

Densities and Excess Molar Volumes for Binary Glycerol + 1-Propanol, + 2-Propanol, + 1,2-Propanediol, and + 1,3-Propanediol Mixtures at Different Temperatures

Qun-Sheng Li, Ming-Gao Su, and Shui Wang*

College of Chemical Engineering, Beijing University of Chemical Technology, Beijing 100029, People's Republic of China

Liquid densities of the binary glycerol + 1-propanol, + 2-propanol, + 1,2-propanediol, and + 1,3-propanediol mixtures were measured at the temperatures in the range from (298.15 to 333.15) K in 5 K intervals. From these data, the excess molar volumes (V^E) and its standard deviations ($\sigma(V^E)$) were calculated. The experimental results have been correlated using the three parameters of the Redlich–Kister equation.

Introduction

Glycerol is important in the pharmaceutical, cosmetic, and food industries because it is nontoxic and possesses good solvent properties for many compounds, both organic and inorganic. It has useful solvent properties, similar to those of water and simple aliphatic alcohols, because it has three hydroxyl groups. It is, accordingly, completely miscible with 1-propanol, 2-propanol, 1,2-propanediol, and 1,3-propanediol. Widespread application of the glycerol mixtures has been found in the manufacturing of solvents. Knowledge of the elementary physicochemical properties such as density of these mixtures is essential in modeling and design of chemical processes. However, no experimental density and V^E measurements have been reported in the previous literature^{1–3} for glycerol + 1-propanol, + 2-propanol, + 1,2-propanediol, and + 1,3-propanediol mixtures.

In this paper, liquid densities and V^E are reported for the binary mixtures glycerol + 1-propanol, + 2-propanol, + 1,2-propanediol, and + 1,3-propanediol between the temperatures of (298.15 to 333.15) K within the whole composition range. The extensive experimental data reported in this work have been correlated with the Redlich–Kister model. The parameters of the model and deviations between experimental and calculated data are given.

Experimental Sections

Materials. Chemical of high purity obtained from different suppliers were purified by simple vacuum fractionation. The purity was checked by gas chromatography (GC). In Table 1, the specifications of the experimental chemicals (mol wt, CASRN, purity) are summarized, and literature data (if available) for comparison are also presented.

Apparatus and Procedure. The densities of the pure components and binary mixtures were measured using a approximately 50 cm³ Gay-Lussac pycnometer, which was calibrated by using pure water. The pycnometer containing the solutions was immersed in a constant-temperature bath. The temperature was controlled within ± 0.05 K of the desired temperature through a thermostat water bath. Once the solutions

Table 1. Pure Compound Specifications: Molecular Weight, CAS Registry Number (CASRN), Purity, Densities at Different Temperatures, and Comparison with Literature Data

| compound | mol wt | CASRN | purity (% GC) | T/K | $\rho/\text{g}\cdot\text{cm}^{-3}$ | | | | | |
|-----------------|--------|-----------------------|---------------|-----------------|------------------------------------|-----------------------|--------|--------|--------|-----------------------|
| | | | | | this work | literature | | | | |
| glycerol | 92.09 | 56-81-5 | > 99.9 | 298.15 | 1.2589 | 1.2581 ⁴ | | | | |
| | | | | 303.15 | 1.2556 | | | | | |
| | | | | 308.15 | 1.2527 | | | | | |
| | | | | 313.15 | 1.2495 | | | | | |
| | | | | 318.15 | 1.2462 | | | | | |
| | | | | 323.15 | 1.2429 | | | | | |
| | | | | 328.15 | 1.2396 | | | | | |
| | | | | 333.15 | 1.2360 | | | | | |
| | | | | 1-propanol | 60.10 | 71-23-8 | > 99.5 | 298.15 | 0.7996 | 0.79978 ⁹ |
| | | | | | | | | 303.15 | 0.7955 | 0.7956 ⁷ |
| 308.15 | 0.7915 | 0.79138 ⁹ | | | | | | | | |
| 313.15 | 0.7873 | 0.7875 ⁷ | | | | | | | | |
| 318.15 | 0.7833 | | | | | | | | | |
| 323.15 | 0.7790 | 0.77926 ¹¹ | | | | | | | | |
| 328.15 | 0.7749 | | | | | | | | | |
| 333.15 | 0.7708 | 0.77065 ¹¹ | | | | | | | | |
| 2-propanol | 60.10 | 67-63-0 | > 99.7 | | | | | 298.15 | 0.7806 | 0.78123 ⁹ |
| | | | | | | | | 303.15 | 0.7766 | 0.7768 ⁸ |
| | | | | 308.15 | 0.7723 | 0.77246 ⁹ | | | | |
| | | | | 313.15 | 0.7679 | 0.7680 ⁸ | | | | |
| | | | | 318.15 | 0.7633 | | | | | |
| | | | | 323.15 | 0.7586 | 0.7589 ⁸ | | | | |
| | | | | 328.15 | 0.7538 | | | | | |
| | | | | 333.15 | 0.7489 | | | | | |
| | | | | 1,2-propanediol | 76.10 | 57-55-6 | > 99.6 | 298.15 | 1.0325 | 1.03277 ¹⁰ |
| | | | | | | | | 303.15 | 1.0292 | 1.02894 ⁵ |
| 308.15 | 1.0253 | 1.02519 ⁵ | | | | | | | | |
| 313.15 | 1.0215 | 1.02140 ⁵ | | | | | | | | |
| 318.15 | 1.0180 | 1.01740 ⁵ | | | | | | | | |
| 323.15 | 1.0140 | | | | | | | | | |
| 328.15 | 1.0102 | 1.00956 ¹⁰ | | | | | | | | |
| 333.15 | 1.0062 | | | | | | | | | |
| 1,3-propanediol | 76.10 | 504-63-2 | > 99.4 | | | | | 298.15 | 1.0499 | 1.04972 ⁶ |
| | | | | | | | | 303.15 | 1.0470 | 1.04672 ⁶ |
| | | | | 308.15 | 1.0441 | 1.04356 ⁶ | | | | |
| | | | | 313.15 | 1.0408 | 1.04028 ⁶ | | | | |
| | | | | 318.15 | 1.0378 | 1.03752 ⁶ | | | | |
| | | | | 323.15 | 1.0348 | 1.03415 ⁶ | | | | |
| | | | | 328.15 | 1.0314 | 1.03097 ¹⁰ | | | | |
| | | | | 333.15 | 1.0282 | | | | | |

reached the desired temperature, they were weighed using an analytical balance (Sartorius CP124S, Germany) with an accuracy of ± 0.0001 g. Each reported value was the average of at least three measurements. The uncertainties of the density were about ± 0.0003 g \cdot cm⁻³.

* Corresponding author. E-mail: wangshui2000@sohu.com. Fax: +0086-10-64413151.

Table 2. Densities and Molar Excess Volumes (V^E) for the Glycerol (1) + 1-Propanol (2) Binary Mixture at Different Temperatures

| x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ |
|----------------|------------------------------|---|--------|------------------------------|---|--------|------------------------------|---|--------|------------------------------|---|
| $T = 298.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7996 | 0.000 | 0.2185 | 0.9035 | -0.466 | 0.4946 | 1.0327 | -0.647 | 0.8545 | 1.1987 | -0.495 |
| 0.0676 | 0.8328 | -0.264 | 0.3031 | 0.9429 | -0.525 | 0.6036 | 1.0831 | -0.630 | 1.0000 | 1.2589 | 0.000 |
| 0.1402 | 0.8673 | -0.409 | 0.3949 | 0.9860 | -0.604 | 0.7230 | 1.1388 | -0.618 | | | |
| $T = 303.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7955 | 0.000 | 0.2185 | 0.9000 | -0.519 | 0.4946 | 1.0295 | -0.704 | 0.8545 | 1.1956 | -0.528 |
| 0.0676 | 0.8289 | -0.284 | 0.3031 | 0.9393 | -0.568 | 0.6036 | 1.0799 | -0.680 | 1.0000 | 1.2556 | 0.000 |
| 0.1402 | 0.8632 | -0.415 | 0.3949 | 0.9821 | -0.618 | 0.7230 | 1.1357 | -0.662 | | | |
| $T = 308.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7915 | 0.000 | 0.2185 | 0.8960 | -0.525 | 0.4946 | 1.0259 | -0.727 | 0.8545 | 1.1927 | -0.553 |
| 0.0676 | 0.8250 | -0.295 | 0.3031 | 0.9356 | -0.596 | 0.6036 | 1.0763 | -0.692 | 1.0000 | 1.2527 | 0.000 |
| 0.1402 | 0.8594 | -0.434 | 0.3949 | 0.9784 | -0.636 | 0.7230 | 1.1324 | -0.681 | | | |
| $T = 313.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7873 | 0.000 | 0.2185 | 0.8921 | -0.552 | 0.4946 | 1.0223 | -0.758 | 0.8545 | 1.1895 | -0.576 |
| 0.0676 | 0.8207 | -0.287 | 0.3031 | 0.9315 | -0.601 | 0.6036 | 1.0727 | -0.714 | 1.0000 | 1.2495 | 0.000 |
| 0.1402 | 0.8554 | -0.456 | 0.3949 | 0.9747 | -0.673 | 0.7230 | 1.1288 | -0.699 | | | |
| $T = 318.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7833 | 0.000 | 0.2185 | 0.8883 | -0.573 | 0.4946 | 1.0184 | -0.774 | 0.8545 | 1.1861 | -0.589 |
| 0.0676 | 0.8168 | -0.304 | 0.3031 | 0.9277 | -0.629 | 0.6036 | 1.0692 | -0.746 | 1.0000 | 1.2462 | 0.000 |
| 0.1402 | 0.8513 | -0.456 | 0.3949 | 0.9708 | -0.690 | 0.7230 | 1.1255 | -0.728 | | | |
| $T = 323.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7790 | 0.000 | 0.2185 | 0.8841 | -0.596 | 0.4946 | 1.0147 | -0.811 | 0.8545 | 1.1827 | -0.610 |
| 0.0676 | 0.8125 | -0.314 | 0.3031 | 0.9236 | -0.651 | 0.6036 | 1.0655 | -0.777 | 1.0000 | 1.2429 | 0.000 |
| 0.1402 | 0.8472 | -0.485 | 0.3949 | 0.9668 | -0.716 | 0.7230 | 1.1220 | -0.761 | | | |
| $T = 328.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7749 | 0.000 | 0.2185 | 0.8803 | -0.627 | 0.4946 | 1.0108 | -0.825 | 0.8545 | 1.1792 | -0.616 |
| 0.0676 | 0.8084 | -0.316 | 0.3031 | 0.9197 | -0.671 | 0.6036 | 1.0618 | -0.799 | 1.0000 | 1.2396 | 0.000 |
| 0.1402 | 0.8431 | -0.492 | 0.3949 | 0.9633 | -0.760 | 0.7230 | 1.1183 | -0.770 | | | |
| $T = 333.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7708 | 0.000 | 0.2185 | 0.8763 | -0.652 | 0.4946 | 1.0068 | -0.840 | 0.8545 | 1.1758 | -0.640 |
| 0.0676 | 0.8043 | -0.331 | 0.3031 | 0.9157 | -0.694 | 0.6036 | 1.0580 | -0.819 | 1.0000 | 1.2360 | 0.000 |
| 0.1402 | 0.8392 | -0.523 | 0.3949 | 0.9594 | -0.794 | 0.7230 | 1.1143 | -0.769 | | | |

Table 3. Densities and Molar Excess Volumes (V^E) for the Glycerol (1) + 2-Propanol (2) Binary Mixture at Different Temperatures

| x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ |
|----------------|------------------------------|---|--------|------------------------------|---|--------|------------------------------|---|--------|------------------------------|---|
| $T = 298.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7806 | 0.000 | 0.2185 | 0.8875 | -0.556 | 0.4946 | 1.0238 | -0.931 | 0.8545 | 1.1965 | -0.631 |
| 0.0676 | 0.8135 | -0.197 | 0.3031 | 0.9291 | -0.703 | 0.6036 | 1.0770 | -0.938 | 1.0000 | 1.2589 | 0.000 |
| 0.1402 | 0.8486 | -0.346 | 0.3949 | 0.9743 | -0.825 | 0.7230 | 1.1352 | -0.894 | | | |
| $T = 303.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7766 | 0.000 | 0.2185 | 0.8838 | -0.593 | 0.4946 | 1.0200 | -0.950 | 0.8545 | 1.1934 | -0.661 |
| 0.0676 | 0.8095 | -0.205 | 0.3031 | 0.9264 | -0.821 | 0.6036 | 1.0734 | -0.965 | 1.0000 | 1.2556 | 0.000 |
| 0.1402 | 0.8447 | -0.365 | 0.3949 | 0.9706 | -0.859 | 0.7230 | 1.1319 | -0.933 | | | |
| $T = 308.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7723 | 0.000 | 0.2185 | 0.8799 | -0.633 | 0.4946 | 1.0162 | -0.975 | 0.8545 | 1.1900 | -0.664 |
| 0.0676 | 0.8055 | -0.235 | 0.3031 | 0.9223 | -0.838 | 0.6036 | 1.0704 | -1.035 | 1.0000 | 1.2527 | 0.000 |
| 0.1402 | 0.8405 | -0.373 | 0.3949 | 0.9673 | -0.927 | 0.7230 | 1.1285 | -0.956 | | | |
| $T = 313.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7679 | 0.000 | 0.2185 | 0.8759 | -0.670 | 0.4946 | 1.0126 | -1.028 | 0.8545 | 1.1868 | -0.686 |
| 0.0676 | 0.8014 | -0.267 | 0.3031 | 0.9184 | -0.887 | 0.6036 | 1.0670 | -1.084 | 1.0000 | 1.2495 | 0.000 |
| 0.1402 | 0.8361 | -0.377 | 0.3949 | 0.9634 | -0.968 | 0.7230 | 1.1250 | -0.985 | | | |
| $T = 318.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7633 | 0.000 | 0.2185 | 0.8717 | -0.712 | 0.4946 | 1.0087 | -1.070 | 0.8545 | 1.1832 | -0.706 |
| 0.0676 | 0.7968 | -0.271 | 0.3031 | 0.9145 | -0.945 | 0.6036 | 1.0631 | -1.118 | 1.0000 | 1.2462 | 0.000 |
| 0.1402 | 0.8319 | -0.420 | 0.3949 | 0.9592 | -0.999 | 0.7230 | 1.1213 | -1.010 | | | |
| $T = 323.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7586 | 0.000 | 0.2185 | 0.8674 | -0.750 | 0.4946 | 1.0048 | -1.125 | 0.8545 | 1.1803 | -0.759 |
| 0.0676 | 0.7922 | -0.277 | 0.3031 | 0.9102 | -0.986 | 0.6036 | 1.0596 | -1.187 | 1.0000 | 1.2429 | 0.000 |
| 0.1402 | 0.8276 | -0.458 | 0.3949 | 0.9553 | -1.064 | 0.7230 | 1.1176 | -1.045 | | | |
| $T = 328.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7538 | 0.000 | 0.2185 | 0.8633 | -0.823 | 0.4946 | 1.0009 | -1.181 | 0.8545 | 1.1766 | -0.776 |
| 0.0676 | 0.7875 | -0.293 | 0.3031 | 0.9062 | -1.059 | 0.6036 | 1.0557 | -1.226 | 1.0000 | 1.2396 | 0.000 |
| 0.1402 | 0.8233 | -0.515 | 0.3949 | 0.9513 | -1.127 | 0.7230 | 1.1141 | -1.091 | | | |
| $T = 333.15$ K | | | | | | | | | | | |
| 0.0000 | 0.7489 | 0.000 | 0.2185 | 0.8588 | -0.872 | 0.4946 | 0.9972 | -1.263 | 0.8545 | 1.1731 | -0.801 |
| 0.0676 | 0.7829 | -0.329 | 0.3031 | 0.9016 | -1.090 | 0.6036 | 1.0519 | -1.290 | 1.0000 | 1.2360 | 0.000 |
| 0.1402 | 0.8184 | -0.526 | 0.3949 | 0.9475 | -1.217 | 0.7230 | 1.1105 | -1.142 | | | |

Table 4. Densities and Molar Excess Volumes (V^E) for the Glycerol (1) + 1,2-Propanediol (2) Binary Mixture at Different Temperatures

| x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ |
|----------------|------------------------------|---|--------|------------------------------|---|--------|------------------------------|---|--------|------------------------------|---|
| $T = 298.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0325 | 0.000 | 0.2615 | 1.0941 | -0.183 | 0.5534 | 1.1610 | -0.224 | 0.8815 | 1.2333 | -0.081 |
| 0.0841 | 1.0526 | -0.081 | 0.3552 | 1.1158 | -0.215 | 0.6585 | 1.1844 | -0.193 | 1.0000 | 1.2589 | 0.000 |
| 0.1712 | 1.0727 | -0.115 | 0.4524 | 1.1383 | -0.240 | 0.7677 | 1.2078 | -0.106 | | | |
| $T = 303.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0292 | 0.000 | 0.2615 | 1.0905 | -0.165 | 0.5534 | 1.1575 | -0.215 | 0.8815 | 1.2301 | -0.088 |
| 0.0841 | 1.0492 | -0.076 | 0.3552 | 1.1126 | -0.221 | 0.6585 | 1.1812 | -0.204 | 1.0000 | 1.2556 | 0.000 |
| 0.1712 | 1.0696 | -0.130 | 0.4524 | 1.1348 | -0.229 | 0.7677 | 1.2050 | -0.139 | | | |
| $T = 308.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0253 | 0.000 | 0.2615 | 1.0871 | -0.182 | 0.5534 | 1.1542 | -0.228 | 0.8815 | 1.2274 | -0.111 |
| 0.0841 | 1.0457 | -0.097 | 0.3552 | 1.1093 | -0.244 | 0.6585 | 1.1780 | -0.217 | 1.0000 | 1.2527 | 0.000 |
| 0.1712 | 1.0661 | -0.149 | 0.4524 | 1.1314 | -0.240 | 0.7677 | 1.2022 | -0.162 | | | |
| $T = 313.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0215 | 0.000 | 0.2615 | 1.0838 | -0.211 | 0.5534 | 1.1512 | -0.263 | 0.8815 | 1.2244 | -0.126 |
| 0.0841 | 1.0420 | -0.108 | 0.3552 | 1.1056 | -0.247 | 0.6585 | 1.1751 | -0.249 | 1.0000 | 1.2495 | 0.000 |
| 0.1712 | 1.0624 | -0.155 | 0.4524 | 1.1282 | -0.271 | 0.7677 | 1.1992 | -0.186 | | | |
| $T = 318.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0180 | 0.000 | 0.2615 | 1.0802 | -0.209 | 0.5534 | 1.1479 | -0.276 | 0.8815 | 1.2210 | -0.132 |
| 0.0841 | 1.0385 | -0.110 | 0.3552 | 1.1023 | -0.259 | 0.6585 | 1.1715 | -0.242 | 1.0000 | 1.2462 | 0.000 |
| 0.1712 | 1.0586 | -0.138 | 0.4524 | 1.1248 | -0.282 | 0.7677 | 1.1956 | -0.181 | | | |
| $T = 323.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0140 | 0.000 | 0.2615 | 1.0763 | -0.209 | 0.5534 | 1.1441 | -0.268 | 0.8815 | 1.2180 | -0.153 |
| 0.0841 | 1.0347 | -0.121 | 0.3552 | 1.0983 | -0.252 | 0.6585 | 1.1681 | -0.255 | 1.0000 | 1.2429 | 0.000 |
| 0.1712 | 1.0550 | -0.158 | 0.4524 | 1.1212 | -0.290 | 0.7677 | 1.1925 | -0.203 | | | |
| $T = 328.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0102 | 0.000 | 0.2615 | 1.0727 | -0.220 | 0.5534 | 1.1405 | -0.267 | 0.8815 | 1.2147 | -0.161 |
| 0.0841 | 1.0310 | -0.127 | 0.3552 | 1.0947 | -0.257 | 0.6585 | 1.1646 | -0.256 | 1.0000 | 1.2396 | 0.000 |
| 0.1712 | 1.0514 | -0.172 | 0.4524 | 1.1175 | -0.290 | 0.7677 | 1.1890 | -0.200 | | | |
| $T = 333.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0062 | 0.000 | 0.2615 | 1.0692 | -0.246 | 0.5534 | 1.1373 | -0.308 | 0.8815 | 1.2113 | -0.170 |
| 0.0841 | 1.0272 | -0.142 | 0.3552 | 1.0912 | -0.282 | 0.6585 | 1.1613 | -0.287 | 1.0000 | 1.2360 | 0.000 |
| 0.1712 | 1.0476 | -0.179 | 0.4524 | 1.1143 | -0.333 | 0.7677 | 1.1858 | -0.234 | | | |

Table 5. Densities and Molar Excess Volumes (V^E) for the Glycerol (1) + 1,3-Propanediol (2) Binary Mixture at Different Temperatures

| x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ | x_1 | ρ g·cm ⁻³ | V^E cm ³ ·mol ⁻¹ |
|----------------|------------------------------|---|--------|------------------------------|---|--------|------------------------------|---|--------|------------------------------|---|
| $T = 298.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0499 | 0.000 | 0.2615 | 1.1057 | -0.048 | 0.5534 | 1.1676 | -0.095 | 0.8815 | 1.2352 | -0.050 |
| 0.0841 | 1.0678 | -0.012 | 0.3552 | 1.1256 | -0.063 | 0.6585 | 1.1893 | -0.082 | 1.0000 | 1.2589 | 0.000 |
| 0.1712 | 1.0864 | -0.028 | 0.4524 | 1.1464 | -0.088 | 0.7677 | 1.2126 | -0.077 | | | |
| $T = 303.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0470 | 0.000 | 0.2615 | 1.1030 | -0.068 | 0.5534 | 1.1646 | -0.099 | 0.8815 | 1.2321 | -0.057 |
| 0.0841 | 1.0650 | -0.015 | 0.3552 | 1.1228 | -0.078 | 0.6585 | 1.1864 | -0.093 | 1.0000 | 1.2556 | 0.000 |
| 0.1712 | 1.0835 | -0.032 | 0.4524 | 1.1434 | -0.092 | 0.7677 | 1.2090 | -0.089 | | | |
| $T = 308.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0441 | 0.000 | 0.2615 | 1.1000 | -0.065 | 0.5534 | 1.1618 | -0.113 | 0.8815 | 1.2293 | -0.067 |
| 0.0841 | 1.0620 | -0.015 | 0.3552 | 1.1198 | -0.080 | 0.6585 | 1.1835 | -0.101 | 1.0000 | 1.2527 | 0.000 |
| 0.1712 | 1.0806 | -0.035 | 0.4524 | 1.1406 | -0.104 | 0.7677 | 1.2061 | -0.096 | | | |
| $T = 313.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0408 | 0.000 | 0.2615 | 1.0969 | -0.072 | 0.5534 | 1.1587 | -0.119 | 0.8815 | 1.2261 | -0.064 |
| 0.0841 | 1.0588 | -0.016 | 0.3552 | 1.1168 | -0.091 | 0.6585 | 1.1804 | -0.106 | 1.0000 | 1.2495 | 0.000 |
| 0.1712 | 1.0775 | -0.043 | 0.4524 | 1.1373 | -0.103 | 0.7677 | 1.2030 | -0.100 | | | |
| $T = 318.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0378 | 0.000 | 0.2615 | 1.0939 | -0.085 | 0.5534 | 1.1556 | -0.129 | 0.8815 | 1.2228 | -0.071 |
| 0.0841 | 1.0557 | -0.018 | 0.3552 | 1.1137 | -0.099 | 0.6585 | 1.1772 | -0.115 | 1.0000 | 1.2462 | 0.000 |
| 0.1712 | 1.0745 | -0.049 | 0.4524 | 1.1343 | -0.114 | 0.7677 | 1.1997 | -0.102 | | | |
| $T = 323.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0348 | 0.000 | 0.2615 | 1.0909 | -0.093 | 0.5534 | 1.1525 | -0.134 | 0.8815 | 1.2198 | -0.086 |
| 0.0841 | 1.0527 | -0.016 | 0.3552 | 1.1107 | -0.108 | 0.6585 | 1.1741 | -0.123 | 1.0000 | 1.2429 | 0.000 |
| 0.1712 | 1.0714 | -0.053 | 0.4524 | 1.1312 | -0.119 | 0.7677 | 1.1966 | -0.110 | | | |
| $T = 328.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0314 | 0.000 | 0.2615 | 1.0876 | -0.102 | 0.5534 | 1.1492 | -0.143 | 0.8815 | 1.2166 | -0.094 |
| 0.0841 | 1.0493 | -0.017 | 0.3552 | 1.1075 | -0.118 | 0.6585 | 1.1708 | -0.124 | 1.0000 | 1.2396 | 0.000 |
| 0.1712 | 1.0681 | -0.058 | 0.4524 | 1.1278 | -0.122 | 0.7677 | 1.1934 | -0.117 | | | |
| $T = 333.15$ K | | | | | | | | | | | |
| 0.0000 | 1.0282 | 0.000 | 0.2615 | 1.0844 | -0.107 | 0.5534 | 1.1459 | -0.148 | 0.8815 | 1.2133 | -0.105 |
| 0.0841 | 1.0461 | -0.022 | 0.3552 | 1.1041 | -0.119 | 0.6585 | 1.1675 | -0.133 | 1.0000 | 1.2360 | 0.000 |
| 0.1712 | 1.0649 | -0.064 | 0.4524 | 1.1246 | -0.129 | 0.7677 | 1.1900 | -0.123 | | | |

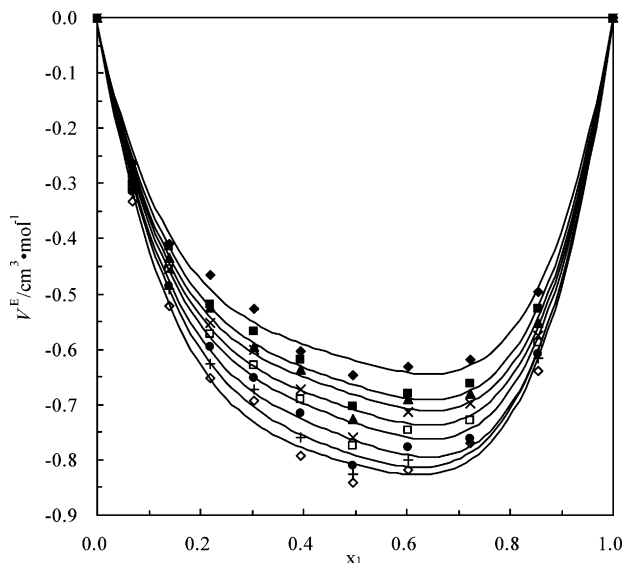


Figure 1. Excess molar volumes (V^E) for the glycerol (1) + 1-propanol (2) mixture at different temperatures: \blacklozenge , 298.15 K; \blacksquare , 303.15 K; \blacktriangle , 308.15 K; \times , 313.15 K; \square , 318.15 K; \bullet , 323.15 K; $+$, 328.15 K; \diamond , 333.15 K.

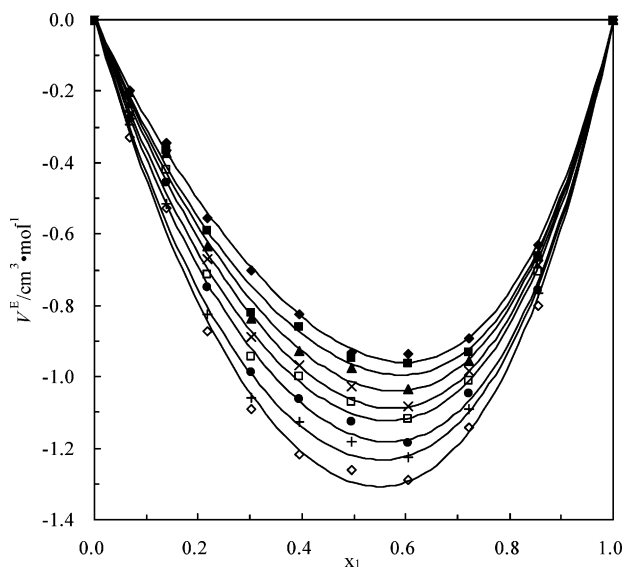


Figure 2. Excess molar volumes (V^E) for the glycerol (1) + 2-propanol (2) mixture at different temperatures: \blacklozenge , 298.15 K; \blacksquare , 303.15 K; \blacktriangle , 308.15 K; \times , 313.15 K; \square , 318.15 K; \bullet , 323.15 K; $+$, 328.15 K; \diamond , 333.15 K.

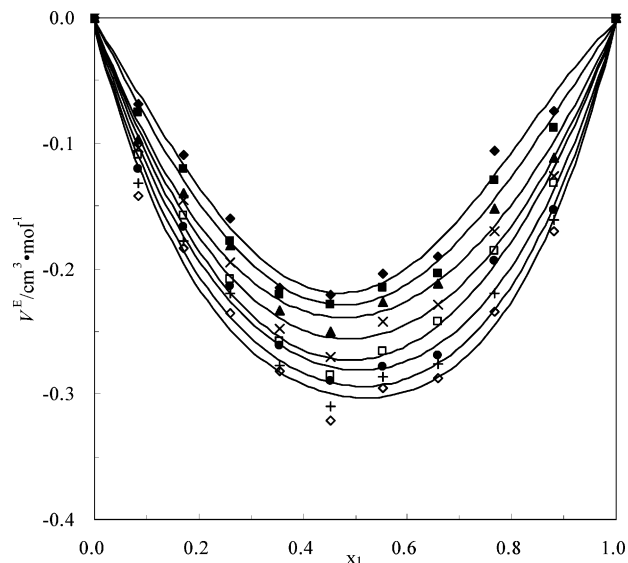


Figure 3. Excess molar volumes (V^E) for the glycerol (1) + 1,2-propanediol (2) mixture at different temperatures: \blacklozenge , 298.15 K; \blacksquare , 303.15 K; \blacktriangle , 308.15 K; \times , 313.15 K; \square , 318.15 K; \bullet , 323.15 K; $+$, 328.15 K; \diamond , 333.15 K.

Values of V^E were calculated from the density of the mixture (ρ) and the density (ρ_i), molar fraction (x_i), and molar masses (M_i) of the pure components (i) using the relation

$$V^E = \frac{(x_1 M_1 + x_2 M_2)}{\rho} - (x_1 M_1 / \rho_1 + x_2 M_2 / \rho_2) \quad (1)$$

Results and Discussion

The densities and excess molar volumes at temperatures between (298.15 and 333.15) K for the glycerol + 1-propanol, 2-propanol, 1,2-propanediol, and 1,3-propanediol binary mixtures are presented in Tables 2 to 5, respectively. The experimental excess molar volumes have been correlated by means of Redlich–Kister expansion in the form

$$V^E = x_1 x_2 \sum_{j=0}^2 a_j (x_2 - x_1)^j \quad (2)$$

The regression was performed by means of the maximum likelihood method using a program with possibility to select the number adjustable parameters and to input estimated standard deviations for the measured properties. The conclusion

Table 6. Redlich–Kister Parameters, a_i , and Standard Deviations of Molar Excess Volumes, $\sigma(V^E)$, for the Investigated Systems at Different Temperatures

| T/K | a_0 | a_1 | a_2 | $\sigma(V^E)/\text{cm}^3 \cdot \text{mol}^{-1}$ | T/K | a_0 | a_1 | a_2 | $\sigma(V^E)/\text{cm}^3 \cdot \text{mol}^{-1}$ |
|------------------------------------|---------|---------|---------|---|--------|---------|---------|---------|---|
| Glycerol (1) + 1-Propanol (2) | | | | | | | | | |
| 298.15 | -2.4762 | 0.5050 | -2.2063 | 0.023 | 318.15 | -2.9264 | 0.6052 | -2.6241 | 0.023 |
| 303.15 | -2.6148 | 0.5283 | -2.3343 | 0.024 | 323.15 | -3.0538 | 0.6424 | -2.6748 | 0.025 |
| 308.15 | -2.7184 | 0.5756 | -2.4249 | 0.025 | 328.15 | -3.1694 | 0.5967 | -2.7216 | 0.023 |
| 313.15 | -2.8303 | 0.5821 | -2.5361 | 0.026 | 333.15 | -3.2711 | 0.5943 | -2.8273 | 0.028 |
| Glycerol (1) + 2-Propanol (2) | | | | | | | | | |
| 298.15 | -3.7197 | 1.3626 | -0.6360 | 0.015 | 318.15 | -4.4478 | 1.1115 | -0.8492 | 0.040 |
| 303.15 | -3.9059 | 1.2781 | -0.7221 | 0.037 | 323.15 | -4.6640 | 1.0370 | -0.8691 | 0.037 |
| 308.15 | -4.0685 | 1.2480 | -0.7520 | 0.033 | 328.15 | -4.8736 | 0.9581 | -0.8818 | 0.038 |
| 313.15 | -4.2642 | 1.1182 | -0.8123 | 0.040 | 333.15 | -5.1964 | 0.9063 | -0.9063 | 0.035 |
| Glycerol (1) + 1,2-Propanediol (2) | | | | | | | | | |
| 298.15 | -0.8722 | -0.1453 | 0.3224 | 0.018 | 318.15 | -1.0906 | -0.0436 | -0.1381 | 0.015 |
| 303.15 | -0.9117 | -0.1107 | 0.1546 | 0.009 | 323.15 | -1.1227 | 0.0205 | -0.2890 | 0.015 |
| 308.15 | -0.9534 | -0.0844 | -0.0735 | 0.011 | 328.15 | -1.1725 | 0.0404 | -0.3908 | 0.021 |
| 313.15 | -1.0223 | -0.0453 | -0.1225 | 0.014 | 333.15 | -1.2090 | 0.0498 | -0.4898 | 0.017 |
| Glycerol (1) + 1,3-Propanediol (2) | | | | | | | | | |
| 298.15 | -0.3490 | 0.1939 | 0.0867 | 0.004 | 318.15 | -0.4854 | 0.2306 | -0.0069 | 0.007 |
| 303.15 | -0.3819 | 0.2063 | 0.0603 | 0.007 | 323.15 | -0.5190 | 0.2343 | -0.0280 | 0.009 |
| 308.15 | -0.4189 | 0.2187 | 0.0439 | 0.005 | 328.15 | -0.5348 | 0.2375 | -0.1152 | 0.011 |
| 313.15 | -0.4511 | 0.2245 | 0.0123 | 0.005 | 333.15 | -0.5525 | 0.2414 | -0.1986 | 0.011 |

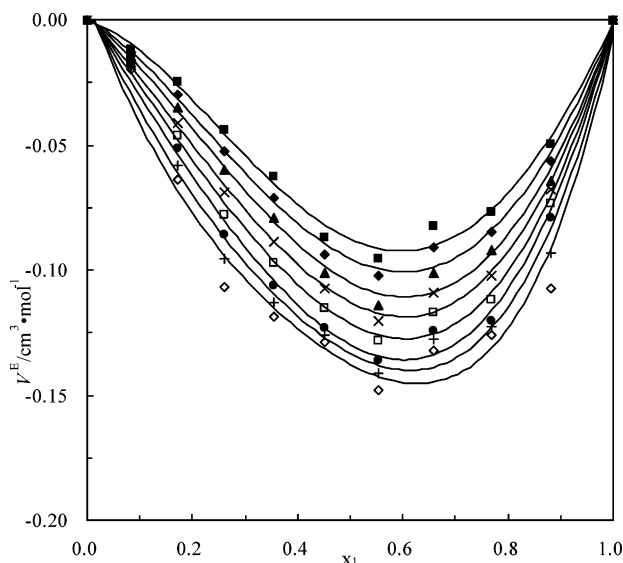


Figure 4. Excess molar volumes (V^E) for the glycerol (1) + 1,3-propanediol (2) mixture at different temperatures: \blacklozenge , 298.15 K; \blacksquare , 303.15 K; \blacktriangle , 308.15 K; \times , 313.15 K; \square , 318.15 K; \bullet , 323.15 K; $+$, 328.15 K; \diamond , 333.15 K.

was to use just three parameters for the Redlich–Kister equation and to find the source of possibly errors. Therefore, the input estimated standard deviation for the composition determinations (in more fractions) was set to 0.001 for all mixtures under investigation.

The Redlich–Kister parameters obtained from the correlation of V^E –composition data are summarized in Table 6 together with the resulting standard deviations in excess molar volume $\sigma(V^E)$. The standard deviation was calculated by

$$\sigma(V^E) = \left[\frac{\sum (V_{\text{expt}}^E - V_{\text{cal}}^E)^2}{D - N} \right]^{0.5} \quad (3)$$

where D and N are the numbers of data points and parameters, respectively.⁵ It was shown that the experimental data provided previously was reliable. From the inspection of Table 1, one may conclude that the pure compound densities at different temperatures are in good agreement with the available literature values.

The graphical presentation of the excess molar volumes (V^E) is shown in Figures 1 to 4. The observed values of V^E are

negative over the entire range of composition in the investigated systems.

Conclusions

The densities of binary mixtures of glycerol + C_3 -alkanol have been measured at different temperatures under atmospheric pressure over the whole concentration range. The values of excess molar volumes are calculated by the densities and have been correlated well using the Redlich–Kister polynomial equation.

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