.1187 | 0.6980 | 1.27496 | 0.311 | 0.3602 | 0.6008 | 1.19237 | 0.351 | 0.1187 | 0.6980 | 1.25086 | 0.346 | 0.3602 | 0.6008 | 1.16994 | 0.448 |
| 0.0788 | 0.7992 | 1.34403 | 0.248 | 0.2698 | 0.6978 | 1.26001 | 0.358 | 0.0788 | 0.7992 | 1.31850 | 0.271 | 0.2698 | 0.6978 | 1.23604 | 0.443 |
| 0.0387 | 0.9007 | 1.41595 | 0.135 | 0.1753 | 0.8042 | 1.33677 | 0.310 | 0.0387 | 0.9007 | 1.38892 | 0.145 | 0.1753 | 0.8042 | 1.31120 | 0.370 |
| | | $T = 298.15$ K | | | | | | | | $T = 313.15$ K | | | | | |
| 0.0893 | 0.1023 | 0.92026 | 0.293 | 0.5393 | 0.1003 | 0.88473 | 0.401 | 0.0893 | 0.1023 | 0.90317 | 0.324 | 0.5393 | 0.1003 | 0.86875 | 0.489 |
| 0.0776 | 0.2164 | 0.98469 | 0.322 | 0.4785 | 0.2021 | 0.94487 | 0.407 | 0.0776 | 0.2164 | 0.96646 | 0.337 | 0.4785 | 0.2021 | 0.92760 | 0.493 |
| 0.0707 | 0.2988 | 1.03215 | 0.329 | 0.4192 | 0.3000 | 1.00383 | 0.440 | 0.0707 | 0.2988 | 1.01302 | 0.336 | 0.4192 | 0.3000 | 0.98527 | 0.525 |
| 0.0592 | 0.4006 | 1.09246 | 0.315 | 0.3617 | 0.3993 | 1.06518 | 0.441 | 0.0592 | 0.4006 | 1.07218 | 0.315 | 0.3617 | 0.3993 | 1.04528 | 0.521 |
| 0.0489 | 0.5008 | 1.15311 | 0.295 | 0.2988 | 0.4987 | 1.12878 | 0.421 | 0.0489 | 0.5008 | 1.13157 | 0.292 | 0.2988 | 0.4987 | 1.10744 | 0.498 |
| 0.0409 | 0.6001 | 1.21438 | 0.270 | 0.2415 | 0.5993 | 1.19403 | 0.414 | 0.0409 | 0.6001 | 1.19158 | 0.265 | 0.2415 | 0.5993 | 1.17126 | 0.484 |
| 0.0318 | 0.6986 | 1.27699 | 0.220 | 0.1819 | 0.6937 | 1.25793 | 0.364 | 0.0318 | 0.6986 | 1.25283 | 0.215 | 0.1819 | 0.6937 | 1.23376 | 0.423 |
| 0.0211 | 0.7895 | 1.33661 | 0.150 | 0.1218 | 0.7944 | 1.32774 | 0.298 | 0.0211 | 0.7895 | 1.31114 | 0.146 | 0.1218 | 0.7944 | 1.30211 | 0.340 |
| 0.1793 | 0.0998 | 0.91109 | 0.394 | 0.0615 | 0.8960 | 1.40098 | 0.177 | 0.1793 | 0.0998 | 0.89416 | 0.449 | 0.0615 | 0.8960 | 1.37385 | 0.200 |
| 0.1589 | 0.1999 | 0.96802 | 0.416 | 0.7190 | 0.1002 | 0.87335 | 0.223 | 0.1589 | 0.1999 | 0.95001 | 0.460 | 0.7190 | 0.1002 | 0.85763 | 0.343 |
| 0.1410 | 0.3031 | 1.02793 | 0.417 | 0.6412 | 0.1996 | 0.93238 | 0.296 | 0.1410 | 0.3031 | 1.00878 | 0.451 | 0.6412 | 0.1996 | 0.91568 | 0.383 |
| 0.1207 | 0.3985 | 1.08512 | 0.394 | 0.5596 | 0.3001 | 0.99416 | 0.327 | 0.1207 | 0.3985 | 1.06483 | 0.421 | 0.5596 | 0.3001 | 0.97599 | 0.422 |
| 0.0994 | 0.5001 | 1.14751 | 0.356 | 0.4795 | 0.4012 | 1.05746 | 0.378 | 0.0994 | 0.5001 | 1.12593 | 0.377 | 0.4795 | 0.4012 | 1.03783 | 0.473 |
| 0.0798 | 0.6005 | 1.21030 | 0.329 | 0.3981 | 0.4995 | 1.12120 | 0.395 | 0.0798 | 0.6005 | 1.18746 | 0.343 | 0.3981 | 0.4995 | 1.10008 | 0.488 |
| 0.0620 | 0.6968 | 1.27231 | 0.267 | 0.3200 | 0.6006 | 1.18804 | 0.406 | 0.0620 | 0.6968 | 1.24814 | 0.277 | 0.3200 | 0.6006 | 1.16537 | 0.494 |
| 0.0388 | 0.8009 | 1.34159 | 0.188 | 0.2374 | 0.7020 | 1.25758 | 0.395 | 0.0388 | 0.8009 | 1.31594 | 0.192 | 0.2374 | 0.7020 | 1.23337 | 0.469 |
| 0.0191 | 0.9009 | 1.40961 | 0.107 | 0.1563 | 0.8031 | 1.32959 | 0.322 | 0.0191 | 0.9009 | 1.38243 | 0.110 | 0.1563 | 0.8031 | 1.30382 | 0.379 |
| 0.3452 | 0.1017 | 0.89924 | 0.451 | 0.0806 | 0.8970 | 1.39929 | 0.204 | 0.3452 | 0.1017 | 0.88269 | 0.528 | 0.0806 | 0.8970 | 1.37212 | 0.235 |
| 0.3190 | 0.1999 | 0.95530 | 0.454 | 0.8103 | 0.1000 | 0.86745 | 0.142 | 0.3190 | 0.1999 | 0.93764 | 0.524 | 0.8103 | 0.1000 | 0.85247 | 0.210 |
| 0.2808 | 0.2987 | 1.01378 | 0.461 | 0.7182 | 0.2020 | 0.92914 | 0.181 | 0.2808 | 0.2987 | 0.99492 | 0.525 | 0.7182 | 0.2020 | 0.91266 | 0.266 |
| 0.2379 | 0.3933 | 1.07172 | 0.450 | 0.6298 | 0.2995 | 0.98896 | 0.273 | 0.2379 | 0.3933 | 1.05160 | 0.512 | 0.6298 | 0.2995 | 0.97101 | 0.372 |
| 0.1893 | 0.5052 | 1.14192 | 0.425 | 0.5383 | 0.4010 | 1.05331 | 0.317 | 0.1893 | 0.5052 | 1.12033 | 0.477 | 0.5383 | 0.4010 | 1.03380 | 0.421 |
| 0.1583 | 0.5986 | 1.20121 | 0.396 | 0.4497 | 0.4984 | 1.11643 | 0.378 | 0.1583 | 0.5986 | 1.17840 | 0.439 | 0.4497 | 0.4984 | 1.09544 | 0.480 |
| 0.1187 | 0.6980 | 1.26698 | 0.323 | 0.3602 | 0.6008 | 1.18495 | 0.383 | 0.1187 | 0.6980 | 1.24274 | 0.359 | 0.3602 | 0.6008 | 1.16235 | 0.480 |
| 0.0788 | 0.7992 | 1.33556 | 0.256 | 0.2698 | 0.6978 | 1.25208 | 0.387 | 0.0788 | 0.7992 | 1.30991 | 0.279 | 0.2698 | 0.6978 | 1.22795 | 0.470 |
| 0.0387 | 0.9007 | 1.40699 | 0.138 | 0.1753 | 0.8042 | 1.32832 | 0.329 | 0.0387 | 0.9007 | 1.37982 | 0.150 | 0.1753 | 0.8042 | 1.30256 | 0.392 |

Tables 2 and 3 list the measured densities $\rho$ and the corresponding values of $V^E$ for the 2-butanol + chloroform and 2-butanol + benzene binary systems as well as for the ternary 2-butanol + chloroform + benzene system. The experimental results for the chloroform + benzene binary system have been presented in our previous paper.[2]

**Table 4. Parameters $A_p/10^{-6}$ m$^3$·mol$^{-1}$ of Equation 2 and the Corresponding rmsd $\sigma/10^{-6}$ m$^3$·mol$^{-1}$ for Binary Mixtures**

| $T$/K | $A_0$ | $A_1$ | $A_2$ | $A_3$ | $\sigma$ |
|---|---|---|---|---|---|
| | | 2-Butanol (1) + Chloroform (2) | | | |
| 288.15 | 1.0504 | −1.1978 | −0.1714 | −0.6499 | 0.004 |
| 293.15 | 1.2009 | −1.1766 | −0.1263 | −0.6160 | 0.004 |
| 298.15 | 1.3494 | −1.1398 | −0.0566 | −0.6362 | 0.003 |
| 303.15 | 1.4992 | −1.1193 | −0.0257 | −0.6102 | 0.003 |
| 308.15 | 1.6393 | −1.1043 | 0.0421 | −0.6028 | 0.006 |
| 313.15 | 1.7762 | −1.0943 | 0.0509 | −0.5588 | 0.003 |
| | | 2-Butanol (1) + Benzene (2) | | | |
| 288.15 | 1.6377 | −0.5773 | 0.1394 | −0.2855 | 0.004 |
| 293.15 | 1.7600 | −0.5555 | 0.1710 | −0.3552 | 0.004 |
| 298.15 | 1.8863 | −0.5394 | 0.2152 | −0.3921 | 0.005 |
| 303.15 | 2.0131 | −0.5161 | 0.2763 | −0.4742 | 0.004 |
| 308.15 | 2.1439 | −0.5051 | 0.3112 | −0.4877 | 0.005 |
| 313.15 | 2.2685 | −0.4595 | 0.3562 | −0.6197 | 0.004 |

**Table 5. Parameters $B_p/10^{-9}$ m$^3$·J$^{-1}$ of Equation 4 and the Corresponding rmsd $\sigma/10^{-6}$ m$^3$·mol$^{-1}$ for the 2-Butanol (1) + Chloroform (2) + Benzene (3) System**

| | $T$/K | | | | | |
|---|---|---|---|---|---|---|
| | 288.15 | 293.15 | 298.15 | 303.15 | 308.15 | 313.15 |
| $B_0$ | 1.104 | 1.338 | 1.720 | 1.911 | 2.082 | 1.957 |
| $B_1$ | 8.815 | 10.784 | 13.545 | 15.280 | 15.882 | 14.745 |
| $B_2$ | −6.720 | −5.925 | −4.259 | −3.790 | −2.710 | −2.830 |
| $B_3$ | −13.151 | −17.186 | −22.933 | −26.300 | −27.083 | −23.816 |
| $B_4$ | 15.597 | 14.097 | 10.986 | 10.878 | 8.283 | 8.173 |
| $B_5$ | 3.817 | 0.022 | −5.937 | −10.227 | −11.548 | −10.755 |
| $B_6$ | 9.405 | 10.548 | 12.540 | 13.257 | 13.395 | 11.032 |
| $B_7$ | −10.538 | −9.178 | −6.581 | −6.469 | −4.349 | −4.416 |
| $B_8$ | −13.300 | −5.270 | 6.147 | 14.698 | 16.538 | 15.225 |
| $\sigma$ | 0.012 | 0.009 | 0.007 | 0.006 | 0.006 | 0.006 |

Data for the binary mixtures were correlated with the Redlich−Kister (RK) equation[6]

$$V^E_{ij}/10^{-6}\ \mathrm{m^3\cdot mol^{-1}} = x_i x_j \sum_{p=0}^{k} A_p (2x_i - 1)^p \qquad (2)$$

where $A_p$ denotes the adjustable parameters and the number of adjustable parameters ($k + 1$) has been determined using the F-test.

Adjustable parameters of the fits at each temperature separately and the corresponding root-mean-square deviations (rmsd) defined by the equation

$$\sigma = \left( \sum_{i=1}^{m} (V^E_{\mathrm{exptl},i} - V^E_{\mathrm{calcd},i})^2/m \right)^{1/2} \qquad (3)$$

are given in Table 4. In eq 3, $m$ is the number of experimental data points.

Comparisons of our experimental results of $V^E$ for the system 2-butanol + benzene at (303.15 and 308.15) K with the data reported previously show that our $V^E$ data are in very good agreement with data reported at 303.15 K[8] (about 1.5 % at $x_1 = 0.5$), while at 308.15 K[9] a larger discrepancy exists (nearly 10 % at $x_1 = 0.5$).

The ternary $V^E$ data were correlated by the Nagata and Tamura[7] equation

$$V^E_{123}/10^{-6}\ \mathrm{m^3\cdot mol^{-1}} = V^E_{12} + V^E_{13} + V^E_{23} + x_1x_2x_3RT(B_0 - B_1x_1 - B_2x_2 - B_3x_1^2 - B_4x_2^2 - B_5x_1x_2 - B_6x_1^3 - B_7x_2^3 - B_8x_1^2x_2) \qquad (4)$$

where $x_1$, $x_2$, and $x_3$ are mole fractions of the ternary system; $V^E_{12}$, $V^E_{13}$, and $V^E_{23}$ represent the excess molar volumes calculated using eq 2 and ternary compositions $x_i$ and $x_j$; and $B_0$, $B_1$,..., $B_8$ are the adjustable parameters of ternary contribution obtained

from ternary experimental $V^E$ data. These fitted parameters of eq 4 along with the corresponding $\sigma$, calculated according to eq 3, are given in Table 5.

**Supporting Information Available:**

Figures S1 to S5 show the $V^E$ data for the binary systems 2-butanol (1) + chloroform (2) (Figure S1a) and 2-butanol (1) + benzene (Figure S1b) for all the investigated temperatures (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K; experimental $V^E$ values at 303.15 K and fitted lines of constant $(x_1/x_3)$ obtained using eq 4 for the ternary system (Figure S2); isolines of the excess molar volume for the ternary system at 288.15 K (Figure S3a) and 313.15 K (Figure S3b); three-dimensional ternary $V^E$ representation of the investigated mixture at 303.15 K generated by eq 4, respectively (Figure S4); and comparison of the experimental values of $V^E$ data at 298.15 K for the systems alcohol (1) + chloroform (2) and alcohol (1) + benzene (2) (Figure S5) (5 pages). This material is available free of charge via the Internet at http://pubs.acs.org.

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