

Supplementary Information

Disruption of self-molecular association of Pentanol in binary mixtures with Alkylbenzoates: A Dielectric Relaxation Spectroscopy Study

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Table S1: Experimental dielectric relaxation parameters for pure pentanols and alkylbenzoates according to Havriliak-Negami model in the 200MHz-20GHz range at room temperature.

| Compound | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R^2 |
|---------------------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|--------|
| 1-Pentanol (1P) | 3.01 | 17.98 | 20.99 | 1209.40 | 0.8563 | 1 | 0.003360 | 0.9985 |
| 2-Pentanol (2P) | 2.97 | 12.73 | 15.7 | 755.31 | 0.8944 | 1 | 0.004344 | 0.9980 |
| 3-Pentanol (3P) | 2.77 | 12.12 | 14.89 | 770.08 | 0.8783 | 1 | 0.005613 | 0.9971 |
| Methylbenzoate (MB) | 3.46 | 3.17 | 6.63 | 34.63 | 1 | 1 | 0.006269 | 0.9981 |
| Ethylbenzoate (EB) | 3.22 | 2.72 | 5.94 | 37.73 | 1 | 1 | 0.004536 | 0.9983 |
| Propylbenzoate (PB) | 3.12 | 2.53 | 5.65 | 48.79 | 1 | 0.9823 | 0.004245 | 0.9982 |
| Butylbenzoate (BB) | 2.89 | 2.14 | 5.03 | 56.93 | 1 | 1 | 0.004696 | 0.9976 |

Table S2: Experimental dielectric relaxation parameters for pentanols and alkylbenzoates binary mixtures at various concentrations according to Havriliak-Negami model in the 200MHz-20GHz range at room temperature.

| BB | | | | | | | | |
|------------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|--------|
| 1-pentanol | | | | | | | | |
| X of 1-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R^2 |
| 0.1119 | 2.91 | 2.37 | 5.28 | 57.86 | 1 | 1 | 0.003428 | 0.9983 |
| 0.2202 | 2.91 | 2.74 | 5.65 | 62.84 | 0.9731 | 0.9808 | 0.003659 | 0.9983 |
| 0.3073 | 2.90 | 3.06 | 5.96 | 66.94 | 0.9347 | 0.9982 | 0.003828 | 0.9982 |
| 0.4032 | 2.87 | 3.57 | 6.44 | 77.07 | 0.8850 | 1 | 0.004200 | 0.9980 |
| 0.4996 | 2.84 | 4.31 | 7.15 | 100.53 | 0.8365 | 1 | 0.004437 | 0.9979 |
| 0.5972 | 2.79 | 5.46 | 8.25 | 145.83 | 0.7784 | 1 | 0.004756 | 0.9978 |
| 0.6964 | 2.74 | 7.46 | 10.20 | 256.83 | 0.7198 | 1 | 0.008281 | 0.9960 |
| 0.7983 | 2.70 | 10.58 | 13.28 | 555.65 | 0.7187 | 1 | 0.003638 | 0.9982 |
| 0.8993 | 2.72 | 13.78 | 16.50 | 919.87 | 0.7913 | 0.9493 | 0.003691 | 0.9981 |
| 2-pentanol | | | | | | | | |
| X of 2-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R^2 |
| 0.1237 | 2.94 | 2.72 | 5.66 | 63.75 | 0.9839 | 0.8475 | 0.004487 | 0.9980 |
| 0.2232 | 2.91 | 2.97 | 5.88 | 69.22 | 0.9851 | 0.7857 | 0.004482 | 0.9981 |
| 0.3073 | 2.90 | 3.23 | 6.13 | 73.58 | 0.9646 | 0.7745 | 0.004851 | 0.9980 |
| 0.4138 | 2.90 | 3.65 | 6.55 | 82.40 | 0.9196 | 0.8001 | 0.005058 | 0.9979 |
| 0.5070 | 2.88 | 4.16 | 7.04 | 94.95 | 0.8646 | 0.8451 | 0.005239 | 0.9978 |
| 0.5996 | 2.88 | 4.87 | 7.75 | 116.36 | 0.8021 | 0.9108 | 0.005342 | 0.9977 |
| 0.6987 | 2.86 | 5.94 | 8.80 | 177.52 | 0.7672 | 0.9216 | 0.005324 | 0.9977 |
| 0.7987 | 2.87 | 7.59 | 10.46 | 304.59 | 0.7567 | 0.9283 | 0.005155 | 0.9977 |
| 0.9010 | 3.02 | 11.77 | 14.79 | 572.83 | 0.7785 | 1 | 0.006728 | 0.9971 |
| 3-pentanol | | | | | | | | |

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| X of 3-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R ² |
|----------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|----------------|
| 0.1149 | 2.93 | 2.61 | 5.54 | 52.50 | 0.9804 | 1 | 0.003557 | 0.9983 |
| 0.2010 | 2.91 | 2.92 | 5.83 | 51.99 | 0.9683 | 1 | 0.011366 | 0.9949 |
| 0.3020 | 2.96 | 3.08 | 6.04 | 54.26 | 0.9388 | 1 | 0.003692 | 0.9983 |
| 0.4019 | 2.96 | 3.47 | 6.43 | 60.50 | 0.9005 | 1 | 0.004270 | 0.9981 |
| 0.5020 | 2.94 | 3.97 | 6.91 | 70.89 | 0.8565 | 1 | 0.005474 | 0.9976 |
| 0.6021 | 2.90 | 4.67 | 7.57 | 91.57 | 0.8100 | 1 | 0.007062 | 0.9969 |
| 0.7011 | 2.85 | 5.63 | 8.48 | 134.81 | 0.7743 | 1 | 0.006183 | 0.9972 |
| 0.7975 | 2.82 | 7.12 | 9.94 | 235.14 | 0.7633 | 1 | 0.003998 | 0.9981 |
| 0.8986 | 2.81 | 9.73 | 12.54 | 465.84 | 0.7769 | 1 | 0.003452 | 0.9983 |

PB

| 1-pentanol | | | | | | | | |
|------------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|----------------|
| X of 1-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R ² |
| 0.0895 | 3.12 | 2.80 | 5.92 | 51.74 | 1 | 0.9371 | 0.004898 | 0.9980 |
| 0.2047 | 3.09 | 3.28 | 6.37 | 57.73 | 0.9458 | 0.9652 | 0.005343 | 0.9978 |
| 0.2917 | 3.11 | 3.66 | 6.77 | 58.36 | 0.8963 | 1 | 0.006090 | 0.9976 |
| 0.3907 | 3.07 | 4.34 | 7.41 | 76.29 | 0.8450 | 1 | 0.006382 | 0.9975 |
| 0.4969 | 3.02 | 5.28 | 8.30 | 94.07 | 0.7716 | 1 | 0.010981 | 0.9957 |
| 0.5974 | 2.93 | 6.84 | 9.77 | 174.94 | 0.7250 | 1 | 0.006334 | 0.9975 |
| 0.6968 | 2.89 | 8.83 | 11.72 | 308.41 | 0.7001 | 1 | 0.005798 | 0.9976 |
| 0.7991 | 2.95 | 11.32 | 14.27 | 495.48 | 0.7162 | 1 | 0.005662 | 0.9976 |
| 0.8999 | 2.98 | 14.43 | 17.41 | 865.36 | 0.8034 | 0.9375 | 0.005560 | 0.9976 |

2-pentanol

| X of 2-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R ² |
|----------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|----------------|
| 0.0996 | 3.27 | 2.60 | 5.87 | 43.09 | 1 | 1 | 0.007585 | 0.9971 |
| 0.2167 | 3.27 | 2.91 | 6.18 | 46.56 | 0.9757 | 1 | 0.005236 | 0.9981 |
| 0.3134 | 3.25 | 3.26 | 6.51 | 52.33 | 0.9392 | 1 | 0.005099 | 0.9981 |
| 0.4072 | 3.21 | 3.67 | 6.88 | 59.34 | 0.8913 | 1 | 0.007547 | 0.9972 |
| 0.5081 | 3.17 | 4.24 | 7.41 | 73.50 | 0.8405 | 1 | 0.010466 | 0.9961 |
| 0.6056 | 3.11 | 5.05 | 8.16 | 102.78 | 0.7922 | 1 | 0.013569 | 0.9947 |
| 0.7004 | 3.05 | 6.04 | 9.09 | 163.39 | 0.7838 | 1 | 0.005172 | 0.9979 |
| 0.7976 | 2.99 | 7.62 | 10.61 | 279.66 | 0.776 | 1 | 0.004659 | 0.9980 |
| 0.9002 | 2.98 | 10.05 | 13.03 | 476.30 | 0.8057 | 1 | 0.007217 | 0.9968 |

3-pentanol

| X of 3-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R ² |
|----------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|----------------|
| 0.1110 | 3.21 | 2.60 | 5.81 | 40.48 | 1 | 1 | 0.010629 | 0.9959 |
| 0.2056 | 3.23 | 2.83 | 6.06 | 41.96 | 1 | 1 | 0.005993 | 0.9978 |
| 0.3018 | 3.25 | 3.06 | 6.31 | 43.13 | 0.9820 | 1 | 0.008210 | 0.9970 |
| 0.4019 | 3.25 | 3.37 | 6.62 | 47.81 | 0.9492 | 1 | 0.008803 | 0.9968 |
| 0.5021 | 3.22 | 3.81 | 7.03 | 56.56 | 0.9065 | 1 | 0.010144 | 0.9963 |
| 0.5991 | 3.17 | 4.40 | 7.57 | 72.07 | 0.8616 | 1 | 0.010583 | 0.9961 |
| 0.6983 | 3.06 | 5.27 | 8.33 | 109.17 | 0.8212 | 1 | 0.008074 | 0.9968 |
| 0.8042 | 2.95 | 6.59 | 9.54 | 200.05 | 0.8131 | 1 | 0.003787 | 0.9984 |
| 0.8986 | 2.92 | 8.30 | 11.22 | 344.83 | 0.8327 | 1 | 0.003408 | 0.9984 |

EB

| 1-pentanol | | | | | | | | |
|------------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|----------------|
| X of 1-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R ² |
| 0.1094 | 3.28 | 2.96 | 6.24 | 38.39 | 0.9936 | 1 | 0.004785 | 0.9983 |
| 0.2211 | 3.30 | 3.40 | 6.70 | 40.43 | 0.9341 | 1 | 0.009158 | 0.9969 |
| 0.3219 | 3.22 | 3.92 | 7.14 | 49.84 | 0.8973 | 1 | 0.005540 | 0.9981 |
| 0.4100 | 3.17 | 4.52 | 7.69 | 61.88 | 0.8492 | 1 | 0.005914 | 0.9980 |
| 0.5042 | 3.07 | 5.46 | 8.53 | 87.23 | 0.7877 | 1 | 0.006782 | 0.9976 |
| 0.5987 | 2.95 | 6.78 | 9.73 | 143.51 | 0.7357 | 1 | 0.006233 | 0.9976 |
| 0.6986 | 2.94 | 8.76 | 11.70 | 266.21 | 0.7072 | 1 | 0.005590 | 0.9978 |
| 0.8065 | 3.06 | 10.95 | 14.01 | 424.38 | 0.7305 | 1 | 0.005281 | 0.9980 |
| 0.9044 | 3.04 | 13.57 | 16.61 | 736.89 | 0.8037 | 0.9518 | 0.004497 | 0.9981 |

2-pentanol

| X of 2-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R ² |
|----------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|----------------|
| 0.1022 | 3.41 | 2.84 | 6.25 | 34.82 | 0.9818 | 1 | 0.008404 | 0.9973 |
| 0.2125 | 3.41 | 3.11 | 6.52 | 35.73 | 0.9490 | 1 | 0.008188 | 0.9974 |
| 0.3129 | 2.82 | 3.88 | 6.70 | 45.61 | 0.8879 | 0.8752 | 0.004776 | 0.9982 |
| 0.4059 | 2.81 | 4.33 | 7.14 | 48.96 | 0.8134 | 0.9778 | 0.004797 | 0.9981 |
| 0.4977 | 2.77 | 4.91 | 7.68 | 61.96 | 0.7604 | 1 | 0.004718 | 0.9981 |
| 0.5975 | 2.72 | 5.83 | 8.55 | 95.20 | 0.7096 | 1 | 0.004774 | 0.9981 |
| 0.6980 | 2.67 | 7.15 | 9.82 | 183.20 | 0.6764 | 0.9894 | 0.004415 | 0.9981 |
| 0.7959 | 3.09 | 8.17 | 11.26 | 294.22 | 0.7455 | 1 | 0.005335 | 0.9979 |
| 0.8952 | 3.08 | 9.95 | 13.03 | 458.26 | 0.7989 | 1 | 0.004833 | 0.9980 |

3-pentanol

| X of 3-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R ² |
|----------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|----------------|
| 0.1044 | 2.91 | 3.08 | 5.99 | 31.04 | 1 | 1 | 0.027726 | 0.9892 |
| 0.2026 | 2.94 | 3.32 | 6.26 | 31.69 | 0.9851 | 1 | 0.029240 | 0.9891 |
| 0.3006 | 2.89 | 3.59 | 6.48 | 34.77 | 0.9586 | 1 | 0.028346 | 0.9892 |
| 0.4012 | 2.81 | 3.99 | 6.80 | 41.17 | 0.9139 | 1 | 0.027414 | 0.9894 |
| 0.4992 | 2.76 | 4.48 | 7.24 | 49.42 | 0.8569 | 1 | 0.028480 | 0.9888 |
| 0.5999 | 2.68 | 5.20 | 7.88 | 68.96 | 0.7996 | 1 | 0.027462 | 0.9889 |
| 0.6999 | 2.64 | 6.33 | 8.97 | 111.52 | 0.7318 | 1 | 0.029871 | 0.9872 |
| 0.7916 | 2.61 | 7.65 | 10.26 | 211.28 | 0.723 | 1 | 0.022445 | 0.9897 |
| 0.8790 | 2.63 | 8.93 | 11.56 | 360.77 | 0.7790 | 1 | 0.005771 | 0.9970 |

MB

1-pentanol

| X of 1-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R ² |
|----------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|----------------|
| 0.1091 | 3.49 | 3.62 | 7.11 | 31.33 | 0.9941 | 1 | 0.014429 | 0.9960 |
| 0.2081 | 3.43 | 3.96 | 7.39 | 32.77 | 0.9510 | 1 | 0.021565 | 0.9940 |
| 0.3121 | 3.47 | 4.52 | 7.99 | 39.43 | 0.9334 | 1 | 0.018442 | 0.9950 |
| 0.4174 | 3.38 | 5.31 | 8.69 | 49.62 | 0.8895 | 1 | 0.016994 | 0.9954 |
| 0.5274 | 3.23 | 6.25 | 9.48 | 68.23 | 0.8336 | 1 | 0.017342 | 0.9949 |
| 0.6178 | 3.12 | 7.38 | 10.50 | 96.56 | 0.7683 | 1 | 0.029228 | 0.9908 |
| 0.7112 | 2.73 | 9.64 | 12.37 | 193.23 | 0.7084 | 1 | 0.009829 | 0.9964 |
| 0.8059 | 2.33 | 11.05 | 13.38 | 493.03 | 0.8365 | 0.6933 | 0.008680 | 0.9962 |
| 0.8994 | 2.80 | 12.95 | 15.75 | 892.53 | 0.9163 | 0.7516 | 0.004800 | 0.9978 |

2-pentanol

| X of 2-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R ² |
|----------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|----------------|
| 0.1026 | 2.75 | 3.65 | 6.40 | 27.44 | 0.9578 | 1 | 0.012046 | 0.9954 |
| 0.2062 | 2.71 | 3.96 | 6.67 | 28.50 | 0.9279 | 1 | 0.011130 | 0.9958 |
| 0.3104 | 2.60 | 4.29 | 6.89 | 31.51 | 0.8863 | 1 | 0.011952 | 0.9953 |
| 0.4068 | 2.54 | 4.83 | 7.37 | 37.93 | 0.8342 | 1 | 0.012348 | 0.9951 |
| 0.5087 | 2.51 | 5.49 | 8.00 | 49.96 | 0.7849 | 1 | 0.011561 | 0.9954 |
| 0.6054 | 2.38 | 6.26 | 8.64 | 69.64 | 0.7277 | 1 | 0.014653 | 0.9938 |
| 0.7013 | 2.33 | 7.58 | 9.91 | 130.50 | 0.6896 | 1 | 0.008947 | 0.9958 |
| 0.7987 | 2.29 | 8.66 | 10.95 | 283.91 | 0.7548 | 0.8403 | 0.008552 | 0.9957 |
| 0.8732 | 2.31 | 9.53 | 11.84 | 448.36 | 0.8391 | 0.7619 | 0.008757 | 0.9953 |

3-pentanol

| X of 3-P | ε_α | $\Delta\varepsilon$ | ε_s | τ (ps) | α | β | χ^2 | R ² |
|----------|----------------------|---------------------|-----------------|-------------|----------|---------|----------|----------------|
| 0.1039 | 2.74 | 3.50 | 6.24 | 24.74 | 0.9538 | 1 | 0.021774 | 0.9911 |
| 0.1993 | 2.67 | 3.86 | 6.53 | 28.81 | 0.9369 | 1 | 0.011309 | 0.9955 |
| 0.3005 | 2.62 | 4.05 | 6.67 | 30.09 | 0.9209 | 1 | 0.014280 | 0.9943 |
| 0.4042 | 2.53 | 4.60 | 7.13 | 36.69 | 0.8568 | 1 | 0.011626 | 0.9952 |
| 0.5106 | 2.37 | 5.19 | 7.56 | 47.37 | 0.7823 | 1 | 0.013692 | 0.9941 |
| 0.5939 | 2.37 | 5.76 | 8.13 | 62.28 | 0.7512 | 1 | 0.011032 | 0.9951 |
| 0.6937 | 2.35 | 6.40 | 8.75 | 93.48 | 0.7329 | 1 | 0.020333 | 0.9903 |
| 0.7947 | 2.34 | 7.97 | 10.31 | 175.88 | 0.7053 | 1 | 0.010657 | 0.9946 |
| 0.8722 | 2.28 | 8.91 | 11.19 | 385.83 | 0.8268 | 0.7874 | 0.009701 | 0.9946 |

Table S3: Values of Bruggeman Factor f_B for pentanol and alkylbenzoate binary mixtures at room temperature.

| 1-pentanol | | | | | | | |
|-----------------|-------|-----------------|-------|-----------------|-------|-----------------|-------|
| BB | | PB | | EB | | MB | |
| \varnothing_2 | f_B | \varnothing_2 | f_B | \varnothing_2 | f_B | \varnothing_2 | f_B |
| 0.9288 | 0.02 | 0.9381 | 0.03 | 0.9155 | 0.03 | 0.9046 | 0.05 |
| 0.8535 | 0.06 | 0.8527 | 0.07 | 0.8243 | 0.07 | 0.8154 | 0.07 |
| 0.7875 | 0.09 | 0.7835 | 0.11 | 0.7373 | 0.11 | 0.7190 | 0.13 |
| 0.7088 | 0.13 | 0.6992 | 0.16 | 0.6571 | 0.16 | 0.6184 | 0.19 |
| 0.6222 | 0.19 | 0.6014 | 0.24 | 0.5670 | 0.23 | 0.5098 | 0.26 |
| 0.5259 | 0.28 | 0.5011 | 0.35 | 0.4717 | 0.33 | 0.4180 | 0.34 |
| 0.4175 | 0.41 | 0.3934 | 0.48 | 0.3649 | 0.47 | 0.3204 | 0.48 |
| 0.2935 | 0.60 | 0.2725 | 0.64 | 0.2422 | 0.61 | 0.2185 | 0.55 |
| 0.1555 | 0.78 | 0.1422 | 0.82 | 0.1234 | 0.77 | 0.1148 | 0.70 |

| 2-pentanol | | | | | | | |
|-----------------|-------|-----------------|-------|-----------------|-------|-----------------|-------|
| BB | | PB | | EB | | MB | |
| \varnothing_2 | f_B | \varnothing_2 | f_B | \varnothing_2 | f_B | \varnothing_2 | f_B |
| 0.9205 | 0.08 | 0.9305 | 0.03 | 0.9208 | 0.04 | 0.9099 | -0.03 |
| 0.8504 | 0.11 | 0.8426 | 0.07 | 0.8307 | 0.08 | 0.8162 | 0.01 |
| 0.7865 | 0.14 | 0.7644 | 0.11 | 0.7440 | 0.10 | 0.7193 | 0.04 |
| 0.6984 | 0.19 | 0.6831 | 0.16 | 0.6596 | 0.16 | 0.6272 | 0.10 |
| 0.6137 | 0.25 | 0.5892 | 0.22 | 0.5719 | 0.23 | 0.5270 | 0.19 |
| 0.5218 | 0.32 | 0.4910 | 0.31 | 0.4714 | 0.33 | 0.4292 | 0.27 |
| 0.4134 | 0.43 | 0.3879 | 0.41 | 0.3642 | 0.46 | 0.3295 | 0.42 |
| 0.2917 | 0.58 | 0.2732 | 0.56 | 0.2534 | 0.61 | 0.2252 | 0.54 |
| 0.1523 | 0.93 | 0.1410 | 0.78 | 0.1342 | 0.77 | 0.1435 | 0.63 |

| 3-pentanol | | | | | | | |
|-----------------|-------|-----------------|-------|-----------------|-------|-----------------|-------|
| BB | | PB | | EB | | MB | |
| \varnothing_2 | f_B | \varnothing_2 | f_B | \varnothing_2 | f_B | \varnothing_2 | f_B |
| 0.9273 | 0.07 | 0.9232 | 0.02 | 0.9200 | 0.01 | 0.9098 | -0.06 |
| 0.8682 | 0.11 | 0.8529 | 0.06 | 0.8408 | 0.05 | 0.8245 | -0.02 |
| 0.7929 | 0.14 | 0.7764 | 0.10 | 0.7574 | 0.08 | 0.7313 | 0.01 |
| 0.7114 | 0.19 | 0.6907 | 0.14 | 0.6669 | 0.12 | 0.6328 | 0.08 |
| 0.6217 | 0.25 | 0.5981 | 0.19 | 0.5737 | 0.18 | 0.5285 | 0.14 |
| 0.5226 | 0.32 | 0.5011 | 0.26 | 0.4723 | 0.27 | 0.4443 | 0.22 |
| 0.4138 | 0.42 | 0.3934 | 0.35 | 0.3651 | 0.40 | 0.3404 | 0.31 |
| 0.2961 | 0.57 | 0.2676 | 0.49 | 0.2610 | 0.55 | 0.2320 | 0.50 |
| 0.1575 | 0.81 | 0.1449 | 0.66 | 0.1603 | 0.68 | 0.1463 | 0.61 |

Table S4: Value of a for pentanol and alkylbenzoate binary mixtures at room temperature.

| | 1-pentanol | 2-pentanol | 3-pentanol |
|-----------|------------|------------|------------|
| BB | 1.71(4) | 1.5(1) | 1.54(5) |
| PB | 1.59(3) | 1.76(2) | 1.97(7) |
| EB | 1.79(2) | 1.77(2) | 1.99(2) |
| MB | 1.94(8) | 2.22(5) | 2.41(6) |

Table S5: Values of Kirkwood Correlation factor g_i for pure pentanol and alkylbenzoate at room temperature.

| | 1P | 2P | 3P | MB | EB | PB | BB |
|-------|------|------|------|------|------|------|------|
| g_i | 2.81 | 2.18 | 2.28 | 0.44 | 0.45 | 0.40 | 0.44 |

Table S6: Values of Effective Kirkwood Correlation factor g^{eff} and Corrective Kirkwood Correlation factor g^f for pentanol and alkylbenzoate binary mixtures at room temperature for various pentanol mole fractions.

| 1-pentanol | | | | | | | | | | | | | | | | | | | | | | | |
|------------|-----------|-------|------------------|-------------------|-------------------|--------|-----------|-------|------------------|-------------------|-------------------|--------|-----------|-------|------------------|-------------------|-------------------|--------|-----------|-------|------------------|-------------------|-------------------|
| BB | | | | | PB | | | | | EB | | | | | MB | | | | | | | | |
| X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} | X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} | X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} | X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} |
| 0.1119 | 0.48 | 0.67 | 3.49 | 3.68 | 0.19 | 0.0895 | 0.44 | 0.75 | 3.42 | 3.56 | 0.14 | 0.1094 | 0.43 | 0.64 | 3.24 | 3.46 | 0.21 | 0.1091 | 0.49 | 0.74 | 3.12 | 3.41 | 0.29 |
| 0.2202 | 0.54 | 0.55 | 3.54 | 3.88 | 0.34 | 0.2047 | 0.52 | 0.62 | 3.49 | 3.77 | 0.29 | 0.2211 | 0.50 | 0.54 | 3.27 | 3.69 | 0.41 | 0.2081 | 0.55 | 0.62 | 3.15 | 3.62 | 0.47 |
| 0.3073 | 0.60 | 0.50 | 3.57 | 4.03 | 0.46 | 0.2917 | 0.58 | 0.55 | 3.49 | 3.94 | 0.45 | 0.3219 | 0.59 | 0.52 | 3.40 | 3.89 | 0.50 | 0.3121 | 0.62 | 0.55 | 3.26 | 3.84 | 0.58 |
| 0.4032 | 0.69 | 0.49 | 3.66 | 4.21 | 0.55 | 0.3907 | 0.69 | 0.54 | 3.65 | 4.13 | 0.48 | 0.4100 | 0.69 | 0.51 | 3.53 | 4.08 | 0.55 | 0.4174 | 0.75 | 0.55 | 3.40 | 4.06 | 0.67 |
| 0.4996 | 0.83 | 0.50 | 3.81 | 4.38 | 0.57 | 0.4969 | 0.85 | 0.56 | 3.77 | 4.33 | 0.56 | 0.5042 | 0.86 | 0.55 | 3.73 | 4.27 | 0.54 | 0.5274 | 0.93 | 0.57 | 3.58 | 4.29 | 0.71 |
| 0.5972 | 1.04 | 0.55 | 4.03 | 4.56 | 0.52 | 0.5974 | 1.13 | 0.64 | 4.14 | 4.52 | 0.38 | 0.5987 | 1.10 | 0.62 | 4.02 | 4.46 | 0.44 | 0.6178 | 1.13 | 0.62 | 3.79 | 4.48 | 0.69 |
| 0.6964 | 1.40 | 0.66 | 4.37 | 4.74 | 0.37 | 0.6968 | 1.46 | 0.72 | 4.48 | 4.71 | 0.23 | 0.6986 | 1.42 | 0.70 | 4.39 | 4.67 | 0.28 | 0.7112 | 1.69 | 0.82 | 4.20 | 4.68 | 0.48 |
| 0.7983 | 1.95 | 0.83 | 4.83 | 4.92 | 0.10 | 0.7991 | 1.82 | 0.80 | 4.76 | 4.91 | 0.15 | 0.8065 | 1.69 | 0.73 | 4.67 | 4.89 | 0.22 | 0.8059 | 2.29 | 0.99 | 4.76 | 4.88 | 0.12 |
| 0.8993 | 2.46 | 0.95 | 5.13 | 5.11 | -0.02 | 0.8999 | 2.29 | 0.90 | 5.09 | 5.10 | 0.01 | 0.9044 | 2.11 | 0.82 | 4.99 | 5.09 | 0.10 | 0.8994 | 2.21 | 0.87 | 5.11 | 5.08 | -0.03 |
| 2-pentanol | | | | | | | | | | | | | | | | | | | | | | | |
| BB | | | | | PB | | | | | EB | | | | | MB | | | | | | | | |
| X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} | X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} | X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} | X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} |
| 0.1237 | 0.54 | 0.82 | 3.54 | 3.67 | 0.12 | 0.0996 | 0.40 | 0.72 | 3.31 | 3.55 | 0.24 | 0.1022 | 0.40 | 0.67 | 3.19 | 3.41 | 0.23 | 0.1026 | 0.65 | 1.10 | 3.04 | 3.37 | 0.33 |
| 0.2232 | 0.59 | 0.71 | 3.59 | 3.82 | 0.23 | 0.2167 | 0.45 | 0.61 | 3.36 | 3.74 | 0.38 | 0.2125 | 0.44 | 0.58 | 3.20 | 3.61 | 0.41 | 0.2062 | 0.72 | 0.96 | 3.07 | 3.56 | 0.49 |
| 0.3073 | 0.64 | 0.66 | 3.63 | 3.95 | 0.32 | 0.3134 | 0.51 | 0.57 | 3.43 | 3.89 | 0.47 | 0.3129 | 0.68 | 0.74 | 3.35 | 3.79 | 0.44 | 0.3104 | 0.83 | 0.90 | 3.13 | 3.75 | 0.62 |
| 0.4138 | 0.71 | 0.62 | 3.70 | 4.11 | 0.41 | 0.4072 | 0.58 | 0.55 | 3.50 | 4.05 | 0.54 | 0.4059 | 0.77 | 0.72 | 3.39 | 3.95 | 0.57 | 0.4068 | 0.96 | 0.89 | 3.24 | 3.93 | 0.69 |
| 0.5070 | 0.81 | 0.61 | 3.78 | 4.25 | 0.47 | 0.5081 | 0.68 | 0.55 | 3.63 | 4.21 | 0.58 | 0.4977 | 0.89 | 0.73 | 3.53 | 4.12 | 0.59 | 0.5087 | 1.11 | 0.88 | 3.40 | 4.11 | 0.71 |
| 0.5996 | 0.93 | 0.63 | 3.90 | 4.40 | 0.49 | 0.6056 | 0.83 | 0.59 | 3.83 | 4.37 | 0.54 | 0.5975 | 1.08 | 0.77 | 3.78 | 4.29 | 0.51 | 0.6054 | 1.34 | 0.94 | 3.60 | 4.29 | 0.69 |
| 0.6987 | 1.13 | 0.68 | 4.15 | 4.55 | 0.40 | 0.7004 | 1.01 | 0.64 | 4.10 | 4.52 | 0.42 | 0.6980 | 1.35 | 0.85 | 4.17 | 4.47 | 0.30 | 0.7013 | 1.66 | 1.04 | 3.97 | 4.46 | 0.49 |
| 0.7987 | 1.40 | 0.77 | 4.47 | 4.70 | 0.23 | 0.7976 | 1.30 | 0.74 | 4.42 | 4.68 | 0.26 | 0.7959 | 1.33 | 0.75 | 4.45 | 4.65 | 0.20 | 0.7987 | 1.94 | 1.09 | 4.43 | 4.64 | 0.21 |
| 0.9010 | 1.99 | 0.99 | 4.84 | 4.86 | 0.01 | 0.9002 | 1.71 | 0.87 | 4.74 | 4.85 | 0.11 | 0.8952 | 1.63 | 0.83 | 4.71 | 4.82 | 0.11 | 0.8732 | 2.13 | 1.10 | 4.70 | 4.78 | 0.08 |
| 3-pentanol | | | | | | | | | | | | | | | | | | | | | | | |
| BB | | | | | PB | | | | | EB | | | | | MB | | | | | | | | |
| X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} | X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} | X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} | X | g^{eff} | g^f | ΔF_{exp} | ΔF_{theo} | ΔF_{diff} |
| 0.1149 | 0.52 | 0.80 | 3.43 | 3.65 | 0.23 | 0.1110 | 0.41 | 0.70 | 3.27 | 3.57 | 0.29 | 0.1044 | 0.52 | 0.85 | 3.12 | 3.42 | 0.30 | 0.1039 | 0.63 | 1.05 | 2.98 | 3.37 | 0.39 |
| 0.2010 | 0.58 | 0.72 | 3.42 | 3.79 | 0.36 | 0.2056 | 0.44 | 0.60 | 3.30 | 3.72 | 0.43 | 0.2026 | 0.56 | 0.73 | 3.13 | 3.60 | 0.47 | 0.1993 | 0.72 | 0.95 | 3.07 | 3.55 | 0.48 |
| 0.3020 | 0.60 | 0.61 | 3.45 | 3.94 | 0.49 | 0.3018 | 0.48 | 0.53 | 3.31 | 3.88 | 0.57 | 0.3006 | 0.62 | 0.67 | 3.18 | 3.77 | 0.59 | 0.3005 | 0.78 | 0.84 | 3.10 | 3.73 | 0.64 |
| 0.4019 | 0.67 | 0.57 | 3.51 | 4.10 | 0.58 | 0.4019 | 0.53 | 0.49 | 3.37 | 4.04 | 0.67 | 0.4012 | 0.72 | 0.66 | 3.28 | 3.95 | 0.67 | 0.4042 | 0.92 | 0.84 | 3.22 | 3.93 | 0.71 |
| 0.5020 | 0.76 | 0.56 | 3.61 | 4.25 | 0.64 | 0.5021 | 0.61 | 0.49 | 3.47 | 4.21 | 0.73 | 0.4992 | 0.83 | 0.65 | 3.39 | 4.13 | 0.73 | 0.5106 | 1.12 | 0.87 | 3.37 | 4.12 | 0.75 |
| 0.6021 | 0.90 | 0.58 | 3.76 | 4.41 | 0.65 | 0.5991 | 0.72 | 0.50 | 3.62 | 4.36 | 0.75 | 0.5999 | 1.00 | 0.69 | 3.59 | 4.31 | 0.71 | 0.5939 | 1.25 | 0.86 | 3.53 | 4.27 | 0.74 |
| 0.7011 | 1.09 | 0.63 | 3.99 | 4.56 | 0.57 | 0.6983 | 0.90 | 0.55 | 3.86 | 4.53 | 0.66 | 0.6999 | 1.24 | 0.75 | 3.88 | 4.48 | 0.61 | 0.6937 | 1.41 | 0.86 | 3.77 | 4.46 | 0.69 |
| 0.7975 | 1.36 | 0.72 | 4.32 | 4.71 | 0.39 | 0.8042 | 1.17 | 0.63 | 4.22 | 4.70 | 0.48 | 0.7916 | 1.52 | 0.83 | 4.25 | 4.65 | 0.39 | 0.7947 | 1.77 | 0.96 | 4.15 | 4.64 | 0.50 |
| 0.8986 | 1.82 | 0.87 | 4.72 | 4.86 | 0.14 | 0.8986 | 1.48 | 0.72 | 4.54 | 4.85 | 0.31 | 0.8790 | 1.77 | 0.88 | 4.57 | 4.80 | 0.23 | 0.8722 | 2.04 | 1.02 | 4.61 | 4.79 | 0.17 |