acetic acid + propionic acid

Sajjad Noshadi, Rahmat Sadeghi, Differential scanning calorimetry determination of solid-liquid equilibria phase diagrams for binary monocarboxylic acids solutions, Fluid Phase Equilibria 486 (2019) 1-10

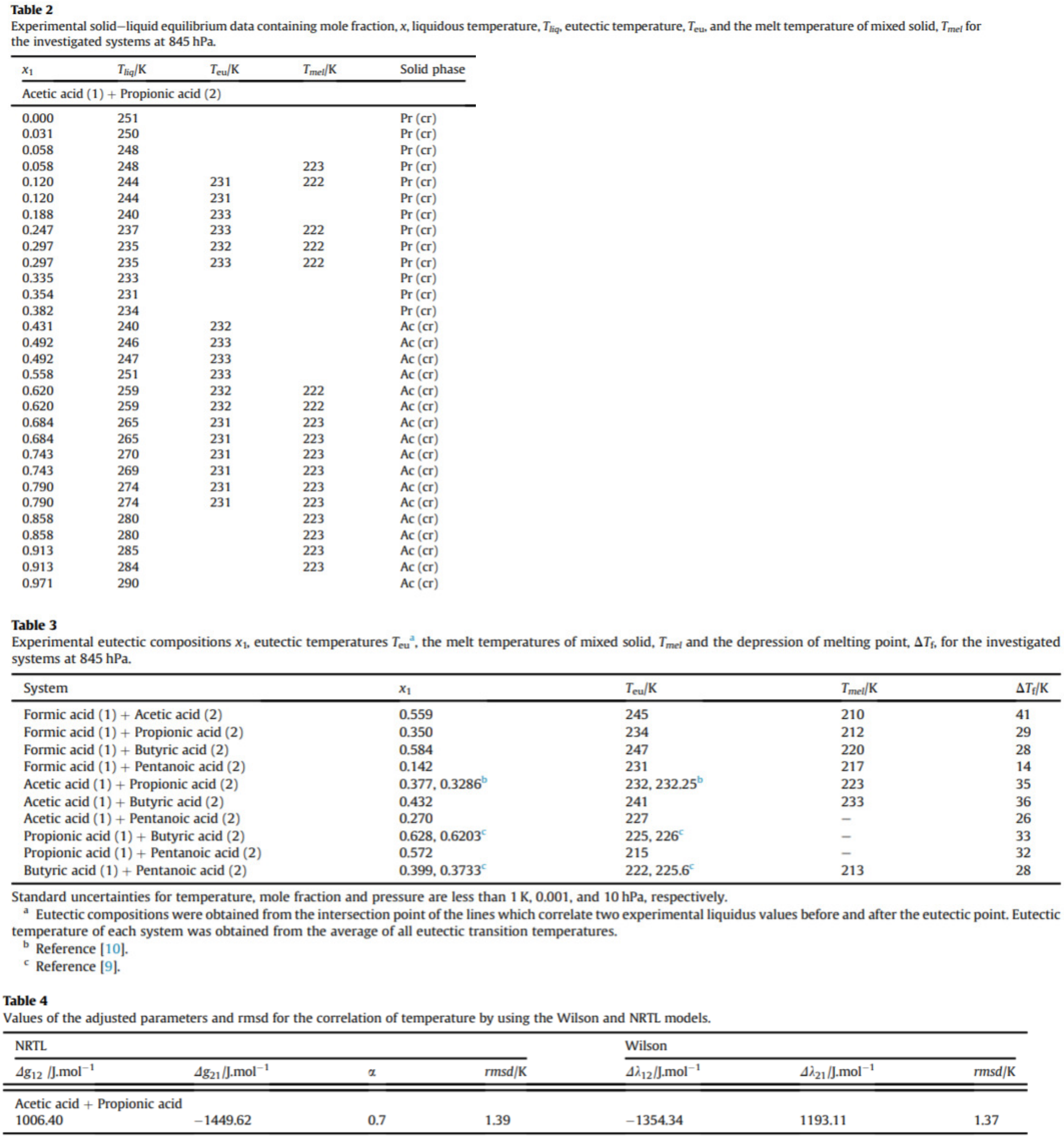


**Table 2**

Experimental solid–liquid equilibrium data containing mole fraction, $x$, liquidous temperature, $T_{liq}$, eutectic temperature, $T_{eu}$, and the melt temperature of mixed solid, $T_{mel}$ for the investigated systems at 845 hPa.

| $x_1$ | $T_{liq}$/K | $T_{eu}$/K | $T_{mel}$/K | Solid phase |
|---|---|---|---|---|
| Acetic acid (1) + Propionic acid (2) | | | | |
| 0.000 | 251 | | | Pr (cr) |
| 0.031 | 250 | | | Pr (cr) |
| 0.058 | 248 | | | Pr (cr) |
| 0.058 | 248 | | 223 | Pr (cr) |
| 0.120 | 244 | 231 | 222 | Pr (cr) |
| 0.120 | 244 | 231 | | Pr (cr) |
| 0.188 | 240 | 233 | | Pr (cr) |
| 0.247 | 237 | 233 | 222 | Pr (cr) |
| 0.297 | 235 | 232 | 222 | Pr (cr) |
| 0.297 | 235 | 233 | 222 | Pr (cr) |
| 0.335 | 233 | | | Pr (cr) |
| 0.354 | 231 | | | Pr (cr) |
| 0.382 | 234 | | | Pr (cr) |
| 0.431 | 240 | 232 | | Ac (cr) |
| 0.492 | 246 | 233 | | Ac (cr) |
| 0.492 | 247 | 233 | | Ac (cr) |
| 0.558 | 251 | 233 | | Ac (cr) |
| 0.620 | 259 | 232 | 222 | Ac (cr) |
| 0.620 | 259 | 232 | 222 | Ac (cr) |
| 0.684 | 265 | 231 | 223 | Ac (cr) |
| 0.684 | 265 | 231 | 223 | Ac (cr) |
| 0.743 | 270 | 231 | 223 | Ac (cr) |
| 0.743 | 269 | 231 | 223 | Ac (cr) |
| 0.790 | 274 | 231 | 223 | Ac (cr) |
| 0.790 | 274 | 231 | 223 | Ac (cr) |
| 0.858 | 280 | | 223 | Ac (cr) |
| 0.858 | 280 | | 223 | Ac (cr) |
| 0.913 | 285 | | 223 | Ac (cr) |
| 0.913 | 284 | | 223 | Ac (cr) |
| 0.971 | 290 | | | Ac (cr) |

**Table 3**

Experimental eutectic compositions $x_1$, eutectic temperatures $T_{eu}$[a], the melt temperatures of mixed solid, $T_{mel}$ and the depression of melting point, $\Delta T_f$, for the investigated systems at 845 hPa.

| System | $x_1$ | $T_{eu}$/K | $T_{mel}$/K | $\Delta T_f$/K |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | 0.559 | 245 | 210 | 41 |
| Formic acid (1) + Propionic acid (2) | 0.350 | 234 | 212 | 29 |
| Formic acid (1) + Butyric acid (2) | 0.584 | 247 | 220 | 28 |
| Formic acid (1) + Pentanoic acid (2) | 0.142 | 231 | 217 | 14 |
| Acetic acid (1) + Propionic acid (2) | 0.377, 0.3286[b] | 232, 232.25[b] | 223 | 35 |
| Acetic acid (1) + Butyric acid (2) | 0.432 | 241 | 233 | 36 |
| Acetic acid (1) + Pentanoic acid (2) | 0.270 | 227 | – | 26 |
| Propionic acid (1) + Butyric acid (2) | 0.628, 0.6203[c] | 225, 226[c] | – | 33 |
| Propionic acid (1) + Pentanoic acid (2) | 0.572 | 215 | – | 32 |
| Butyric acid (1) + Pentanoic acid (2) | 0.399, 0.3733[c] | 222, 225.6[c] | 213 | 28 |

Standard uncertainties for temperature, mole fraction and pressure are less than 1 K, 0.001, and 10 hPa, respectively.

[a] Eutectic compositions were obtained from the intersection point of the lines which correlate two experimental liquidus values before and after the eutectic point. Eutectic temperature of each system was obtained from the average of all eutectic transition temperatures.

[b] Reference [10].

[c] Reference [9].

**Table 4**

Values of the adjusted parameters and rmsd for the correlation of temperature by using the Wilson and NRTL models.

| NRTL | | | | Wilson | | |
|---|---|---|---|---|---|---|
| $\Delta g_{12}$ /J.mol$^{-1}$ | $\Delta g_{21}$ /J.mol$^{-1}$ | $\alpha$ | rmsd/K | $\Delta\lambda_{12}$/J.mol$^{-1}$ | $\Delta\lambda_{21}$/J.mol$^{-1}$ | rmsd/K |
| Acetic acid + Propionic acid | | | | | | |
| 1006.40 | −1449.62 | 0.7 | 1.39 | −1354.34 | 1193.11 | 1.37 |

ODABRATI JEDAN MODEL!

butyric acid + acetic acid

Sajjad Noshadi, Rahmat Sadeghi, Differential scanning calorimetry determination of solid-liquid equilibria phase diagrams for binary monocarboxylic acids solutions, Fluid Phase Equilibria 486 (2019) 1-10

---

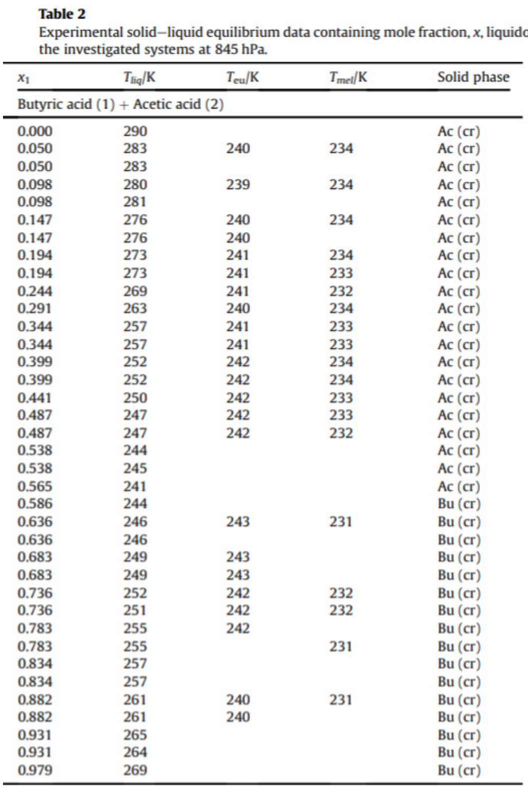


**Table 2**
Experimental solid–liquid equilibrium data containing mole fraction, $x$, liquidous temperature, $T_{liq}$, eutectic temperature, $T_{eu}$, and the melt temperature of mixed solid, $T_{mel}$ for the investigated systems at 845 hPa.

| $x_1$ | $T_{liq}$/K | $T_{eu}$/K | $T_{mel}$/K | Solid phase |
|---|---|---|---|---|
| Butyric acid (1) + Acetic acid (2) | | | | |
| 0.000 | 290 | | | Ac (cr) |
| 0.050 | 283 | 240 | 234 | Ac (cr) |
| 0.050 | 283 | | | Ac (cr) |
| 0.098 | 280 | 239 | 234 | Ac (cr) |
| 0.098 | 281 | | | Ac (cr) |
| 0.147 | 276 | 240 | 234 | Ac (cr) |
| 0.147 | 276 | 240 | | Ac (cr) |
| 0.194 | 273 | 241 | 234 | Ac (cr) |
| 0.194 | 273 | 241 | 233 | Ac (cr) |
| 0.244 | 269 | 241 | 232 | Ac (cr) |
| 0.291 | 263 | 240 | 234 | Ac (cr) |
| 0.344 | 257 | 241 | 233 | Ac (cr) |
| 0.344 | 257 | 241 | 233 | Ac (cr) |
| 0.399 | 252 | 242 | 234 | Ac (cr) |
| 0.399 | 252 | 242 | 234 | Ac (cr) |
| 0.441 | 250 | 242 | 233 | Ac (cr) |
| 0.487 | 247 | 242 | 233 | Ac (cr) |
| 0.487 | 247 | 242 | 232 | Ac (cr) |
| 0.538 | 244 | | | Ac (cr) |
| 0.538 | 245 | | | Ac (cr) |
| 0.565 | 241 | | | Ac (cr) |
| 0.586 | 244 | | | Bu (cr) |
| 0.636 | 246 | 243 | 231 | Bu (cr) |
| 0.636 | 246 | | | Bu (cr) |
| 0.683 | 249 | 243 | | Bu (cr) |
| 0.683 | 249 | 243 | | Bu (cr) |
| 0.736 | 252 | 242 | 232 | Bu (cr) |
| 0.736 | 251 | 242 | 232 | Bu (cr) |
| 0.783 | 255 | 242 | | Bu (cr) |
| 0.783 | 255 | | 231 | Bu (cr) |
| 0.834 | 257 | | | Bu (cr) |
| 0.834 | 257 | | | Bu (cr) |
| 0.882 | 261 | 240 | 231 | Bu (cr) |
| 0.882 | 261 | 240 | | Bu (cr) |
| 0.931 | 265 | | | Bu (cr) |
| 0.931 | 264 | | | Bu (cr) |
| 0.979 | 269 | | | Bu (cr) |

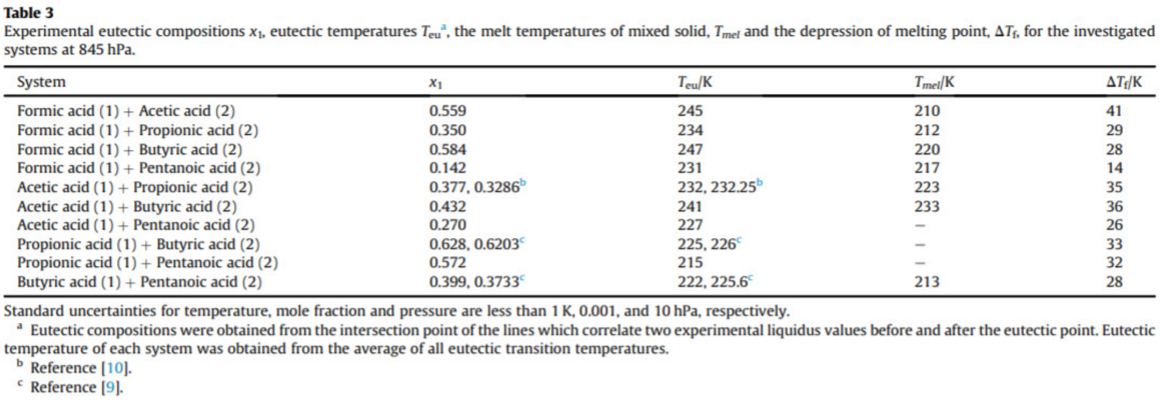


**Table 3**
Experimental eutectic compositions $x_1$, eutectic temperatures $T_{eu}$[a], the melt temperatures of mixed solid, $T_{mel}$ and the depression of melting point, $\Delta T_f$, for the investigated systems at 845 hPa.

| System | $x_1$ | $T_{eu}$/K | $T_{mel}$/K | $\Delta T_f$/K |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | 0.559 | 245 | 210 | 41 |
| Formic acid (1) + Propionic acid (2) | 0.350 | 234 | 212 | 29 |
| Formic acid (1) + Butyric acid (2) | 0.584 | 247 | 220 | 28 |
| Formic acid (1) + Pentanoic acid (2) | 0.142 | 231 | 217 | 14 |
| Acetic acid (1) + Propionic acid (2) | 0.377, 0.3286[b] | 232, 232.25[b] | 223 | 35 |
| Acetic acid (1) + Butyric acid (2) | 0.432 | 241 | 233 | 36 |
| Acetic acid (1) + Pentanoic acid (2) | 0.270 | 227 | – | 26 |
| Propionic acid (1) + Butyric acid (2) | 0.628, 0.6203[c] | 225, 226[c] | – | 33 |
| Propionic acid (1) + Pentanoic acid (2) | 0.572 | 215 | – | 32 |
| Butyric acid (1) + Pentanoic acid (2) | 0.399, 0.3733[c] | 222, 225.6[c] | 213 | 28 |

Standard uncertainties for temperature, mole fraction and pressure are less than 1 K, 0.001, and 10 hPa, respectively.

[a] Eutectic compositions were obtained from the intersection point of the lines which correlate two experimental liquidus values before and after the eutectic point. Eutectic temperature of each system was obtained from the average of all eutectic transition temperatures.

[b] Reference [10].

[c] Reference [9].

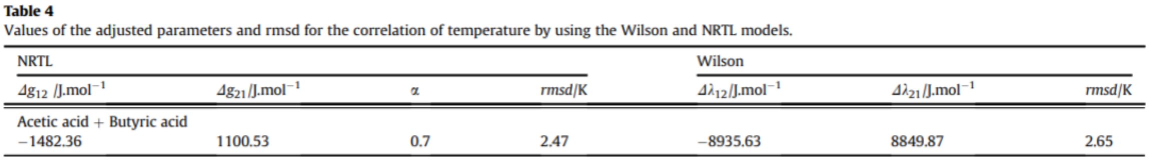


**Table 4**
Values of the adjusted parameters and rmsd for the correlation of temperature by using the Wilson and NRTL models.

| NRTL | | | | Wilson | | |
|---|---|---|---|---|---|---|
| $\Delta g_{12}$ /J.mol$^{-1}$ | $\Delta g_{21}$ /J.mol$^{-1}$ | $\alpha$ | rmsd/K | $\Delta\lambda_{12}$/J.mol$^{-1}$ | $\Delta\lambda_{21}$ /J.mol$^{-1}$ | rmsd/K |
| Acetic acid + Butyric acid | | | | | | |
| −1482.36 | 1100.53 | 0.7 | 2.47 | −8935.63 | 8849.87 | 2.65 |

ODABRATI JEDAN MODEL!

formic acid + acetic acid

Sajjad Noshadi, Rahmat Sadeghi, Differential scanning calorimetry determination of solid-liquid equilibria phase diagrams for binary monocarboxylic acids solutions, Fluid Phase Equilibria 486 (2019) 1-10

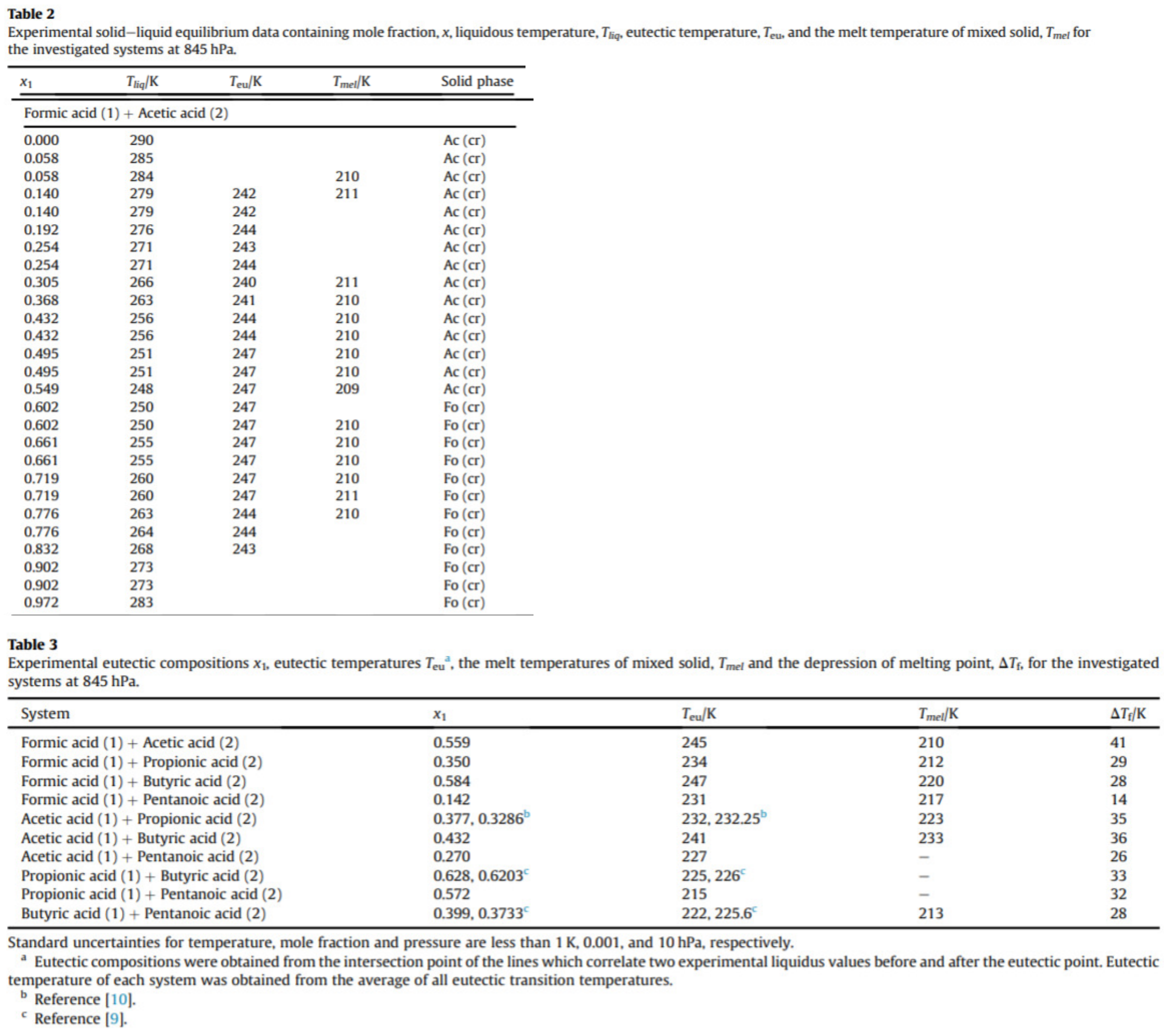


**Table 2**
Experimental solid–liquid equilibrium data containing mole fraction, $x$, liquidous temperature, $T_{liq}$, eutectic temperature, $T_{eu}$, and the melt temperature of mixed solid, $T_{mel}$ for the investigated systems at 845 hPa.

| $x_1$ | $T_{liq}$/K | $T_{eu}$/K | $T_{mel}$/K | Solid phase |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | | | | |
| 0.000 | 290 | | | Ac (cr) |
| 0.058 | 285 | | | Ac (cr) |
| 0.058 | 284 | | 210 | Ac (cr) |
| 0.140 | 279 | 242 | 211 | Ac (cr) |
| 0.140 | 279 | 242 | | Ac (cr) |
| 0.192 | 276 | 244 | | Ac (cr) |
| 0.254 | 271 | 243 | | Ac (cr) |
| 0.254 | 271 | 244 | | Ac (cr) |
| 0.305 | 266 | 240 | 211 | Ac (cr) |
| 0.368 | 263 | 241 | 210 | Ac (cr) |
| 0.432 | 256 | 244 | 210 | Ac (cr) |
| 0.432 | 256 | 244 | 210 | Ac (cr) |
| 0.495 | 251 | 247 | 210 | Ac (cr) |
| 0.495 | 251 | 247 | 210 | Ac (cr) |
| 0.549 | 248 | 247 | 209 | Ac (cr) |
| 0.602 | 250 | 247 | | Fo (cr) |
| 0.602 | 250 | 247 | 210 | Fo (cr) |
| 0.661 | 255 | 247 | 210 | Fo (cr) |
| 0.661 | 255 | 247 | 210 | Fo (cr) |
| 0.719 | 260 | 247 | 210 | Fo (cr) |
| 0.719 | 260 | 247 | 211 | Fo (cr) |
| 0.776 | 263 | 244 | 210 | Fo (cr) |
| 0.776 | 264 | 244 | | Fo (cr) |
| 0.832 | 268 | 243 | | Fo (cr) |
| 0.902 | 273 | | | Fo (cr) |
| 0.902 | 273 | | | Fo (cr) |
| 0.972 | 283 | | | Fo (cr) |

**Table 3**
Experimental eutectic compositions $x_1$, eutectic temperatures $T_{eu}$[a], the melt temperatures of mixed solid, $T_{mel}$ and the depression of melting point, $\Delta T_f$, for the investigated systems at 845 hPa.

| System | $x_1$ | $T_{eu}$/K | $T_{mel}$/K | $\Delta T_f$/K |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | 0.559 | 245 | 210 | 41 |
| Formic acid (1) + Propionic acid (2) | 0.350 | 234 | 212 | 29 |
| Formic acid (1) + Butyric acid (2) | 0.584 | 247 | 220 | 28 |
| Formic acid (1) + Pentanoic acid (2) | 0.142 | 231 | 217 | 14 |
| Acetic acid (1) + Propionic acid (2) | 0.377, 0.3286[b] | 232, 232.25[b] | 223 | 35 |
| Acetic acid (1) + Butyric acid (2) | 0.432 | 241 | 233 | 36 |
| Acetic acid (1) + Pentanoic acid (2) | 0.270 | 227 | – | 26 |
| Propionic acid (1) + Butyric acid (2) | 0.628, 0.6203[c] | 225, 226[c] | – | 33 |
| Propionic acid (1) + Pentanoic acid (2) | 0.572 | 215 | – | 32 |
| Butyric acid (1) + Pentanoic acid (2) | 0.399, 0.3733[c] | 222, 225.6[c] | 213 | 28 |

Standard uncertainties for temperature, mole fraction and pressure are less than 1 K, 0.001, and 10 hPa, respectively.

[a] Eutectic compositions were obtained from the intersection point of the lines which correlate two experimental liquidus values before and after the eutectic point. Eutectic temperature of each system was obtained from the average of all eutectic transition temperatures.

[b] Reference [10].

[c] Reference [9].

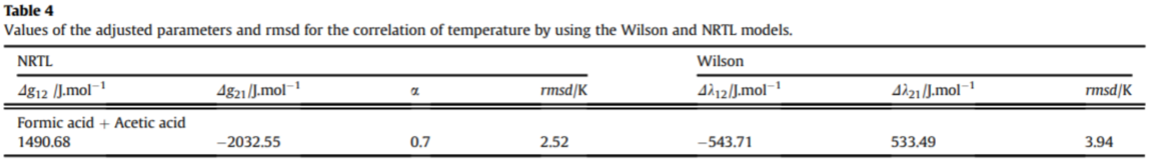


**Table 4**
Values of the adjusted parameters and rmsd for the correlation of temperature by using the Wilson and NRTL models.

| NRTL | | | | Wilson | | |
|---|---|---|---|---|---|---|
| $\Delta g_{12}$ /J.mol$^{-1}$ | $\Delta g_{21}$ /J.mol$^{-1}$ | $\alpha$ | *rmsd*/K | $\Delta\lambda_{12}$ /J.mol$^{-1}$ | $\Delta\lambda_{21}$ /J.mol$^{-1}$ | *rmsd*/K |
| Formic acid + Acetic acid | | | | | | |
| 1490.68 | −2032.55 | 0.7 | 2.52 | −543.71 | 533.49 | 3.94 |

ODABRATI JEDAN MODEL!

formic acid + butyric acid

Sajjad Noshadi, Rahmat Sadeghi, Differential scanning calorimetry determination of solid-liquid equilibria phase diagrams for binary monocarboxylic acids solutions, Fluid Phase Equilibria 486 (2019) 1-10

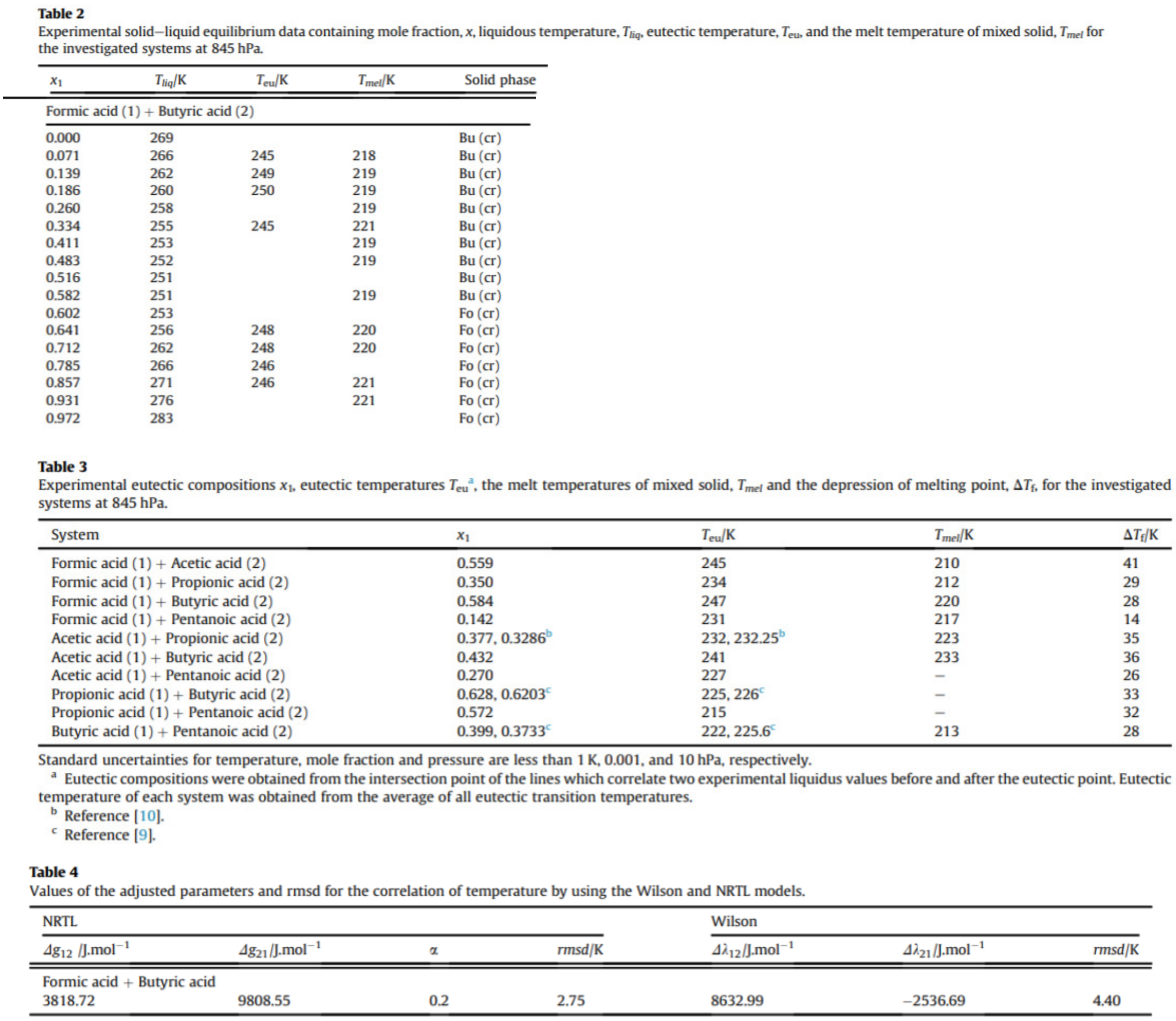


**Table 2**

Experimental solid–liquid equilibrium data containing mole fraction, *x*, liquidous temperature, $T_{liq}$, eutectic temperature, $T_{eu}$, and the melt temperature of mixed solid, $T_{mel}$ for the investigated systems at 845 hPa.

| $x_1$ | $T_{liq}$/K | $T_{eu}$/K | $T_{mel}$/K | Solid phase |
|---|---|---|---|---|
| Formic acid (1) + Butyric acid (2) | | | | |
| 0.000 | 269 | | | Bu (cr) |
| 0.071 | 266 | 245 | 218 | Bu (cr) |
| 0.139 | 262 | 249 | 219 | Bu (cr) |
| 0.186 | 260 | 250 | 219 | Bu (cr) |
| 0.260 | 258 | | 219 | Bu (cr) |
| 0.334 | 255 | 245 | 221 | Bu (cr) |
| 0.411 | 253 | | 219 | Bu (cr) |
| 0.483 | 252 | | 219 | Bu (cr) |
| 0.516 | 251 | | | Bu (cr) |
| 0.582 | 251 | | 219 | Bu (cr) |
| 0.602 | 253 | | | Fo (cr) |
| 0.641 | 256 | 248 | 220 | Fo (cr) |
| 0.712 | 262 | 248 | 220 | Fo (cr) |
| 0.785 | 266 | 246 | | Fo (cr) |
| 0.857 | 271 | 246 | 221 | Fo (cr) |
| 0.931 | 276 | | 221 | Fo (cr) |
| 0.972 | 283 | | | Fo (cr) |

**Table 3**

Experimental eutectic compositions $x_1$, eutectic temperatures $T_{eu}$[a], the melt temperatures of mixed solid, $T_{mel}$ and the depression of melting point, $\Delta T_f$, for the investigated systems at 845 hPa.

| System | $x_1$ | $T_{eu}$/K | $T_{mel}$/K | $\Delta T_f$/K |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | 0.559 | 245 | 210 | 41 |
| Formic acid (1) + Propionic acid (2) | 0.350 | 234 | 212 | 29 |
| Formic acid (1) + Butyric acid (2) | 0.584 | 247 | 220 | 28 |
| Formic acid (1) + Pentanoic acid (2) | 0.142 | 231 | 217 | 14 |
| Acetic acid (1) + Propionic acid (2) | 0.377, 0.3286[b] | 232, 232.25[b] | 223 | 35 |
| Acetic acid (1) + Butyric acid (2) | 0.432 | 241 | 233 | 36 |
| Acetic acid (1) + Pentanoic acid (2) | 0.270 | 227 | – | 26 |
| Propionic acid (1) + Butyric acid (2) | 0.628, 0.6203[c] | 225, 226[c] | – | 33 |
| Propionic acid (1) + Pentanoic acid (2) | 0.572 | 215 | – | 32 |
| Butyric acid (1) + Pentanoic acid (2) | 0.399, 0.3733[c] | 222, 225.6[c] | 213 | 28 |

Standard uncertainties for temperature, mole fraction and pressure are less than 1 K, 0.001, and 10 hPa, respectively.

[a] Eutectic compositions were obtained from the intersection point of the lines which correlate two experimental liquidus values before and after the eutectic point. Eutectic temperature of each system was obtained from the average of all eutectic transition temperatures.

[b] Reference [10].

[c] Reference [9].

**Table 4**

Values of the adjusted parameters and rmsd for the correlation of temperature by using the Wilson and NRTL models.

| NRTL | | | | Wilson | | |
|---|---|---|---|---|---|---|
| $\Delta g_{12}$ /J.mol$^{-1}$ | $\Delta g_{21}$ /J.mol$^{-1}$ | $\alpha$ | *rmsd*/K | $\Delta\lambda_{12}$/J.mol$^{-1}$ | $\Delta\lambda_{21}$ /J.mol$^{-1}$ | *rmsd*/K |
| Formic acid + Butyric acid | | | | | | |
| 3818.72 | 9808.55 | 0.2 | 2.75 | 8632.99 | −2536.69 | 4.40 |

ODABRATI JEDAN MODEL!

formic acid + propionic acid

Sajjad Noshadi, Rahmat Sadeghi, Differential scanning calorimetry determination of solid-liquid equilibria phase diagrams for binary monocarboxylic acids solutions, Fluid Phase Equilibria 486 (2019) 1-10

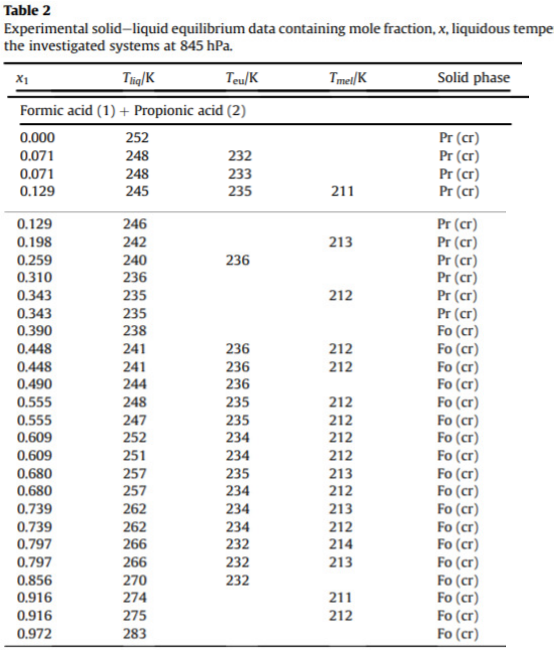


**Table 2**
Experimental solid–liquid equilibrium data containing mole fraction, $x$, liquidous temperature, $T_{liq}$, eutectic temperature, $T_{eu}$, and the melt temperature of mixed solid, $T_{mel}$ for the investigated systems at 845 hPa.

| $x_1$ | $T_{liq}$/K | $T_{eu}$/K | $T_{mel}$/K | Solid phase |
|---|---|---|---|---|
| Formic acid (1) + Propionic acid (2) | | | | |
| 0.000 | 252 | | | Pr (cr) |
| 0.071 | 248 | 232 | | Pr (cr) |
| 0.071 | 248 | 233 | | Pr (cr) |
| 0.129 | 245 | 235 | 211 | Pr (cr) |
| 0.129 | 246 | | | Pr (cr) |
| 0.198 | 242 | | 213 | Pr (cr) |
| 0.259 | 240 | 236 | | Pr (cr) |
| 0.310 | 236 | | | Pr (cr) |
| 0.343 | 235 | | 212 | Pr (cr) |
| 0.343 | 235 | | | Pr (cr) |
| 0.390 | 238 | | | Fo (cr) |
| 0.448 | 241 | 236 | 212 | Fo (cr) |
| 0.448 | 241 | 236 | 212 | Fo (cr) |
| 0.490 | 244 | 236 | | Fo (cr) |
| 0.555 | 248 | 235 | 212 | Fo (cr) |
| 0.555 | 247 | 235 | 212 | Fo (cr) |
| 0.609 | 252 | 234 | 212 | Fo (cr) |
| 0.609 | 251 | 234 | 212 | Fo (cr) |
| 0.680 | 257 | 235 | 213 | Fo (cr) |
| 0.680 | 257 | 234 | 212 | Fo (cr) |
| 0.739 | 262 | 234 | 213 | Fo (cr) |
| 0.739 | 262 | 234 | 212 | Fo (cr) |
| 0.797 | 266 | 232 | 214 | Fo (cr) |
| 0.797 | 266 | 232 | 213 | Fo (cr) |
| 0.856 | 270 | 232 | | Fo (cr) |
| 0.916 | 274 | | 211 | Fo (cr) |
| 0.916 | 275 | | 212 | Fo (cr) |
| 0.972 | 283 | | | Fo (cr) |

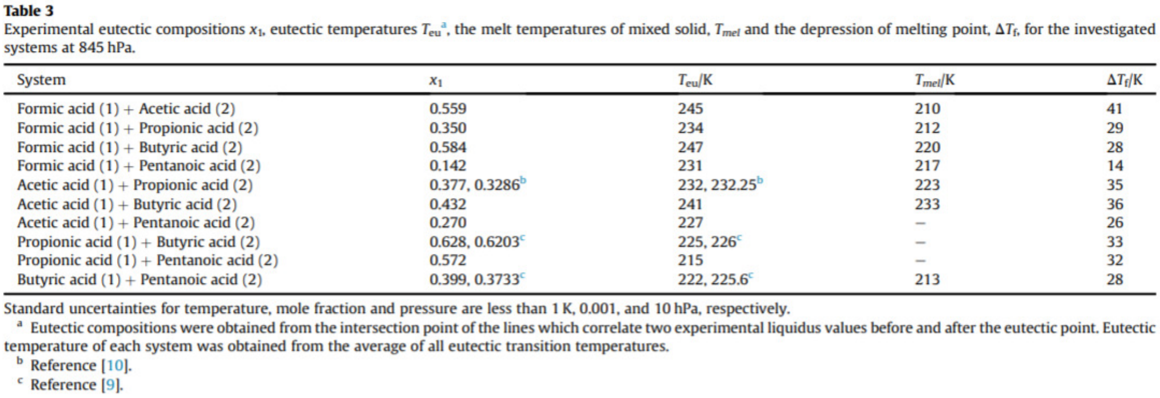


**Table 3**
Experimental eutectic compositions $x_1$, eutectic temperatures $T_{eu}$[a], the melt temperatures of mixed solid, $T_{mel}$ and the depression of melting point, $\Delta T_f$, for the investigated systems at 845 hPa.

| System | $x_1$ | $T_{eu}$/K | $T_{mel}$/K | $\Delta T_f$/K |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | 0.559 | 245 | 210 | 41 |
| Formic acid (1) + Propionic acid (2) | 0.350 | 234 | 212 | 29 |
| Formic acid (1) + Butyric acid (2) | 0.584 | 247 | 220 | 28 |
| Formic acid (1) + Pentanoic acid (2) | 0.142 | 231 | 217 | 14 |
| Acetic acid (1) + Propionic acid (2) | 0.377, 0.3286[b] | 232, 232.25[b] | 223 | 35 |
| Acetic acid (1) + Butyric acid (2) | 0.432 | 241 | 233 | 36 |
| Acetic acid (1) + Pentanoic acid (2) | 0.270 | 227 | – | 26 |
| Propionic acid (1) + Butyric acid (2) | 0.628, 0.6203[c] | 225, 226[c] | – | 33 |
| Propionic acid (1) + Pentanoic acid (2) | 0.572 | 215 | – | 32 |
| Butyric acid (1) + Pentanoic acid (2) | 0.399, 0.3733[c] | 222, 225.6[c] | 213 | 28 |

Standard uncertainties for temperature, mole fraction and pressure are less than 1 K, 0.001, and 10 hPa, respectively.

[a] Eutectic compositions were obtained from the intersection point of the lines which correlate two experimental liquidus values before and after the eutectic point. Eutectic temperature of each system was obtained from the average of all eutectic transition temperatures.

[b] Reference [10].

[c] Reference [9].

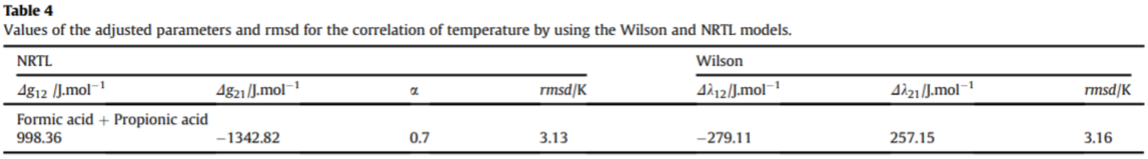


**Table 4**
Values of the adjusted parameters and rmsd for the correlation of temperature by using the Wilson and NRTL models.

| NRTL | | | | Wilson | | |
|---|---|---|---|---|---|---|
| $\Delta g_{12}$ /J.mol$^{-1}$ | $\Delta g_{21}$ /J.mol$^{-1}$ | $\alpha$ | rmsd/K | $\Delta\lambda_{12}$/J.mol$^{-1}$ | $\Delta\lambda_{21}$/J.mol$^{-1}$ | rmsd/K |
| Formic acid + Propionic acid | | | | | | |
| 998.36 | −1342.82 | 0.7 | 3.13 | −279.11 | 257.15 | 3.16 |

ODABRATI JEDAN MODEL!

formic acid + pentanoic acid

Sajjad Noshadi, Rahmat Sadeghi, Differential scanning calorimetry determination of solid-liquid equilibria phase diagrams for binary monocarboxylic acids solutions, Fluid Phase Equilibria 486 (2019) 1-10

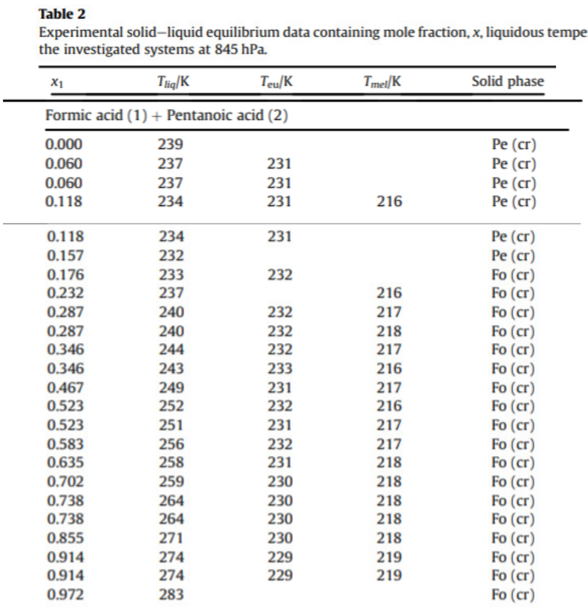


**Table 2**
Experimental solid–liquid equilibrium data containing mole fraction, *x*, liquidous temperature, $T_{liq}$, eutectic temperature, $T_{eu}$, and the melt temperature of mixed solid, $T_{mel}$ for the investigated systems at 845 hPa.

| $x_1$ | $T_{liq}$/K | $T_{eu}$/K | $T_{mel}$/K | Solid phase |
|---|---|---|---|---|
| Formic acid (1) + Pentanoic acid (2) | | | | |
| 0.000 | 239 | | | Pe (cr) |
| 0.060 | 237 | 231 | | Pe (cr) |
| 0.060 | 237 | 231 | | Pe (cr) |
| 0.118 | 234 | 231 | 216 | Pe (cr) |
| 0.118 | 234 | 231 | | Pe (cr) |
| 0.157 | 232 | | | Pe (cr) |
| 0.176 | 233 | 232 | | Fo (cr) |
| 0.232 | 237 | | 216 | Fo (cr) |
| 0.287 | 240 | 232 | 217 | Fo (cr) |
| 0.287 | 240 | 232 | 218 | Fo (cr) |
| 0.346 | 244 | 232 | 217 | Fo (cr) |
| 0.346 | 243 | 233 | 216 | Fo (cr) |
| 0.467 | 249 | 231 | 217 | Fo (cr) |
| 0.523 | 252 | 232 | 216 | Fo (cr) |
| 0.523 | 251 | 231 | 217 | Fo (cr) |
| 0.583 | 256 | 232 | 217 | Fo (cr) |
| 0.635 | 258 | 231 | 218 | Fo (cr) |
| 0.702 | 259 | 230 | 218 | Fo (cr) |
| 0.738 | 264 | 230 | 218 | Fo (cr) |
| 0.738 | 264 | 230 | 218 | Fo (cr) |
| 0.855 | 271 | 230 | 218 | Fo (cr) |
| 0.914 | 274 | 229 | 219 | Fo (cr) |
| 0.914 | 274 | 229 | 219 | Fo (cr) |
| 0.972 | 283 | | | Fo (cr) |

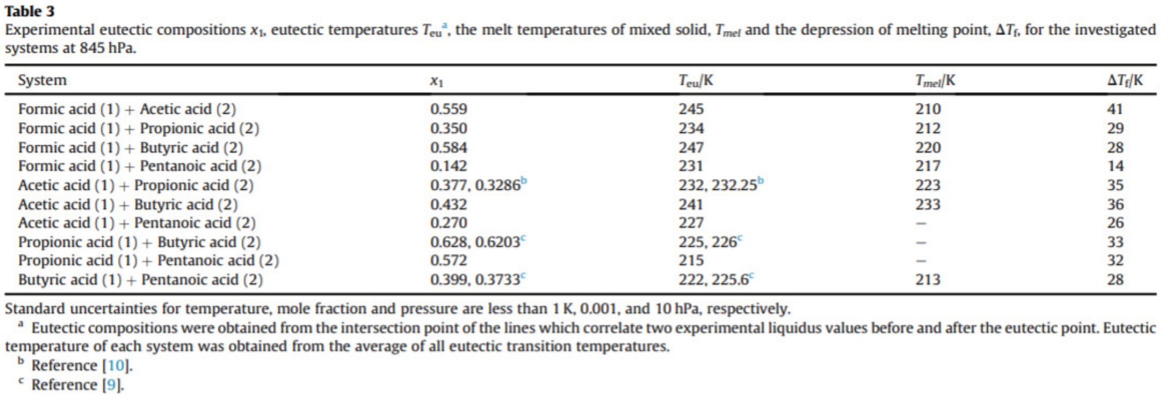


**Table 3**
Experimental eutectic compositions $x_1$, eutectic temperatures $T_{eu}$[a], the melt temperatures of mixed solid, $T_{mel}$ and the depression of melting point, $\Delta T_f$, for the investigated systems at 845 hPa.

| System | $x_1$ | $T_{eu}$/K | $T_{mel}$/K | $\Delta T_f$/K |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | 0.559 | 245 | 210 | 41 |
| Formic acid (1) + Propionic acid (2) | 0.350 | 234 | 212 | 29 |
| Formic acid (1) + Butyric acid (2) | 0.584 | 247 | 220 | 28 |
| Formic acid (1) + Pentanoic acid (2) | 0.142 | 231 | 217 | 14 |
| Acetic acid (1) + Propionic acid (2) | 0.377, 0.3286[b] | 232, 232.25[b] | 223 | 35 |
| Acetic acid (1) + Butyric acid (2) | 0.432 | 241 | 233 | 36 |
| Acetic acid (1) + Pentanoic acid (2) | 0.270 | 227 | – | 26 |
| Propionic acid (1) + Butyric acid (2) | 0.628, 0.6203[c] | 225, 226[c] | – | 33 |
| Propionic acid (1) + Pentanoic acid (2) | 0.572 | 215 | – | 32 |
| Butyric acid (1) + Pentanoic acid (2) | 0.399, 0.3733[c] | 222, 225.6[c] | 213 | 28 |

Standard uncertainties for temperature, mole fraction and pressure are less than 1 K, 0.001, and 10 hPa, respectively.

[a] Eutectic compositions were obtained from the intersection point of the lines which correlate two experimental liquidus values before and after the eutectic point. Eutectic temperature of each system was obtained from the average of all eutectic transition temperatures.

[b] Reference [10].

[c] Reference [9].

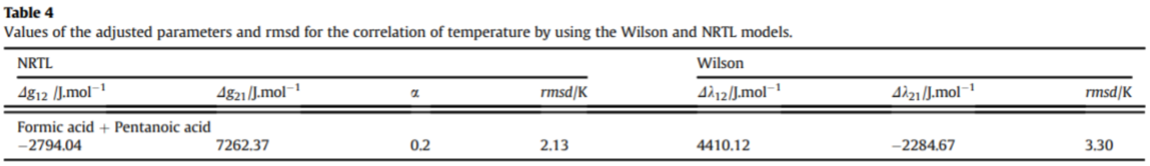


**Table 4**
Values of the adjusted parameters and rmsd for the correlation of temperature by using the Wilson and NRTL models.

| NRTL | | | | Wilson | | |
|---|---|---|---|---|---|---|
| $\Delta g_{12}$ /J.mol$^{-1}$ | $\Delta g_{21}$ /J.mol$^{-1}$ | $\alpha$ | *rmsd*/K | $\Delta\lambda_{12}$/J.mol$^{-1}$ | $\Delta\lambda_{21}$ /J.mol$^{-1}$ | *rmsd*/K |
| Formic acid + Pentanoic acid | | | | | | |
| −2794.04 | 7262.37 | 0.2 | 2.13 | 4410.12 | −2284.67 | 3.30 |

ODABRATI JEDAN MODEL!

butyric acid + pentanoic acid
Sajjad Noshadi, Rahmat Sadeghi, Differential scanning calorimetry determination of solid-liquid equilibria phase diagrams for binary monocarboxylic acids solutions, Fluid Phase Equilibria 486 (2019) 1-10

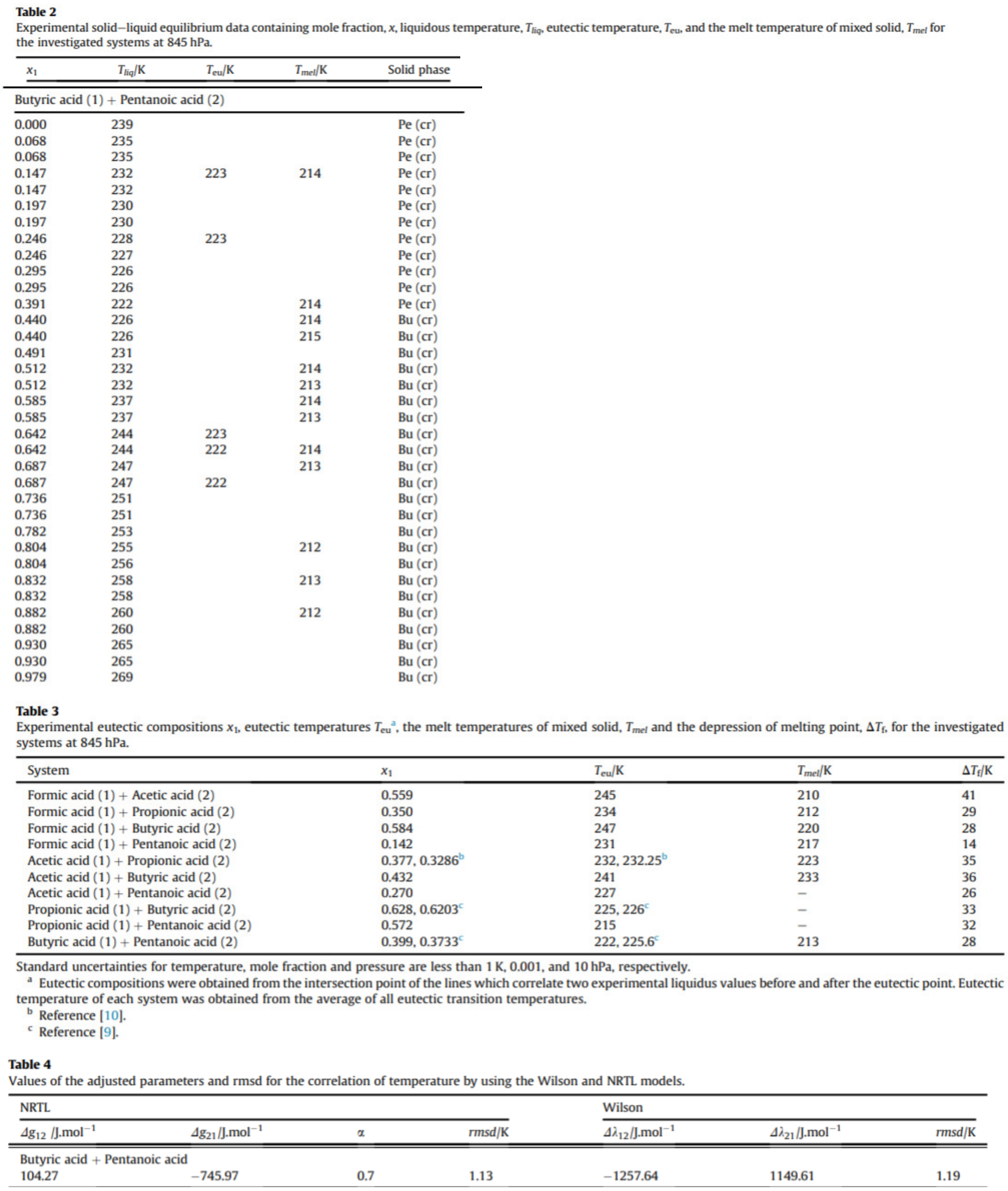


**Table 2**
Experimental solid–liquid equilibrium data containing mole fraction, $x$, liquidous temperature, $T_{liq}$, eutectic temperature, $T_{eu}$, and the melt temperature of mixed solid, $T_{mel}$ for the investigated systems at 845 hPa.

| $x_1$ | $T_{liq}$/K | $T_{eu}$/K | $T_{mel}$/K | Solid phase |
|---|---|---|---|---|
| Butyric acid (1) + Pentanoic acid (2) | | | | |
| 0.000 | 239 | | | Pe (cr) |
| 0.068 | 235 | | | Pe (cr) |
| 0.068 | 235 | | | Pe (cr) |
| 0.147 | 232 | 223 | 214 | Pe (cr) |
| 0.147 | 232 | | | Pe (cr) |
| 0.197 | 230 | | | Pe (cr) |
| 0.197 | 230 | | | Pe (cr) |
| 0.246 | 228 | 223 | | Pe (cr) |
| 0.246 | 227 | | | Pe (cr) |
| 0.295 | 226 | | | Pe (cr) |
| 0.295 | 226 | | | Pe (cr) |
| 0.391 | 222 | | 214 | Pe (cr) |
| 0.440 | 226 | | 214 | Bu (cr) |
| 0.440 | 226 | | 215 | Bu (cr) |
| 0.491 | 231 | | | Bu (cr) |
| 0.512 | 232 | | 214 | Bu (cr) |
| 0.512 | 232 | | 213 | Bu (cr) |
| 0.585 | 237 | | 214 | Bu (cr) |
| 0.585 | 237 | | 213 | Bu (cr) |
| 0.642 | 244 | 223 | | Bu (cr) |
| 0.642 | 244 | 222 | 214 | Bu (cr) |
| 0.687 | 247 | | 213 | Bu (cr) |
| 0.687 | 247 | 222 | | Bu (cr) |
| 0.736 | 251 | | | Bu (cr) |
| 0.736 | 251 | | | Bu (cr) |
| 0.782 | 253 | | | Bu (cr) |
| 0.804 | 255 | | 212 | Bu (cr) |
| 0.804 | 256 | | | Bu (cr) |
| 0.832 | 258 | | 213 | Bu (cr) |
| 0.832 | 258 | | | Bu (cr) |
| 0.882 | 260 | | 212 | Bu (cr) |
| 0.882 | 260 | | | Bu (cr) |
| 0.930 | 265 | | | Bu (cr) |
| 0.930 | 265 | | | Bu (cr) |
| 0.979 | 269 | | | Bu (cr) |

**Table 3**
Experimental eutectic compositions $x_1$, eutectic temperatures $T_{eu}$[a], the melt temperatures of mixed solid, $T_{mel}$ and the depression of melting point, $\Delta T_f$, for the investigated systems at 845 hPa.

| System | $x_1$ | $T_{eu}$/K | $T_{mel}$/K | $\Delta T_f$/K |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | 0.559 | 245 | 210 | 41 |
| Formic acid (1) + Propionic acid (2) | 0.350 | 234 | 212 | 29 |
| Formic acid (1) + Butyric acid (2) | 0.584 | 247 | 220 | 28 |
| Formic acid (1) + Pentanoic acid (2) | 0.142 | 231 | 217 | 14 |
| Acetic acid (1) + Propionic acid (2) | 0.377, 0.3286[b] | 232, 232.25[b] | 223 | 35 |
| Acetic acid (1) + Butyric acid (2) | 0.432 | 241 | 233 | 36 |
| Acetic acid (1) + Pentanoic acid (2) | 0.270 | 227 | – | 26 |
| Propionic acid (1) + Butyric acid (2) | 0.628, 0.6203[c] | 225, 226[c] | – | 33 |
| Propionic acid (1) + Pentanoic acid (2) | 0.572 | 215 | – | 32 |
| Butyric acid (1) + Pentanoic acid (2) | 0.399, 0.3733[c] | 222, 225.6[c] | 213 | 28 |

Standard uncertainties for temperature, mole fraction and pressure are less than 1 K, 0.001, and 10 hPa, respectively.

[a] Eutectic compositions were obtained from the intersection point of the lines which correlate two experimental liquidus values before and after the eutectic point. Eutectic temperature of each system was obtained from the average of all eutectic transition temperatures.

[b] Reference [10].

[c] Reference [9].

**Table 4**
Values of the adjusted parameters and rmsd for the correlation of temperature by using the Wilson and NRTL models.

| NRTL | | | | Wilson | | |
|---|---|---|---|---|---|---|
| $\Delta g_{12}$ /J.mol$^{-1}$ | $\Delta g_{21}$ /J.mol$^{-1}$ | $\alpha$ | rmsd/K | $\Delta\lambda_{12}$/J.mol$^{-1}$ | $\Delta\lambda_{21}$/J.mol$^{-1}$ | rmsd/K |
| Butyric acid + Pentanoic acid | | | | | | |
| 104.27 | −745.97 | 0.7 | 1.13 | −1257.64 | 1149.61 | 1.19 |

ODABRATI JEDAN MODEL!

butyric acid + propionic acid

Sajjad Noshadi, Rahmat Sadeghi, Differential scanning calorimetry determination of solid-liquid equilibria phase diagrams for binary monocarboxylic acids solutions, Fluid Phase Equilibria 486 (2019) 1-10

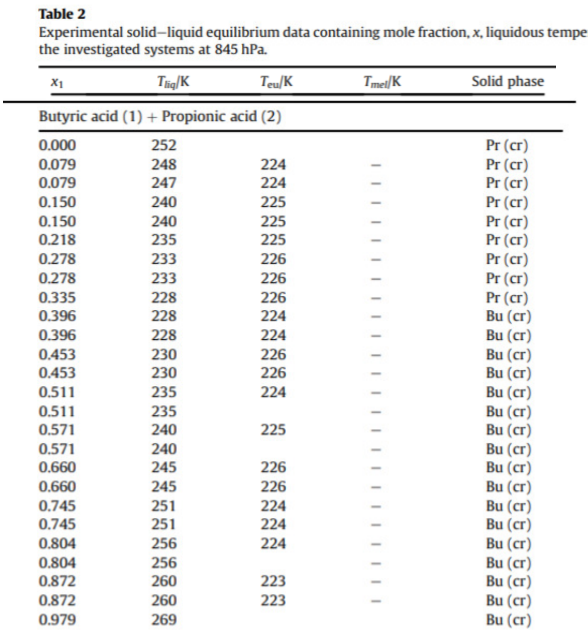


**Table 2**
Experimental solid–liquid equilibrium data containing mole fraction, $x$, liquidous temperature, $T_{liq}$, eutectic temperature, $T_{eu}$, and the melt temperature of mixed solid, $T_{mel}$ for the investigated systems at 845 hPa.

| $x_1$ | $T_{liq}$/K | $T_{eu}$/K | $T_{mel}$/K | Solid phase |
|---|---|---|---|---|
| Butyric acid (1) + Propionic acid (2) | | | | |
| 0.000 | 252 | | | Pr (cr) |
| 0.079 | 248 | 224 | – | Pr (cr) |
| 0.079 | 247 | 224 | – | Pr (cr) |
| 0.150 | 240 | 225 | – | Pr (cr) |
| 0.150 | 240 | 225 | – | Pr (cr) |
| 0.218 | 235 | 225 | – | Pr (cr) |
| 0.278 | 233 | 226 | – | Pr (cr) |
| 0.278 | 233 | 226 | – | Pr (cr) |
| 0.335 | 228 | 226 | – | Pr (cr) |
| 0.396 | 228 | 224 | – | Bu (cr) |
| 0.396 | 228 | 224 | – | Bu (cr) |
| 0.453 | 230 | 226 | – | Bu (cr) |
| 0.453 | 230 | 226 | – | Bu (cr) |
| 0.511 | 235 | 224 | – | Bu (cr) |
| 0.511 | 235 | | – | Bu (cr) |
| 0.571 | 240 | 225 | – | Bu (cr) |
| 0.571 | 240 | | – | Bu (cr) |
| 0.660 | 245 | 226 | – | Bu (cr) |
| 0.660 | 245 | 226 | – | Bu (cr) |
| 0.745 | 251 | 224 | – | Bu (cr) |
| 0.745 | 251 | 224 | – | Bu (cr) |
| 0.804 | 256 | 224 | – | Bu (cr) |
| 0.804 | 256 | | – | Bu (cr) |
| 0.872 | 260 | 223 | – | Bu (cr) |
| 0.872 | 260 | 223 | – | Bu (cr) |
| 0.979 | 269 | | | Bu (cr) |

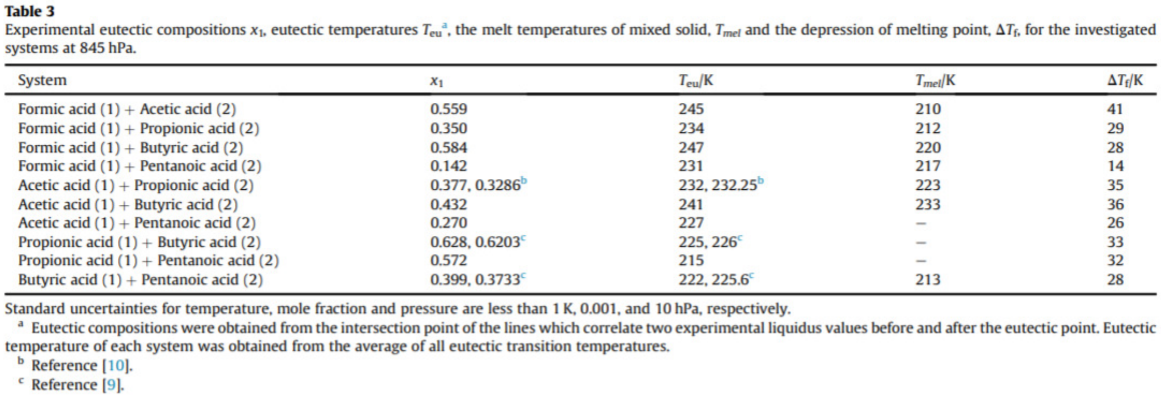


**Table 3**
Experimental eutectic compositions $x_1$, eutectic temperatures $T_{eu}$[a], the melt temperatures of mixed solid, $T_{mel}$ and the depression of melting point, $\Delta T_f$, for the investigated systems at 845 hPa.

| System | $x_1$ | $T_{eu}$/K | $T_{mel}$/K | $\Delta T_f$/K |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | 0.559 | 245 | 210 | 41 |
| Formic acid (1) + Propionic acid (2) | 0.350 | 234 | 212 | 29 |
| Formic acid (1) + Butyric acid (2) | 0.584 | 247 | 220 | 28 |
| Formic acid (1) + Pentanoic acid (2) | 0.142 | 231 | 217 | 14 |
| Acetic acid (1) + Propionic acid (2) | 0.377, 0.3286[b] | 232, 232.25[b] | 223 | 35 |
| Acetic acid (1) + Butyric acid (2) | 0.432 | 241 | 233 | 36 |
| Acetic acid (1) + Pentanoic acid (2) | 0.270 | 227 | – | 26 |
| Propionic acid (1) + Butyric acid (2) | 0.628, 0.6203[c] | 225, 226[c] | – | 33 |
| Propionic acid (1) + Pentanoic acid (2) | 0.572 | 215 | – | 32 |
| Butyric acid (1) + Pentanoic acid (2) | 0.399, 0.3733[c] | 222, 225.6[c] | 213 | 28 |

Standard uncertainties for temperature, mole fraction and pressure are less than 1 K, 0.001, and 10 hPa, respectively.

[a] Eutectic compositions were obtained from the intersection point of the lines which correlate two experimental liquidus values before and after the eutectic point. Eutectic temperature of each system was obtained from the average of all eutectic transition temperatures.

[b] Reference [10].

[c] Reference [9].

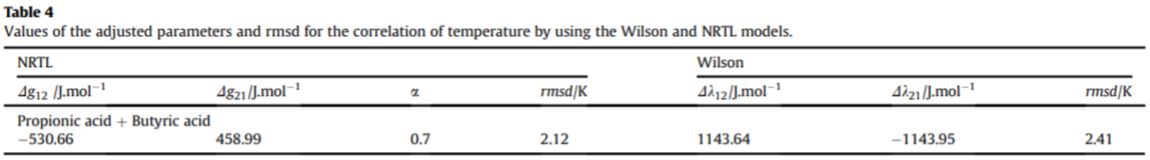


**Table 4**
Values of the adjusted parameters and rmsd for the correlation of temperature by using the Wilson and NRTL models.

| NRTL | | | | Wilson | | |
|---|---|---|---|---|---|---|
| $\Delta g_{12}$ /J.mol$^{-1}$ | $\Delta g_{21}$ /J.mol$^{-1}$ | $\alpha$ | rmsd/K | $\Delta\lambda_{12}$/J.mol$^{-1}$ | $\Delta\lambda_{21}$ /J.mol$^{-1}$ | rmsd/K |
| Propionic acid + Butyric acid | | | | | | |
| −530.66 | 458.99 | 0.7 | 2.12 | 1143.64 | −1143.95 | 2.41 |

ODABRATI JEDAN MODEL!

propionic acid + pentanoic acid

Sajjad Noshadi, Rahmat Sadeghi, Differential scanning calorimetry determination of solid-liquid equilibria phase diagrams for binary monocarboxylic acids solutions, Fluid Phase Equilibria 486 (2019) 1-10

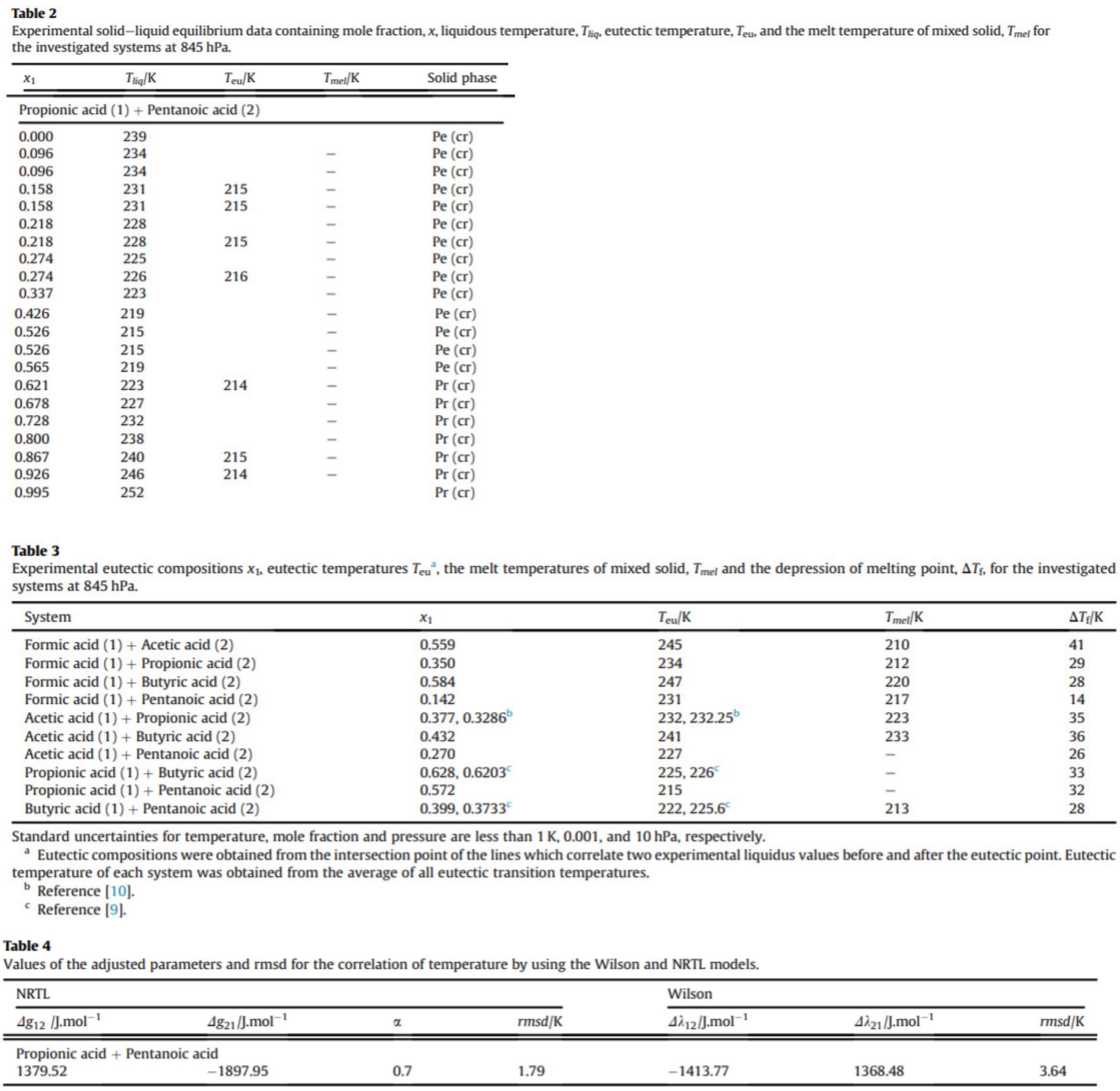


**Table 2**

Experimental solid–liquid equilibrium data containing mole fraction, $x$, liquidous temperature, $T_{liq}$, eutectic temperature, $T_{eu}$, and the melt temperature of mixed solid, $T_{mel}$ for the investigated systems at 845 hPa.

| $x_1$ | $T_{liq}$/K | $T_{eu}$/K | $T_{mel}$/K | Solid phase |
|---|---|---|---|---|
| Propionic acid (1) + Pentanoic acid (2) | | | | |
| 0.000 | 239 | | | Pe (cr) |
| 0.096 | 234 | | – | Pe (cr) |
| 0.096 | 234 | | – | Pe (cr) |
| 0.158 | 231 | 215 | – | Pe (cr) |
| 0.158 | 231 | 215 | – | Pe (cr) |
| 0.218 | 228 | | – | Pe (cr) |
| 0.218 | 228 | 215 | – | Pe (cr) |
| 0.274 | 225 | | – | Pe (cr) |
| 0.274 | 226 | 216 | – | Pe (cr) |
| 0.337 | 223 | | – | Pe (cr) |
| 0.426 | 219 | | – | Pe (cr) |
| 0.526 | 215 | | – | Pe (cr) |
| 0.526 | 215 | | – | Pe (cr) |
| 0.565 | 219 | | – | Pe (cr) |
| 0.621 | 223 | 214 | – | Pr (cr) |
| 0.678 | 227 | | – | Pr (cr) |
| 0.728 | 232 | | – | Pr (cr) |
| 0.800 | 238 | | – | Pr (cr) |
| 0.867 | 240 | 215 | – | Pr (cr) |
| 0.926 | 246 | 214 | – | Pr (cr) |
| 0.995 | 252 | | | Pr (cr) |

**Table 3**

Experimental eutectic compositions $x_1$, eutectic temperatures $T_{eu}$[a], the melt temperatures of mixed solid, $T_{mel}$ and the depression of melting point, $\Delta T_f$, for the investigated systems at 845 hPa.

| System | $x_1$ | $T_{eu}$/K | $T_{mel}$/K | $\Delta T_f$/K |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | 0.559 | 245 | 210 | 41 |
| Formic acid (1) + Propionic acid (2) | 0.350 | 234 | 212 | 29 |
| Formic acid (1) + Butyric acid (2) | 0.584 | 247 | 220 | 28 |
| Formic acid (1) + Pentanoic acid (2) | 0.142 | 231 | 217 | 14 |
| Acetic acid (1) + Propionic acid (2) | 0.377, 0.3286[b] | 232, 232.25[b] | 223 | 35 |
| Acetic acid (1) + Butyric acid (2) | 0.432 | 241 | 233 | 36 |
| Acetic acid (1) + Pentanoic acid (2) | 0.270 | 227 | – | 26 |
| Propionic acid (1) + Butyric acid (2) | 0.628, 0.6203[c] | 225, 226[c] | – | 33 |
| Propionic acid (1) + Pentanoic acid (2) | 0.572 | 215 | – | 32 |
| Butyric acid (1) + Pentanoic acid (2) | 0.399, 0.3733[c] | 222, 225.6[c] | 213 | 28 |

Standard uncertainties for temperature, mole fraction and pressure are less than 1 K, 0.001, and 10 hPa, respectively.

[a] Eutectic compositions were obtained from the intersection point of the lines which correlate two experimental liquidus values before and after the eutectic point. Eutectic temperature of each system was obtained from the average of all eutectic transition temperatures.

[b] Reference [10].

[c] Reference [9].

**Table 4**

Values of the adjusted parameters and rmsd for the correlation of temperature by using the Wilson and NRTL models.

| NRTL | | | | Wilson | | |
|---|---|---|---|---|---|---|
| $\Delta g_{12}$ /J.mol$^{-1}$ | $\Delta g_{21}$ /J.mol$^{-1}$ | $\alpha$ | rmsd/K | $\Delta\lambda_{12}$ /J.mol$^{-1}$ | $\Delta\lambda_{21}$ /J.mol$^{-1}$ | rmsd/K |
| Propionic acid + Pentanoic acid | | | | | | |
| 1379.52 | −1897.95 | 0.7 | 1.79 | −1413.77 | 1368.48 | 3.64 |

ODABRATI JEDAN MODEL!

acetic acid + pentanoic acid

Sajjad Noshadi, Rahmat Sadeghi, Differential scanning calorimetry determination of solid-liquid equilibria phase diagrams for binary monocarboxylic acids solutions, Fluid Phase Equilibria 486 (2019) 1-10

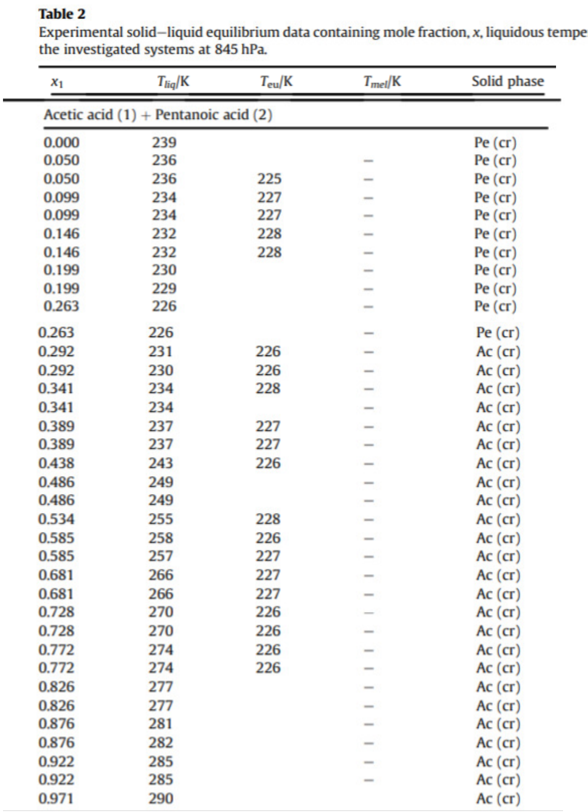


**Table 2**

Experimental solid–liquid equilibrium data containing mole fraction, *x*, liquidous temperature, $T_{liq}$, eutectic temperature, $T_{eu}$, and the melt temperature of mixed solid, $T_{mel}$ for the investigated systems at 845 hPa.

| $x_1$ | $T_{liq}$/K | $T_{eu}$/K | $T_{mel}$/K | Solid phase |
|---|---|---|---|---|
| Acetic acid (1) + Pentanoic acid (2) | | | | |
| 0.000 | 239 | | | Pe (cr) |
| 0.050 | 236 | | – | Pe (cr) |
| 0.050 | 236 | 225 | – | Pe (cr) |
| 0.099 | 234 | 227 | – | Pe (cr) |
| 0.099 | 234 | 227 | – | Pe (cr) |
| 0.146 | 232 | 228 | – | Pe (cr) |
| 0.146 | 232 | 228 | – | Pe (cr) |
| 0.199 | 230 | | – | Pe (cr) |
| 0.199 | 229 | | – | Pe (cr) |
| 0.263 | 226 | | – | Pe (cr) |
| 0.263 | 226 | | – | Pe (cr) |
| 0.292 | 231 | 226 | – | Ac (cr) |
| 0.292 | 230 | 226 | – | Ac (cr) |
| 0.341 | 234 | 228 | – | Ac (cr) |
| 0.341 | 234 | | – | Ac (cr) |
| 0.389 | 237 | 227 | – | Ac (cr) |
| 0.389 | 237 | 227 | – | Ac (cr) |
| 0.438 | 243 | 226 | – | Ac (cr) |
| 0.486 | 249 | | – | Ac (cr) |
| 0.486 | 249 | | – | Ac (cr) |
| 0.534 | 255 | 228 | – | Ac (cr) |
| 0.585 | 258 | 226 | – | Ac (cr) |
| 0.585 | 257 | 227 | – | Ac (cr) |
| 0.681 | 266 | 227 | – | Ac (cr) |
| 0.681 | 266 | 227 | – | Ac (cr) |
| 0.728 | 270 | 226 | – | Ac (cr) |
| 0.728 | 270 | 226 | – | Ac (cr) |
| 0.772 | 274 | 226 | – | Ac (cr) |
| 0.772 | 274 | 226 | – | Ac (cr) |
| 0.826 | 277 | | – | Ac (cr) |
| 0.826 | 277 | | – | Ac (cr) |
| 0.876 | 281 | | – | Ac (cr) |
| 0.876 | 282 | | – | Ac (cr) |
| 0.922 | 285 | | – | Ac (cr) |
| 0.922 | 285 | | – | Ac (cr) |
| 0.971 | 290 | | | Ac (cr) |

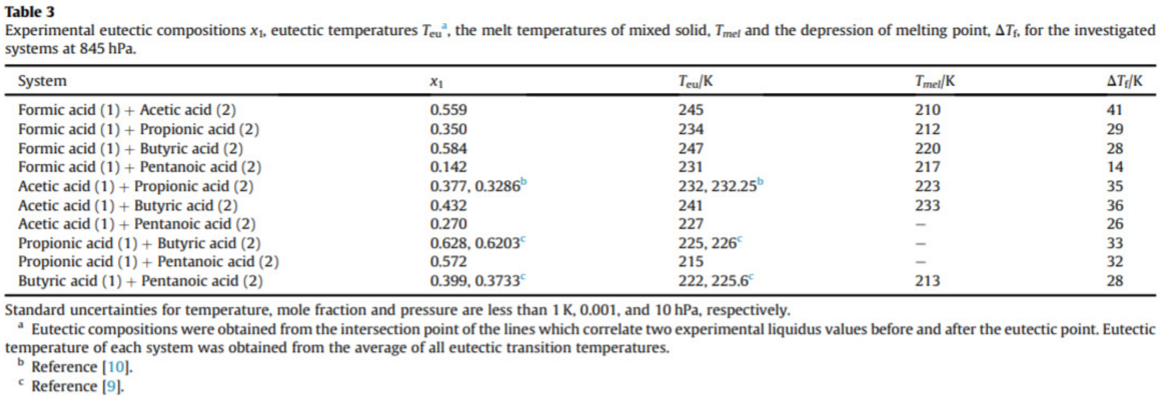


**Table 3**

Experimental eutectic compositions $x_1$, eutectic temperatures $T_{eu}$[a], the melt temperatures of mixed solid, $T_{mel}$ and the depression of melting point, $\Delta T_f$, for the investigated systems at 845 hPa.

| System | $x_1$ | $T_{eu}$/K | $T_{mel}$/K | $\Delta T_f$/K |
|---|---|---|---|---|
| Formic acid (1) + Acetic acid (2) | 0.559 | 245 | 210 | 41 |
| Formic acid (1) + Propionic acid (2) | 0.350 | 234 | 212 | 29 |
| Formic acid (1) + Butyric acid (2) | 0.584 | 247 | 220 | 28 |
| Formic acid (1) + Pentanoic acid (2) | 0.142 | 231 | 217 | 14 |
| Acetic acid (1) + Propionic acid (2) | 0.377, 0.3286[b] | 232, 232.25[b] | 223 | 35 |
| Acetic acid (1) + Butyric acid (2) | 0.432 | 241 | 233 | 36 |
| Acetic acid (1) + Pentanoic acid (2) | 0.270 | 227 | – | 26 |
| Propionic acid (1) + Butyric acid (2) | 0.628, 0.6203[c] | 225, 226[c] | – | 33 |
| Propionic acid (1) + Pentanoic acid (2) | 0.572 | 215 | – | 32 |
| Butyric acid (1) + Pentanoic acid (2) | 0.399, 0.3733[c] | 222, 225.6[c] | 213 | 28 |

Standard uncertainties for temperature, mole fraction and pressure are less than 1 K, 0.001, and 10 hPa, respectively.

[a] Eutectic compositions were obtained from the intersection point of the lines which correlate two experimental liquidus values before and after the eutectic point. Eutectic temperature of each system was obtained from the average of all eutectic transition temperatures.

[b] Reference [10].

[c] Reference [9].

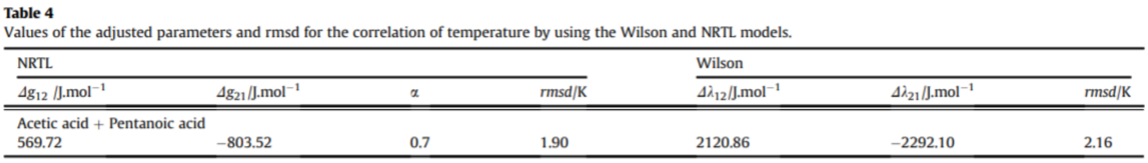


**Table 4**

Values of the adjusted parameters and rmsd for the correlation of temperature by using the Wilson and NRTL models.

| NRTL | | | | Wilson | | |
|---|---|---|---|---|---|---|
| $\Delta g_{12}$ /J.mol$^{-1}$ | $\Delta g_{21}$ /J.mol$^{-1}$ | $\alpha$ | *rmsd*/K | $\Delta\lambda_{12}$ /J.mol$^{-1}$ | $\Delta\lambda_{21}$ /J.mol$^{-1}$ | *rmsd*/K |
| Acetic acid + Pentanoic acid | | | | | | |
| 569.72 | −803.52 | 0.7 | 1.90 | 2120.86 | −2292.10 | 2.16 |

ODABRATI JEDAN MODEL!

naphthalene + phenanthrene
Kazuhiro Tamura, Tsuyoshi Kasuga, Tomoyuki Nakagawa, Phase behavior and solid-liquid equilibria of aliphatic and aromatic carboxylic acid mixtures, Fluid Phase Equilibria 420, 25 July 2016, Pages 24-29

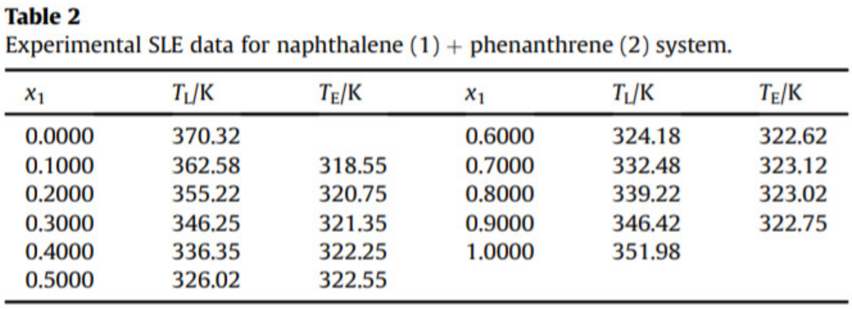


**Table 2**
Experimental SLE data for naphthalene (1) + phenanthrene (2) system.

| $x_1$ | $T_L$/K | $T_E$/K | $x_1$ | $T_L$/K | $T_E$/K |
|---|---|---|---|---|---|
| 0.0000 | 370.32 | | 0.6000 | 324.18 | 322.62 |
| 0.1000 | 362.58 | 318.55 | 0.7000 | 332.48 | 323.12 |
| 0.2000 | 355.22 | 320.75 | 0.8000 | 339.22 | 323.02 |
| 0.3000 | 346.25 | 321.35 | 0.9000 | 346.42 | 322.75 |
| 0.4000 | 336.35 | 322.25 | 1.0000 | 351.98 | |
| 0.5000 | 326.02 | 322.55 | | | |

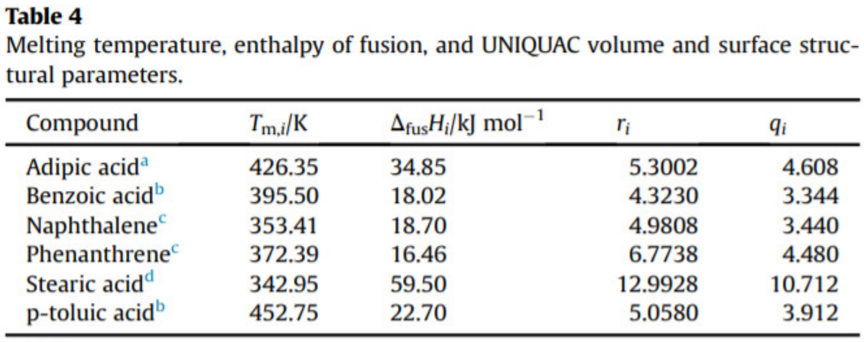


**Table 4**
Melting temperature, enthalpy of fusion, and UNIQUAC volume and surface structural parameters.

| Compound | $T_{m,i}$/K | $\Delta_{fus}H_i$/kJ mol$^{-1}$ | $r_i$ | $q_i$ |
|---|---|---|---|---|
| Adipic acid[a] | 426.35 | 34.85 | 5.3002 | 4.608 |
| Benzoic acid[b] | 395.50 | 18.02 | 4.3230 | 3.344 |
| Naphthalene[c] | 353.41 | 18.70 | 4.9808 | 3.440 |
| Phenanthrene[c] | 372.39 | 16.46 | 6.7738 | 4.480 |
| Stearic acid[d] | 342.95 | 59.50 | 12.9928 | 10.712 |
| p-toluic acid[b] | 452.75 | 22.70 | 5.0580 | 3.912 |

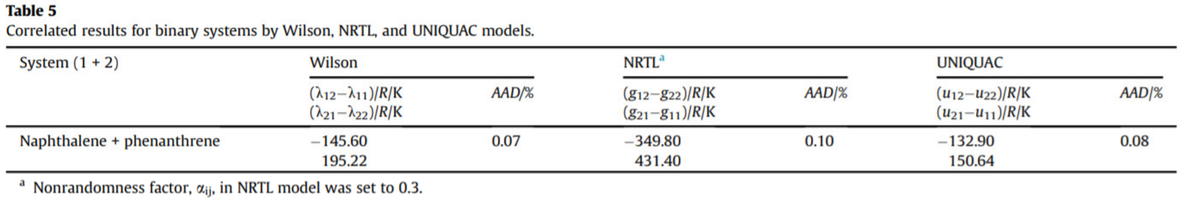


**Table 5**
Correlated results for binary systems by Wilson, NRTL, and UNIQUAC models.

| System (1 + 2) | Wilson | | NRTL[a] | | UNIQUAC | |
|---|---|---|---|---|---|---|
| | $(\lambda_{12}-\lambda_{11})/R$/K<br>$(\lambda_{21}-\lambda_{22})/R$/K | AAD/% | $(g_{12}-g_{22})/R$/K<br>$(g_{21}-g_{11})/R$/K | AAD/% | $(u_{12}-u_{22})/R$/K<br>$(u_{21}-u_{11})/R$/K | AAD/% |
| Naphthalene + phenanthrene | −145.60<br>195.22 | 0.07 | −349.80<br>431.40 | 0.10 | −132.90<br>150.64 | 0.08 |

[a] Nonrandomness factor, $\alpha_{ij}$, in NRTL model was set to 0.3.

ODABRATI JEDAN MODEL!

*p*-toluic acid + benzoic acid

Kazuhiro Tamura, Tsuyoshi Kasuga, Tomoyuki Nakagawa, Phase behavior and solid-liquid equilibria of aliphatic and aromatic carboxylic acid mixtures, Fluid Phase Equilibria 420, 25 July 2016, Pages 24-29

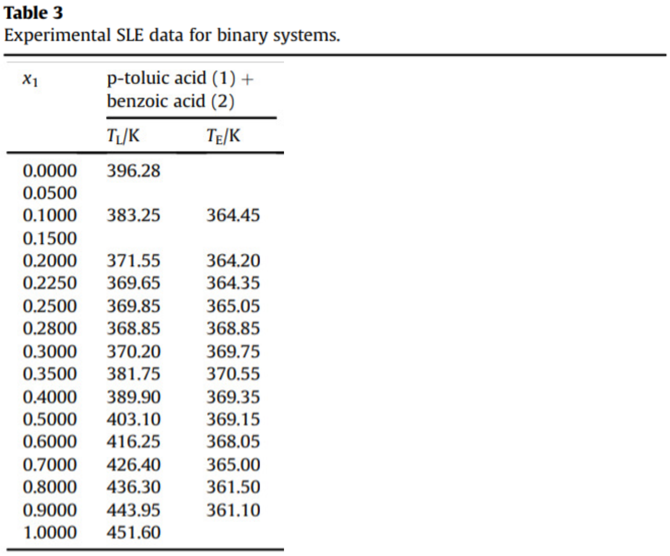


**Table 3**

Experimental SLE data for binary systems.

| $x_1$ | p-toluic acid (1) + benzoic acid (2) $T_L$/K | $T_E$/K |
|---|---|---|
| 0.0000 | 396.28 | |
| 0.0500 | | |
| 0.1000 | 383.25 | 364.45 |
| 0.1500 | | |
| 0.2000 | 371.55 | 364.20 |
| 0.2250 | 369.65 | 364.35 |
| 0.2500 | 369.85 | 365.05 |
| 0.2800 | 368.85 | 368.85 |
| 0.3000 | 370.20 | 369.75 |
| 0.3500 | 381.75 | 370.55 |
| 0.4000 | 389.90 | 369.35 |
| 0.5000 | 403.10 | 369.15 |
| 0.6000 | 416.25 | 368.05 |
| 0.7000 | 426.40 | 365.00 |
| 0.8000 | 436.30 | 361.50 |
| 0.9000 | 443.95 | 361.10 |
| 1.0000 | 451.60 | |

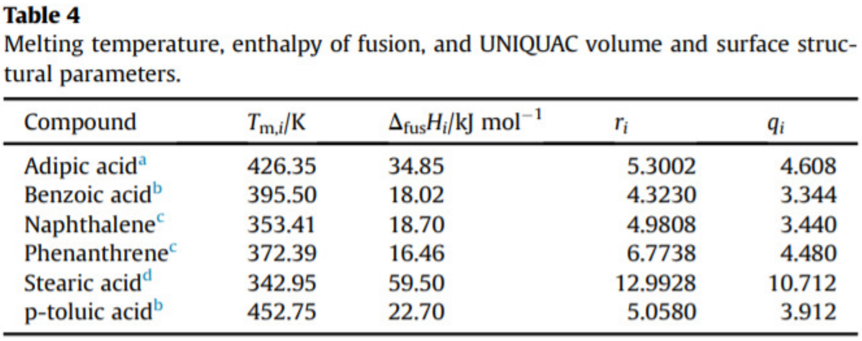


**Table 4**

Melting temperature, enthalpy of fusion, and UNIQUAC volume and surface structural parameters.

| Compound | $T_{m,i}$/K | $\Delta_{fus}H_i$/kJ mol$^{-1}$ | $r_i$ | $q_i$ |
|---|---|---|---|---|
| Adipic acid[a] | 426.35 | 34.85 | 5.3002 | 4.608 |
| Benzoic acid[b] | 395.50 | 18.02 | 4.3230 | 3.344 |
| Naphthalene[c] | 353.41 | 18.70 | 4.9808 | 3.440 |
| Phenanthrene[c] | 372.39 | 16.46 | 6.7738 | 4.480 |
| Stearic acid[d] | 342.95 | 59.50 | 12.9928 | 10.712 |
| p-toluic acid[b] | 452.75 | 22.70 | 5.0580 | 3.912 |

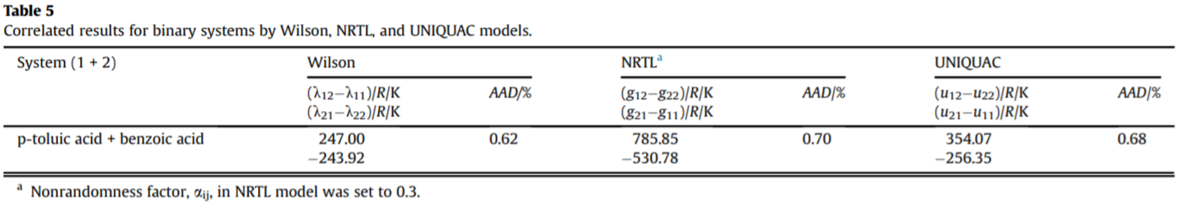


**Table 5**

Correlated results for binary systems by Wilson, NRTL, and UNIQUAC models.

| System (1 + 2) | Wilson $(\lambda_{12}-\lambda_{11})/R$/K<br>$(\lambda_{21}-\lambda_{22})/R$/K | Wilson AAD/% | NRTL[a] $(g_{12}-g_{22})/R$/K<br>$(g_{21}-g_{11})/R$/K | NRTL[a] AAD/% | UNIQUAC $(u_{12}-u_{22})/R$/K<br>$(u_{21}-u_{11})/R$/K | UNIQUAC AAD/% |
|---|---|---|---|---|---|---|
| p-toluic acid + benzoic acid | 247.00<br>−243.92 | 0.62 | 785.85<br>−530.78 | 0.70 | 354.07<br>−256.35 | 0.68 |

[a] Nonrandomness factor, $\alpha_{ij}$, in NRTL model was set to 0.3.

ODABRATI JEDAN MODEL!

adipic acid + benzoic acid

Kazuhiro Tamura, Tsuyoshi Kasuga, Tomoyuki Nakagawa, Phase behavior and solid-liquid equilibria of aliphatic and aromatic carboxylic acid mixtures, Fluid Phase Equilibria 420, 25 July 2016, Pages 24-29

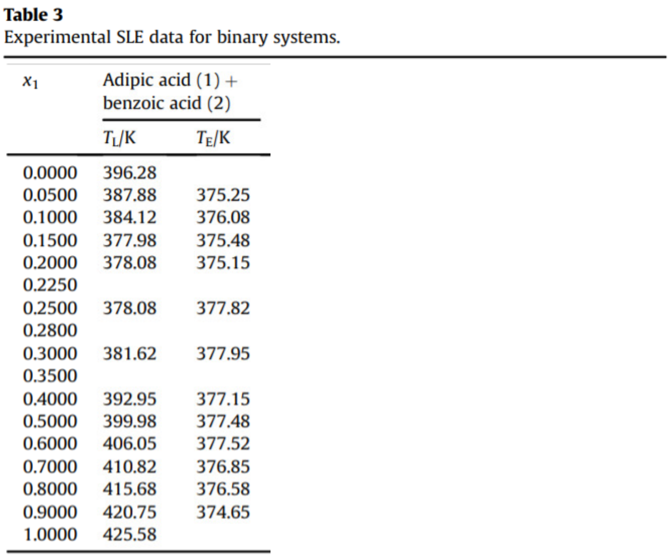


**Table 3**
Experimental SLE data for binary systems.

| $x_1$ | Adipic acid (1) + benzoic acid (2) | |
|---|---|---|
| | $T_L$/K | $T_E$/K |
| 0.0000 | 396.28 | |
| 0.0500 | 387.88 | 375.25 |
| 0.1000 | 384.12 | 376.08 |
| 0.1500 | 377.98 | 375.48 |
| 0.2000 | 378.08 | 375.15 |
| 0.2250 | | |
| 0.2500 | 378.08 | 377.82 |
| 0.2800 | | |
| 0.3000 | 381.62 | 377.95 |
| 0.3500 | | |
| 0.4000 | 392.95 | 377.15 |
| 0.5000 | 399.98 | 377.48 |
| 0.6000 | 406.05 | 377.52 |
| 0.7000 | 410.82 | 376.85 |
| 0.8000 | 415.68 | 376.58 |
| 0.9000 | 420.75 | 374.65 |
| 1.0000 | 425.58 | |

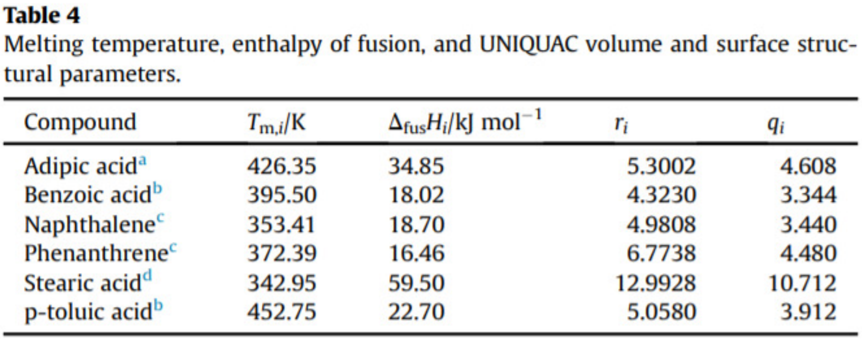


**Table 4**
Melting temperature, enthalpy of fusion, and UNIQUAC volume and surface structural parameters.

| Compound | $T_{m,i}$/K | $\Delta_{fus}H_i$/kJ mol$^{-1}$ | $r_i$ | $q_i$ |
|---|---|---|---|---|
| Adipic acid[a] | 426.35 | 34.85 | 5.3002 | 4.608 |
| Benzoic acid[b] | 395.50 | 18.02 | 4.3230 | 3.344 |
| Naphthalene[c] | 353.41 | 18.70 | 4.9808 | 3.440 |
| Phenanthrene[c] | 372.39 | 16.46 | 6.7738 | 4.480 |
| Stearic acid[d] | 342.95 | 59.50 | 12.9928 | 10.712 |
| p-toluic acid[b] | 452.75 | 22.70 | 5.0580 | 3.912 |

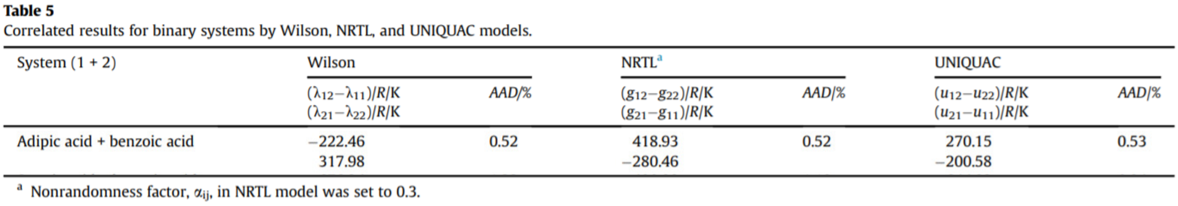


**Table 5**
Correlated results for binary systems by Wilson, NRTL, and UNIQUAC models.

| System (1 + 2) | Wilson | | NRTL[a] | | UNIQUAC | |
|---|---|---|---|---|---|---|
| | $(\lambda_{12}-\lambda_{11})/R$/K<br>$(\lambda_{21}-\lambda_{22})/R$/K | AAD/% | $(g_{12}-g_{22})/R$/K<br>$(g_{21}-g_{11})/R$/K | AAD/% | $(u_{12}-u_{22})/R$/K<br>$(u_{21}-u_{11})/R$/K | AAD/% |
| Adipic acid + benzoic acid | −222.46<br>317.98 | 0.52 | 418.93<br>−280.46 | 0.52 | 270.15<br>−200.58 | 0.53 |

[a] Nonrandomness factor, $\alpha_{ij}$, in NRTL model was set to 0.3.

ODABRATI JEDAN MODEL!

stearic acid + benzoic acid

Kazuhiro Tamura, Tsuyoshi Kasuga, Tomoyuki Nakagawa, Phase behavior and solid-liquid equilibria of aliphatic and aromatic carboxylic acid mixtures, Fluid Phase Equilibria 420, 25 July 2016, Pages 24-29

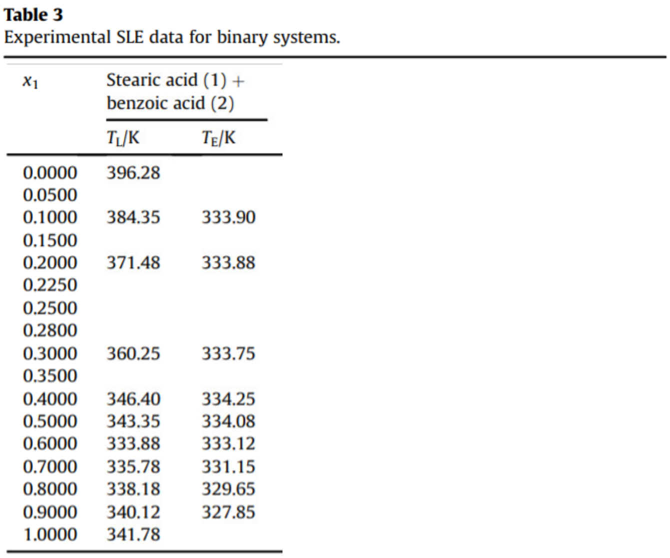


**Table 3**
Experimental SLE data for binary systems.

| $x_1$ | Stearic acid (1) + benzoic acid (2) | |
|---|---|---|
| | $T_L$/K | $T_E$/K |
| 0.0000 | 396.28 | |
| 0.0500 | | |
| 0.1000 | 384.35 | 333.90 |
| 0.1500 | | |
| 0.2000 | 371.48 | 333.88 |
| 0.2250 | | |
| 0.2500 | | |
| 0.2800 | | |
| 0.3000 | 360.25 | 333.75 |
| 0.3500 | | |
| 0.4000 | 346.40 | 334.25 |
| 0.5000 | 343.35 | 334.08 |
| 0.6000 | 333.88 | 333.12 |
| 0.7000 | 335.78 | 331.15 |
| 0.8000 | 338.18 | 329.65 |
| 0.9000 | 340.12 | 327.85 |
| 1.0000 | 341.78 | |

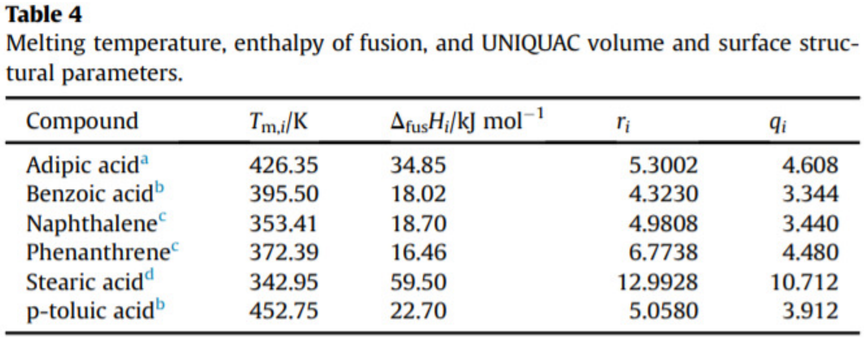


**Table 4**
Melting temperature, enthalpy of fusion, and UNIQUAC volume and surface structural parameters.

| Compound | $T_{m,i}$/K | $\Delta_{fus}H_i$/kJ mol$^{-1}$ | $r_i$ | $q_i$ |
|---|---|---|---|---|
| Adipic acid[a] | 426.35 | 34.85 | 5.3002 | 4.608 |
| Benzoic acid[b] | 395.50 | 18.02 | 4.3230 | 3.344 |
| Naphthalene[c] | 353.41 | 18.70 | 4.9808 | 3.440 |
| Phenanthrene[c] | 372.39 | 16.46 | 6.7738 | 4.480 |
| Stearic acid[d] | 342.95 | 59.50 | 12.9928 | 10.712 |
| p-toluic acid[b] | 452.75 | 22.70 | 5.0580 | 3.912 |

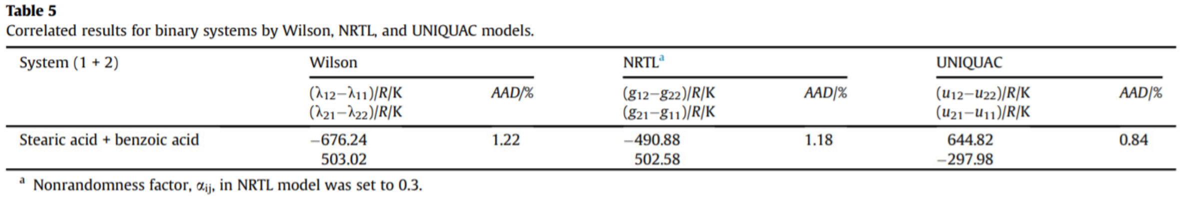


**Table 5**
Correlated results for binary systems by Wilson, NRTL, and UNIQUAC models.

| System (1 + 2) | Wilson | | NRTL[a] | | UNIQUAC | |
|---|---|---|---|---|---|---|
| | $(\lambda_{12}-\lambda_{11})/R$/K<br>$(\lambda_{21}-\lambda_{22})/R$/K | AAD/% | $(g_{12}-g_{22})/R$/K<br>$(g_{21}-g_{11})/R$/K | AAD/% | $(u_{12}-u_{22})/R$/K<br>$(u_{21}-u_{11})/R$/K | AAD/% |
| Stearic acid + benzoic acid | −676.24<br>503.02 | 1.22 | −490.88<br>502.58 | 1.18 | 644.82<br>−297.98 | 0.84 |

[a] Nonrandomness factor, $\alpha_{ij}$, in NRTL model was set to 0.3.

ODABRATI JEDAN MODEL!

$N_2O$ + Pentafluoroethane
Cheonkyu Lee, Junghyun Yoo, Jisung Lee, Sangkwon Jeong, Visualization of the solid-liquid equilibria for non-flammable mixed refrigerants, Cryogenics, Volume 75, April 2016, Pages 26-34

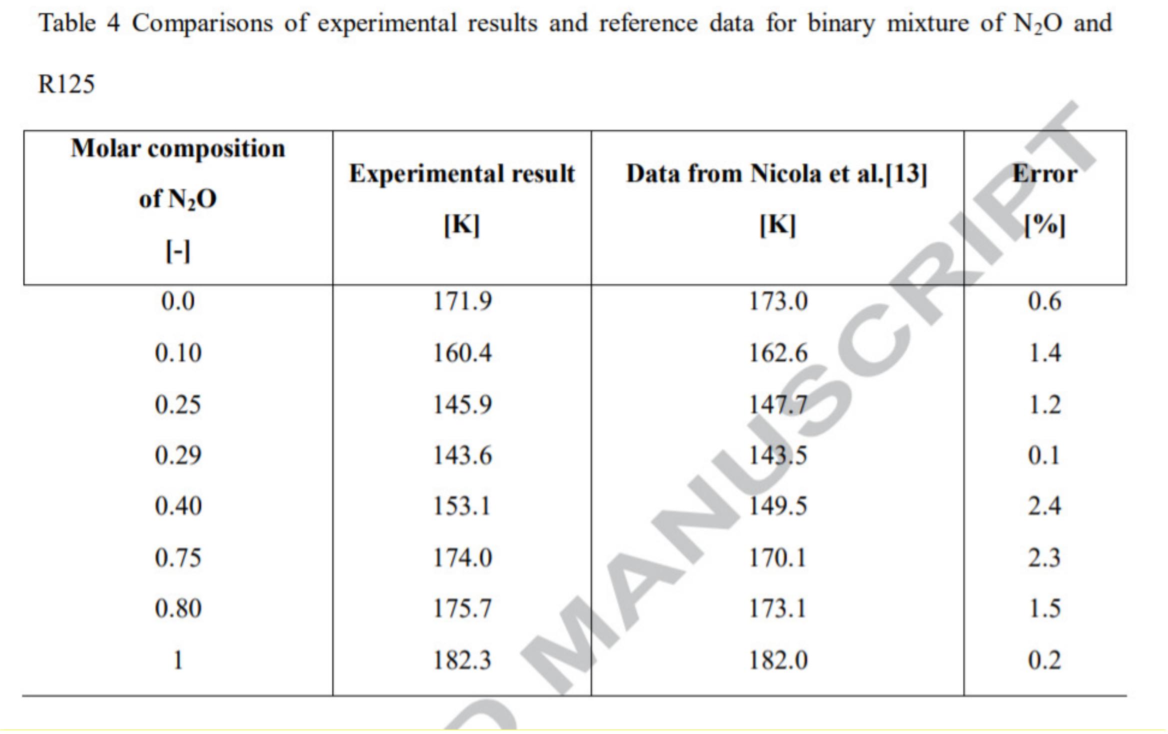


Table 4 Comparisons of experimental results and reference data for binary mixture of $N_2O$ and R125

| **Molar composition of $N_2O$ [-]** | **Experimental result [K]** | **Data from Nicola et al.[13] [K]** | **Error [%]** |
|---|---|---|---|
| 0.0 | 171.9 | 173.0 | 0.6 |
| 0.10 | 160.4 | 162.6 | 1.4 |
| 0.25 | 145.9 | 147.7 | 1.2 |
| 0.29 | 143.6 | 143.5 | 0.1 |
| 0.40 | 153.1 | 149.5 | 2.4 |
| 0.75 | 174.0 | 170.1 | 2.3 |
| 0.80 | 175.7 | 173.1 | 1.5 |
| 1 | 182.3 | 182.0 | 0.2 |

dimethyl carbonate + diphenyl carbonate
Hiroyuki Matsuda, Yuki Ohashi, Kiyofumi Kurihara, Katsumi Tochigi, Kenji Ochi, Solid–liquid equilibria for selected binary systems containing diphenyl carbonate, Fluid Phase Equilibria, Volume 479, 15 January 2019, Pages 17-24

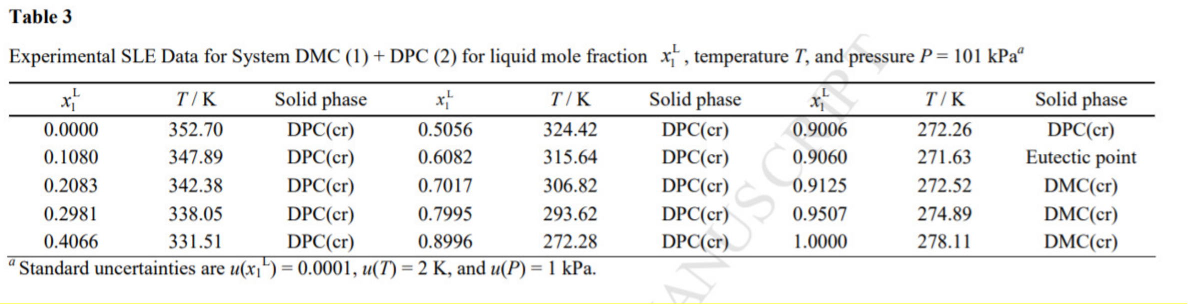


**Table 3**

Experimental SLE Data for System DMC (1) + DPC (2) for liquid mole fraction $x_1^L$, temperature $T$, and pressure $P = 101$ kPa[a]

| $x_1^L$ | $T$ / K | Solid phase | $x_1^L$ | $T$ / K | Solid phase | $x_1^L$ | $T$ / K | Solid phase |
|---|---|---|---|---|---|---|---|---|
| 0.0000 | 352.70 | DPC(cr) | 0.5056 | 324.42 | DPC(cr) | 0.9006 | 272.26 | DPC(cr) |
| 0.1080 | 347.89 | DPC(cr) | 0.6082 | 315.64 | DPC(cr) | 0.9060 | 271.63 | Eutectic point |
| 0.2083 | 342.38 | DPC(cr) | 0.7017 | 306.82 | DPC(cr) | 0.9125 | 272.52 | DMC(cr) |
| 0.2981 | 338.05 | DPC(cr) | 0.7995 | 293.62 | DPC(cr) | 0.9507 | 274.89 | DMC(cr) |
| 0.4066 | 331.51 | DPC(cr) | 0.8996 | 272.28 | DPC(cr) | 1.0000 | 278.11 | DMC(cr) |

[a] Standard uncertainties are $u(x_1^L) = 0.0001$, $u(T) = 2$ K, and $u(P) = 1$ kPa.

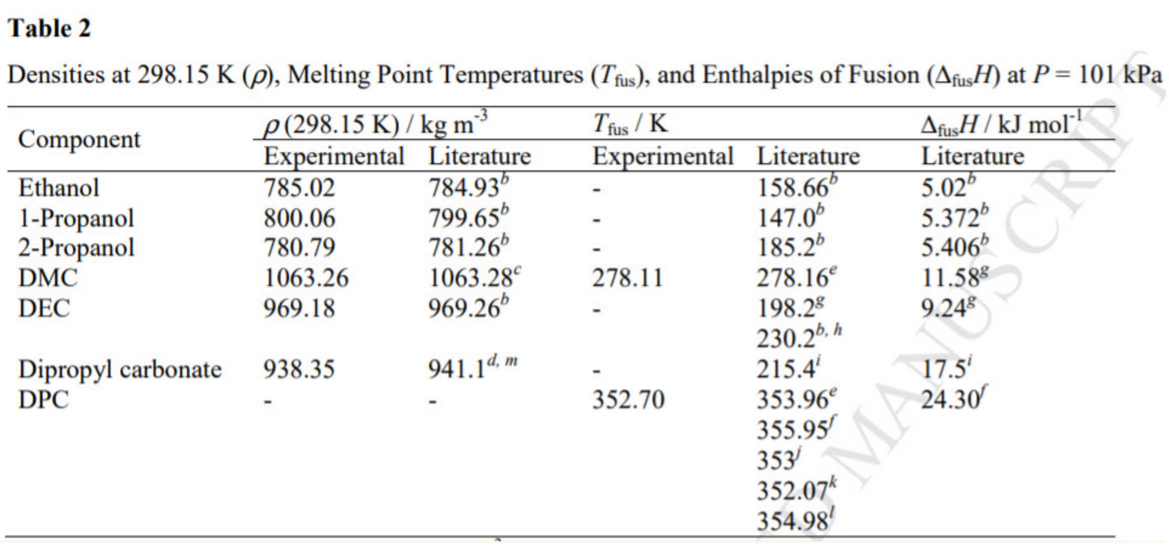


**Table 2**

Densities at 298.15 K ($\rho$), Melting Point Temperatures ($T_{fus}$), and Enthalpies of Fusion ($\Delta_{fus}H$) at $P = 101$ kPa

| Component | $\rho$ (298.15 K) / kg m$^{-3}$ | | $T_{fus}$ / K | | $\Delta_{fus}H$ / kJ mol$^{-1}$ |
|---|---|---|---|---|---|
| | Experimental | Literature | Experimental | Literature | Literature |
| Ethanol | 785.02 | 784.93[b] | - | 158.66[b] | 5.02[b] |
| 1-Propanol | 800.06 | 799.65[b] | - | 147.0[b] | 5.372[b] |
| 2-Propanol | 780.79 | 781.26[b] | - | 185.2[b] | 5.406[b] |
| DMC | 1063.26 | 1063.28[c] | 278.11 | 278.16[e] | 11.58[g] |
| DEC | 969.18 | 969.26[b] | - | 198.2[g]<br>230.2[b, h] | 9.24[g] |
| Dipropyl carbonate | 938.35 | 941.1[d, m] | - | 215.4[i] | 17.5[i] |
| DPC | - | - | 352.70 | 353.96[e]<br>355.95[f]<br>353[j]<br>352.07[k]<br>354.98[l] | 24.30[f] |

ethanol + diphenyl carbonate

Hiroyuki Matsuda, Yuki Ohashi, Kiyofumi Kurihara, Katsumi Tochigi, Kenji Ochi, Solid–liquid equilibria for selected binary systems containing diphenyl carbonate, Fluid Phase Equilibria, Volume 479, 15 January 2019, Pages 17-24

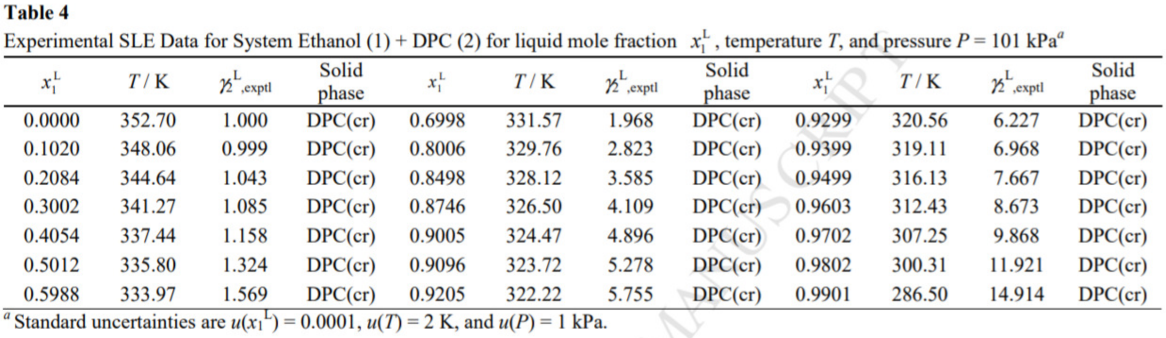


**Table 4**

Experimental SLE Data for System Ethanol (1) + DPC (2) for liquid mole fraction $x_1^L$, temperature $T$, and pressure $P$ = 101 kPa[a]

| $x_1^L$ | $T$ / K | $\gamma_2^L$,exptl | Solid phase | $x_1^L$ | $T$ / K | $\gamma_2^L$,exptl | Solid phase | $x_1^L$ | $T$ / K | $\gamma_2^L$,exptl | Solid phase |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.0000 | 352.70 | 1.000 | DPC(cr) | 0.6998 | 331.57 | 1.968 | DPC(cr) | 0.9299 | 320.56 | 6.227 | DPC(cr) |
| 0.1020 | 348.06 | 0.999 | DPC(cr) | 0.8006 | 329.76 | 2.823 | DPC(cr) | 0.9399 | 319.11 | 6.968 | DPC(cr) |
| 0.2084 | 344.64 | 1.043 | DPC(cr) | 0.8498 | 328.12 | 3.585 | DPC(cr) | 0.9499 | 316.13 | 7.667 | DPC(cr) |
| 0.3002 | 341.27 | 1.085 | DPC(cr) | 0.8746 | 326.50 | 4.109 | DPC(cr) | 0.9603 | 312.43 | 8.673 | DPC(cr) |
| 0.4054 | 337.44 | 1.158 | DPC(cr) | 0.9005 | 324.47 | 4.896 | DPC(cr) | 0.9702 | 307.25 | 9.868 | DPC(cr) |
| 0.5012 | 335.80 | 1.324 | DPC(cr) | 0.9096 | 323.72 | 5.278 | DPC(cr) | 0.9802 | 300.31 | 11.921 | DPC(cr) |
| 0.5988 | 333.97 | 1.569 | DPC(cr) | 0.9205 | 322.22 | 5.755 | DPC(cr) | 0.9901 | 286.50 | 14.914 | DPC(cr) |

[a] Standard uncertainties are $u(x_1^L)$ = 0.0001, $u(T)$ = 2 K, and $u(P)$ = 1 kPa.

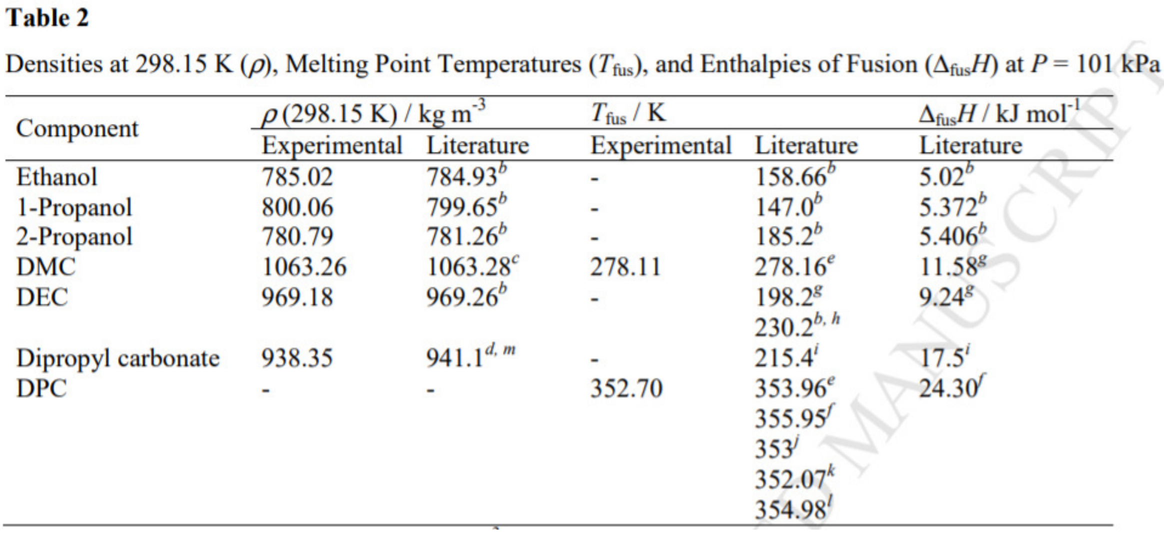


**Table 2**

Densities at 298.15 K ($\rho$), Melting Point Temperatures ($T_{fus}$), and Enthalpies of Fusion ($\Delta_{fus}H$) at $P$ = 101 kPa

| Component | $\rho$(298.15 K) / kg m$^{-3}$ |  | $T_{fus}$ / K |  | $\Delta_{fus}H$ / kJ mol$^{-1}$ |
|---|---|---|---|---|---|
|  | Experimental | Literature | Experimental | Literature | Literature |
| Ethanol | 785.02 | 784.93[b] | - | 158.66[b] | 5.02[b] |
| 1-Propanol | 800.06 | 799.65[b] | - | 147.0[b] | 5.372[b] |
| 2-Propanol | 780.79 | 781.26[b] | - | 185.2[b] | 5.406[b] |
| DMC | 1063.26 | 1063.28[c] | 278.11 | 278.16[e] | 11.58[g] |
| DEC | 969.18 | 969.26[b] | - | 198.2[g]<br>230.2[b, h] | 9.24[g] |
| Dipropyl carbonate | 938.35 | 941.1[d, m] | - | 215.4[i] | 17.5[i] |
| DPC | - | - | 352.70 | 353.96[e]<br>355.95[f]<br>353[j]<br>352.07[k]<br>354.98[l] | 24.30[f] |

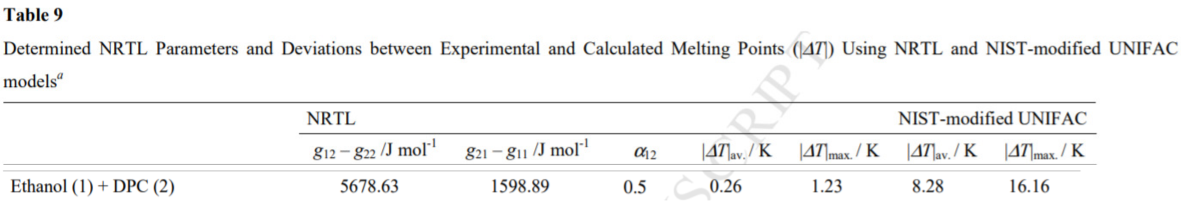


**Table 9**

Determined NRTL Parameters and Deviations between Experimental and Calculated Melting Points (|$\Delta T$|) Using NRTL and NIST-modified UNIFAC models[a]

|  | NRTL |  |  |  |  | NIST-modified UNIFAC |  |
|---|---|---|---|---|---|---|---|
|  | $g_{12} - g_{22}$ /J mol$^{-1}$ | $g_{21} - g_{11}$ /J mol$^{-1}$ | $\alpha_{12}$ | $\vert\Delta T\vert_{av.}$ / K | $\vert\Delta T\vert_{max.}$ / K | $\vert\Delta T\vert_{av.}$ / K | $\vert\Delta T\vert_{max.}$ / K |
| Ethanol (1) + DPC (2) | 5678.63 | 1598.89 | 0.5 | 0.26 | 1.23 | 8.28 | 16.16 |

1-propanol + diphenyl carbonate

Hiroyuki Matsuda, Yuki Ohashi, Kiyofumi Kurihara, Katsumi Tochigi, Kenji Ochi, Solid–liquid equilibria for selected binary systems containing diphenyl carbonate, Fluid Phase Equilibria, Volume 479, 15 January 2019, Pages 17-24

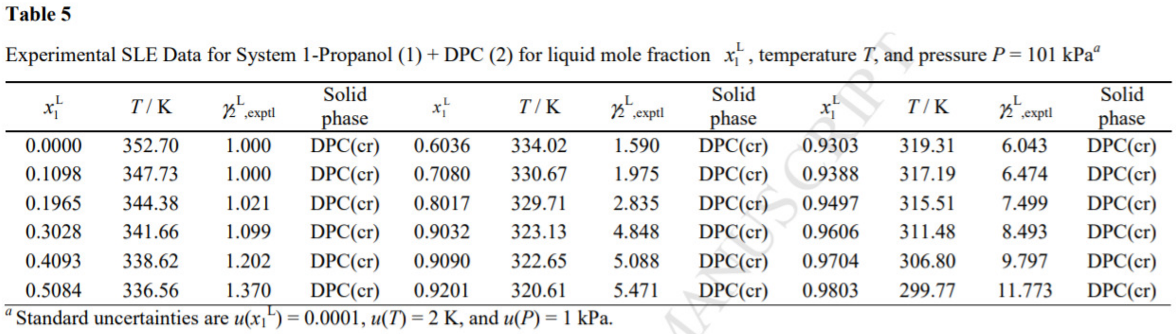


**Table 5**

Experimental SLE Data for System 1-Propanol (1) + DPC (2) for liquid mole fraction $x_1^{\mathrm{L}}$, temperature $T$, and pressure $P$ = 101 kPa[a]

| $x_1^{\mathrm{L}}$ | $T$ / K | $\gamma_{2,\mathrm{exptl}}^{\mathrm{L}}$ | Solid phase | $x_1^{\mathrm{L}}$ | $T$ / K | $\gamma_{2,\mathrm{exptl}}^{\mathrm{L}}$ | Solid phase | $x_1^{\mathrm{L}}$ | $T$ / K | $\gamma_{2,\mathrm{exptl}}^{\mathrm{L}}$ | Solid phase |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.0000 | 352.70 | 1.000 | DPC(cr) | 0.6036 | 334.02 | 1.590 | DPC(cr) | 0.9303 | 319.31 | 6.043 | DPC(cr) |
| 0.1098 | 347.73 | 1.000 | DPC(cr) | 0.7080 | 330.67 | 1.975 | DPC(cr) | 0.9388 | 317.19 | 6.474 | DPC(cr) |
| 0.1965 | 344.38 | 1.021 | DPC(cr) | 0.8017 | 329.71 | 2.835 | DPC(cr) | 0.9497 | 315.51 | 7.499 | DPC(cr) |
| 0.3028 | 341.66 | 1.099 | DPC(cr) | 0.9032 | 323.13 | 4.848 | DPC(cr) | 0.9606 | 311.48 | 8.493 | DPC(cr) |
| 0.4093 | 338.62 | 1.202 | DPC(cr) | 0.9090 | 322.65 | 5.088 | DPC(cr) | 0.9704 | 306.80 | 9.797 | DPC(cr) |
| 0.5084 | 336.56 | 1.370 | DPC(cr) | 0.9201 | 320.61 | 5.471 | DPC(cr) | 0.9803 | 299.77 | 11.773 | DPC(cr) |

[a] Standard uncertainties are $u(x_1^{\mathrm{L}})$ = 0.0001, $u(T)$ = 2 K, and $u(P)$ = 1 kPa.

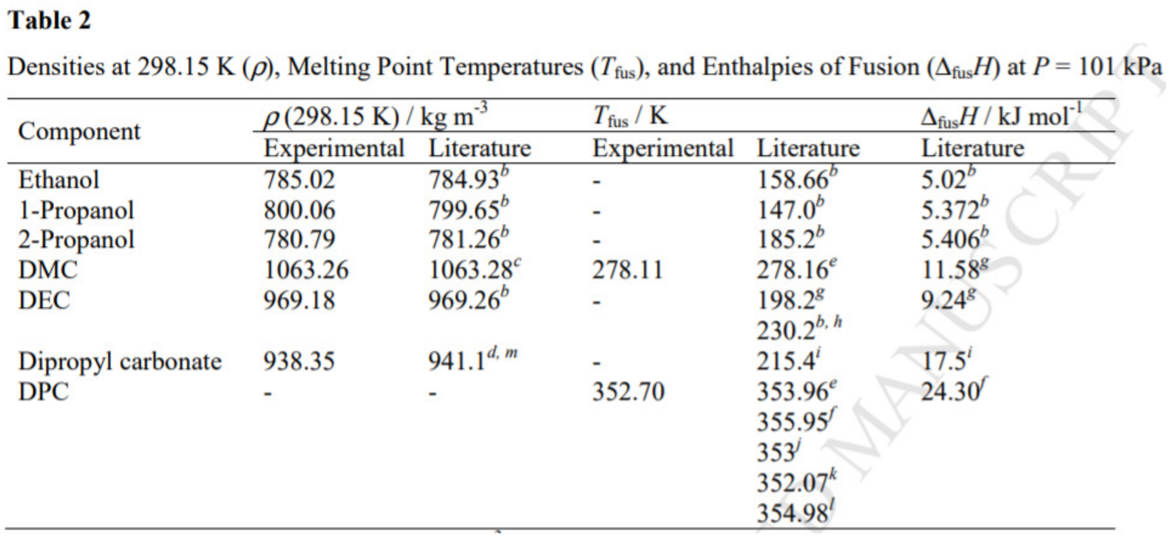


**Table 2**

Densities at 298.15 K ($\rho$), Melting Point Temperatures ($T_{\mathrm{fus}}$), and Enthalpies of Fusion ($\Delta_{\mathrm{fus}}H$) at $P$ = 101 kPa

| Component | $\rho$ (298.15 K) / kg m$^{-3}$ | | $T_{\mathrm{fus}}$ / K | | $\Delta_{\mathrm{fus}}H$ / kJ mol$^{-1}$ |
|---|---|---|---|---|---|
| | Experimental | Literature | Experimental | Literature | Literature |
| Ethanol | 785.02 | 784.93$^b$ | - | 158.66$^b$ | 5.02$^b$ |
| 1-Propanol | 800.06 | 799.65$^b$ | - | 147.0$^b$ | 5.372$^b$ |
| 2-Propanol | 780.79 | 781.26$^b$ | - | 185.2$^b$ | 5.406$^b$ |
| DMC | 1063.26 | 1063.28$^c$ | 278.11 | 278.16$^e$ | 11.58$^g$ |
| DEC | 969.18 | 969.26$^b$ | - | 198.2$^g$<br>230.2$^{b,h}$ | 9.24$^g$ |
| Dipropyl carbonate | 938.35 | 941.1$^{d,m}$ | - | 215.4$^i$ | 17.5$^i$ |
| DPC | - | - | 352.70 | 353.96$^e$<br>355.95$^f$<br>353$^j$<br>352.07$^k$<br>354.98$^l$ | 24.30$^f$ |

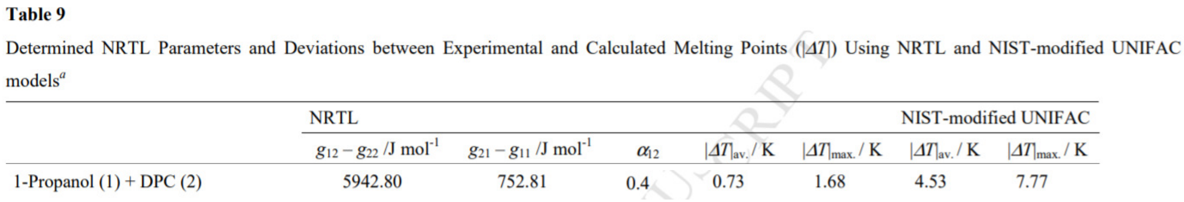


**Table 9**

Determined NRTL Parameters and Deviations between Experimental and Calculated Melting Points (|$\Delta T$|) Using NRTL and NIST-modified UNIFAC models[a]

| | NRTL | | | | | NIST-modified UNIFAC | |
|---|---|---|---|---|---|---|---|
| | $g_{12} - g_{22}$ /J mol$^{-1}$ | $g_{21} - g_{11}$ /J mol$^{-1}$ | $\alpha_{12}$ | $\lvert\Delta T\rvert_{\mathrm{av.}}$ / K | $\lvert\Delta T\rvert_{\mathrm{max.}}$ / K | $\lvert\Delta T\rvert_{\mathrm{av.}}$ / K | $\lvert\Delta T\rvert_{\mathrm{max.}}$ / K |
| 1-Propanol (1) + DPC (2) | 5942.80 | 752.81 | 0.4 | 0.73 | 1.68 | 4.53 | 7.77 |

2-propanol + diphenyl carbonate

Hiroyuki Matsuda, Yuki Ohashi, Kiyofumi Kurihara, Katsumi Tochigi, Kenji Ochi, Solid–liquid equilibria for selected binary systems containing diphenyl carbonate, Fluid Phase Equilibria, Volume 479, 15 January 2019, Pages 17-24

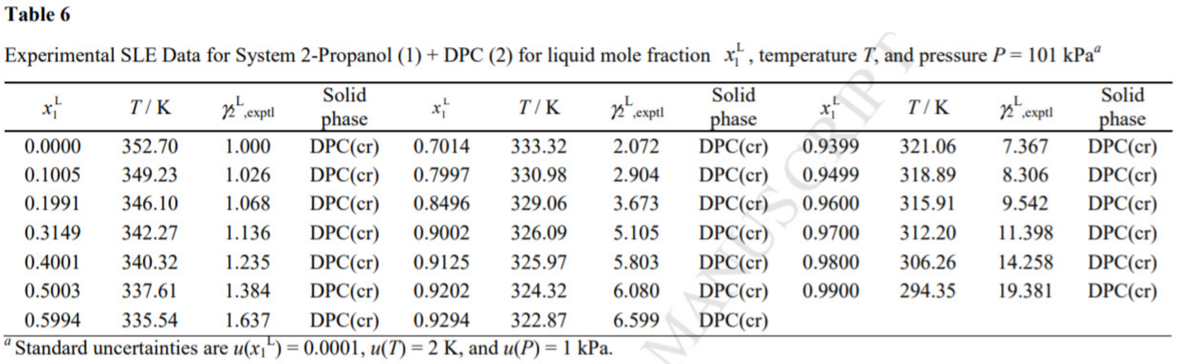


**Table 6**

Experimental SLE Data for System 2-Propanol (1) + DPC (2) for liquid mole fraction $x_1^L$, temperature $T$, and pressure $P$ = 101 kPa[a]

| $x_1^L$ | $T$ / K | $\gamma_{1,\text{exptl}}^L$ | Solid phase | $x_1^L$ | $T$ / K | $\gamma_{1,\text{exptl}}^L$ | Solid phase | $x_1^L$ | $T$ / K | $\gamma_{1,\text{exptl}}^L$ | Solid phase |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.0000 | 352.70 | 1.000 | DPC(cr) | 0.7014 | 333.32 | 2.072 | DPC(cr) | 0.9399 | 321.06 | 7.367 | DPC(cr) |
| 0.1005 | 349.23 | 1.026 | DPC(cr) | 0.7997 | 330.98 | 2.904 | DPC(cr) | 0.9499 | 318.89 | 8.306 | DPC(cr) |
| 0.1991 | 346.10 | 1.068 | DPC(cr) | 0.8496 | 329.06 | 3.673 | DPC(cr) | 0.9600 | 315.91 | 9.542 | DPC(cr) |
| 0.3149 | 342.27 | 1.136 | DPC(cr) | 0.9002 | 326.09 | 5.105 | DPC(cr) | 0.9700 | 312.20 | 11.398 | DPC(cr) |
| 0.4001 | 340.32 | 1.235 | DPC(cr) | 0.9125 | 325.97 | 5.803 | DPC(cr) | 0.9800 | 306.26 | 14.258 | DPC(cr) |
| 0.5003 | 337.61 | 1.384 | DPC(cr) | 0.9202 | 324.32 | 6.080 | DPC(cr) | 0.9900 | 294.35 | 19.381 | DPC(cr) |
| 0.5994 | 335.54 | 1.637 | DPC(cr) | 0.9294 | 322.87 | 6.599 | DPC(cr) | | | | |

[a] Standard uncertainties are $u(x_1^L)$ = 0.0001, $u(T)$ = 2 K, and $u(P)$ = 1 kPa.

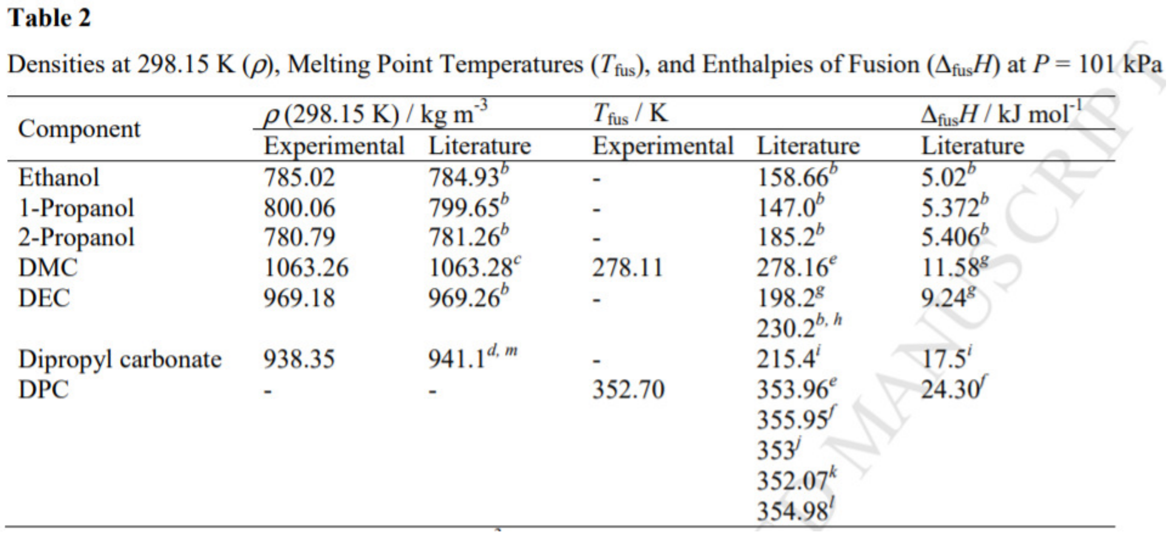


**Table 2**

Densities at 298.15 K ($\rho$), Melting Point Temperatures ($T_{\text{fus}}$), and Enthalpies of Fusion ($\Delta_{\text{fus}}H$) at $P$ = 101 kPa

| Component | $\rho$ (298.15 K) / kg m$^{-3}$ | | $T_{\text{fus}}$ / K | | $\Delta_{\text{fus}}H$ / kJ mol$^{-1}$ |
|---|---|---|---|---|---|
| | Experimental | Literature | Experimental | Literature | Literature |
| Ethanol | 785.02 | 784.93[b] | - | 158.66[b] | 5.02[b] |
| 1-Propanol | 800.06 | 799.65[b] | - | 147.0[b] | 5.372[b] |
| 2-Propanol | 780.79 | 781.26[b] | - | 185.2[b] | 5.406[b] |
| DMC | 1063.26 | 1063.28[c] | 278.11 | 278.16[e] | 11.58[g] |
| DEC | 969.18 | 969.26[b] | - | 198.2[g]<br>230.2[b, h] | 9.24[g] |
| Dipropyl carbonate | 938.35 | 941.1[d, m] | - | 215.4[i] | 17.5[i] |
| DPC | - | - | 352.70 | 353.96[e]<br>355.95[f]<br>353[j]<br>352.07[k]<br>354.98[l] | 24.30[f] |

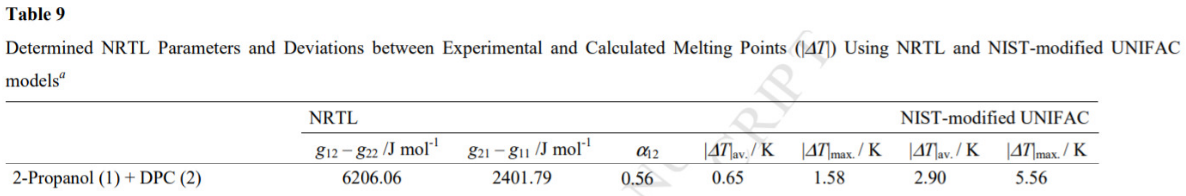


**Table 9**

Determined NRTL Parameters and Deviations between Experimental and Calculated Melting Points ($|\Delta T|$) Using NRTL and NIST-modified UNIFAC models[a]

| | NRTL | | | | | NIST-modified UNIFAC | |
|---|---|---|---|---|---|---|---|
| | $g_{12} - g_{22}$ /J mol$^{-1}$ | $g_{21} - g_{11}$ /J mol$^{-1}$ | $\alpha_{12}$ | $\|\Delta T\|_{\text{av.}}$ / K | $\|\Delta T\|_{\text{max.}}$ / K | $\|\Delta T\|_{\text{av.}}$ / K | $\|\Delta T\|_{\text{max.}}$ / K |
| 2-Propanol (1) + DPC (2) | 6206.06 | 2401.79 | 0.56 | 0.65 | 1.58 | 2.90 | 5.56 |

diethyl carbonate + diphenyl carbonate
Hiroyuki Matsuda, Yuki Ohashi, Kiyofumi Kurihara, Katsumi Tochigi, Kenji Ochi, Solid–liquid equilibria for selected binary systems containing diphenyl carbonate, Fluid Phase Equilibria, Volume 479, 15 January 2019, Pages 17-24

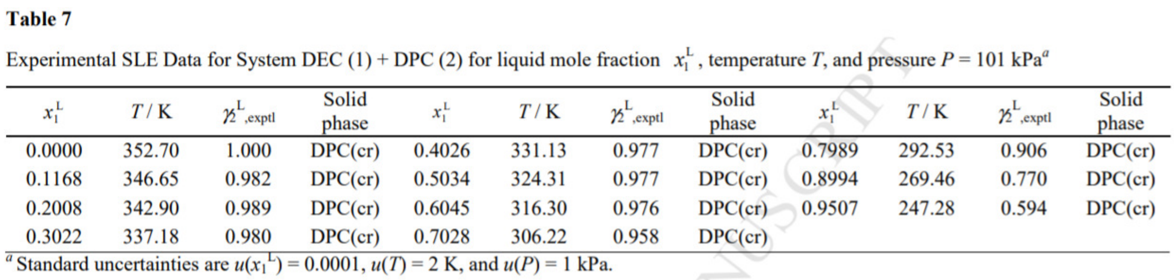


**Table 7**

Experimental SLE Data for System DEC (1) + DPC (2) for liquid mole fraction $x_1^L$, temperature $T$, and pressure $P$ = 101 kPa[a]

| $x_1^L$ | $T$ / K | $\gamma_{2,\mathrm{exptl}}^L$ | Solid phase | $x_1^L$ | $T$ / K | $\gamma_{2,\mathrm{exptl}}^L$ | Solid phase | $x_1^L$ | $T$ / K | $\gamma_{2,\mathrm{exptl}}^L$ | Solid phase |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.0000 | 352.70 | 1.000 | DPC(cr) | 0.4026 | 331.13 | 0.977 | DPC(cr) | 0.7989 | 292.53 | 0.906 | DPC(cr) |
| 0.1168 | 346.65 | 0.982 | DPC(cr) | 0.5034 | 324.31 | 0.977 | DPC(cr) | 0.8994 | 269.46 | 0.770 | DPC(cr) |
| 0.2008 | 342.90 | 0.989 | DPC(cr) | 0.6045 | 316.30 | 0.976 | DPC(cr) | 0.9507 | 247.28 | 0.594 | DPC(cr) |
| 0.3022 | 337.18 | 0.980 | DPC(cr) | 0.7028 | 306.22 | 0.958 | DPC(cr) | | | | |

[a] Standard uncertainties are $u(x_1^L)$ = 0.0001, $u(T)$ = 2 K, and $u(P)$ = 1 kPa.

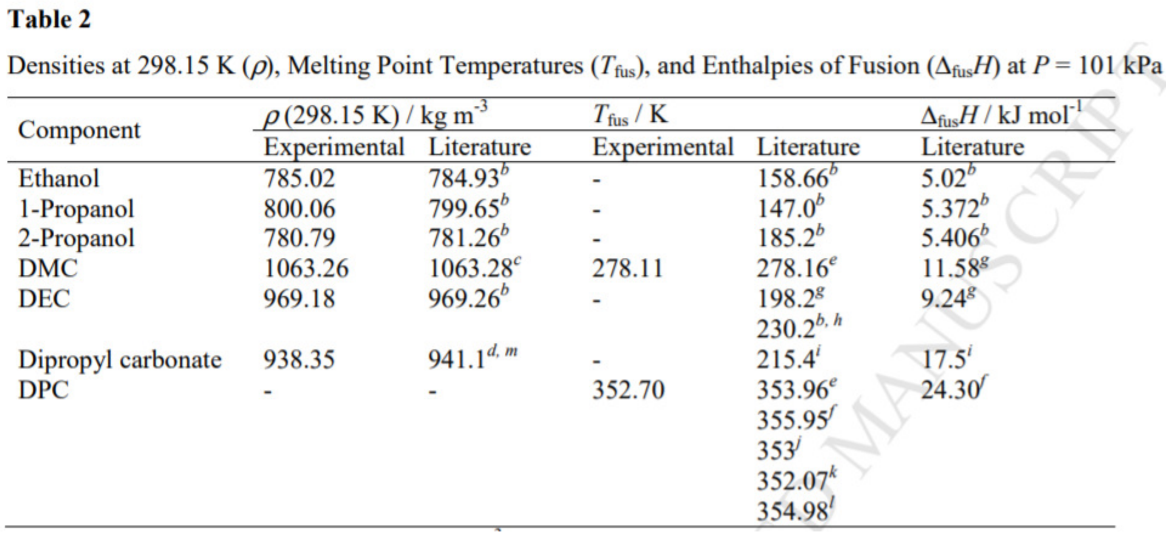


**Table 2**

Densities at 298.15 K ($\rho$), Melting Point Temperatures ($T_{\mathrm{fus}}$), and Enthalpies of Fusion ($\Delta_{\mathrm{fus}}H$) at $P$ = 101 kPa

| Component | $\rho$(298.15 K) / kg m$^{-3}$ | | $T_{\mathrm{fus}}$ / K | | $\Delta_{\mathrm{fus}}H$ / kJ mol$^{-1}$ |
|---|---|---|---|---|---|
| | Experimental | Literature | Experimental | Literature | Literature |
| Ethanol | 785.02 | 784.93[b] | - | 158.66[b] | 5.02[b] |
| 1-Propanol | 800.06 | 799.65[b] | - | 147.0[b] | 5.372[b] |
| 2-Propanol | 780.79 | 781.26[b] | - | 185.2[b] | 5.406[b] |
| DMC | 1063.26 | 1063.28[c] | 278.11 | 278.16[e] | 11.58[g] |
| DEC | 969.18 | 969.26[b] | - | 198.2[g]<br>230.2[b, h] | 9.24[g] |
| Dipropyl carbonate | 938.35 | 941.1[d, m] | - | 215.4[i] | 17.5[i] |
| DPC | - | - | 352.70 | 353.96[e]<br>355.95[f]<br>353[j]<br>352.07[k]<br>354.98[l] | 24.30[f] |

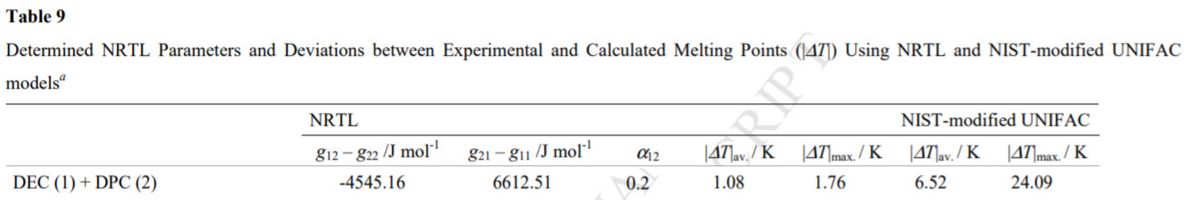


**Table 9**

Determined NRTL Parameters and Deviations between Experimental and Calculated Melting Points ($|\Delta T|$) Using NRTL and NIST-modified UNIFAC models[a]

| | NRTL | | | | | NIST-modified UNIFAC | |
|---|---|---|---|---|---|---|---|
| | $g_{12}-g_{22}$ /J mol$^{-1}$ | $g_{21}-g_{11}$ /J mol$^{-1}$ | $\alpha_{12}$ | $\lvert\Delta T\rvert_{\mathrm{av.}}$ / K | $\lvert\Delta T\rvert_{\mathrm{max.}}$ / K | $\lvert\Delta T\rvert_{\mathrm{av.}}$ / K | $\lvert\Delta T\rvert_{\mathrm{max.}}$ / K |
| DEC (1) + DPC (2) | -4545.16 | 6612.51 | 0.2 | 1.08 | 1.76 | 6.52 | 24.09 |

dipropyl carbonate + diphenyl carbonate

Hiroyuki Matsuda, Yuki Ohashi, Kiyofumi Kurihara, Katsumi Tochigi, Kenji Ochi, Solid–liquid equilibria for selected binary systems containing diphenyl carbonate, Fluid Phase Equilibria, Volume 479, 15 January 2019, Pages 17-24

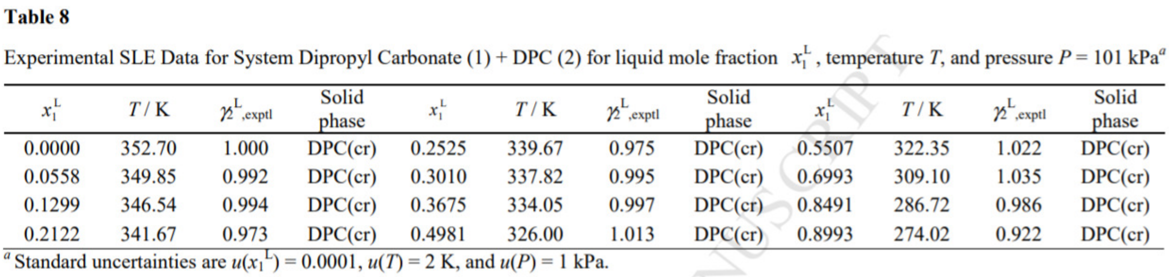


**Table 8**

Experimental SLE Data for System Dipropyl Carbonate (1) + DPC (2) for liquid mole fraction $x_1^{\mathrm{L}}$, temperature $T$, and pressure $P$ = 101 kPa[a]

| $x_1^{\mathrm{L}}$ | $T$ / K | $\gamma_{2,\mathrm{exptl}}^{\mathrm{L}}$ | Solid phase | $x_1^{\mathrm{L}}$ | $T$ / K | $\gamma_{2,\mathrm{exptl}}^{\mathrm{L}}$ | Solid phase | $x_1^{\mathrm{L}}$ | $T$ / K | $\gamma_{2,\mathrm{exptl}}^{\mathrm{L}}$ | Solid phase |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.0000 | 352.70 | 1.000 | DPC(cr) | 0.2525 | 339.67 | 0.975 | DPC(cr) | 0.5507 | 322.35 | 1.022 | DPC(cr) |
| 0.0558 | 349.85 | 0.992 | DPC(cr) | 0.3010 | 337.82 | 0.995 | DPC(cr) | 0.6993 | 309.10 | 1.035 | DPC(cr) |
| 0.1299 | 346.54 | 0.994 | DPC(cr) | 0.3675 | 334.05 | 0.997 | DPC(cr) | 0.8491 | 286.72 | 0.986 | DPC(cr) |
| 0.2122 | 341.67 | 0.973 | DPC(cr) | 0.4981 | 326.00 | 1.013 | DPC(cr) | 0.8993 | 274.02 | 0.922 | DPC(cr) |

[a] Standard uncertainties are $u(x_1^{\mathrm{L}})$ = 0.0001, $u(T)$ = 2 K, and $u(P)$ = 1 kPa.

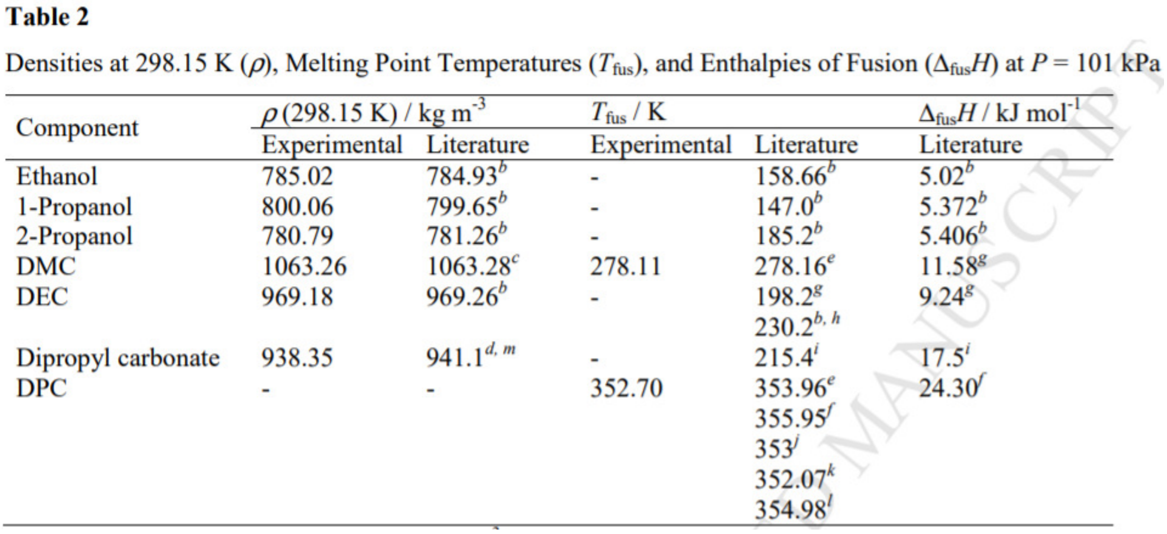


**Table 2**

Densities at 298.15 K ($\rho$), Melting Point Temperatures ($T_{\mathrm{fus}}$), and Enthalpies of Fusion ($\Delta_{\mathrm{fus}}H$) at $P$ = 101 kPa

| Component | $\rho$ (298.15 K) / kg m$^{-3}$ |  | $T_{\mathrm{fus}}$ / K |  | $\Delta_{\mathrm{fus}}H$ / kJ mol$^{-1}$ |
|---|---|---|---|---|---|
|  | Experimental | Literature | Experimental | Literature | Literature |
| Ethanol | 785.02 | 784.93[b] | - | 158.66[b] | 5.02[b] |
| 1-Propanol | 800.06 | 799.65[b] | - | 147.0[b] | 5.372[b] |
| 2-Propanol | 780.79 | 781.26[b] | - | 185.2[b] | 5.406[b] |
| DMC | 1063.26 | 1063.28[c] | 278.11 | 278.16[e] | 11.58[g] |
| DEC | 969.18 | 969.26[b] | - | 198.2[g]<br>230.2[b, h] | 9.24[g] |
| Dipropyl carbonate | 938.35 | 941.1[d, m] | - | 215.4[i] | 17.5[i] |
| DPC | - | - | 352.70 | 353.96[e]<br>355.95[f]<br>353[j]<br>352.07[k]<br>354.98[l] | 24.30[f] |

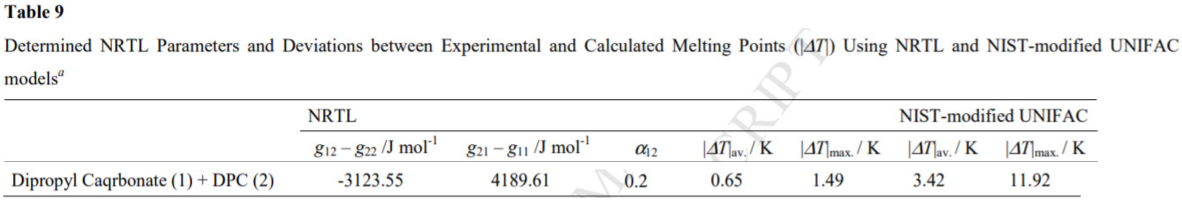


**Table 9**

Determined NRTL Parameters and Deviations between Experimental and Calculated Melting Points ($|\Delta T|$) Using NRTL and NIST-modified UNIFAC models[a]

|  | NRTL |  |  |  |  | NIST-modified UNIFAC |  |
|---|---|---|---|---|---|---|---|
|  | $g_{12} - g_{22}$ /J mol$^{-1}$ | $g_{21} - g_{11}$ /J mol$^{-1}$ | $\alpha_{12}$ | $\lvert\Delta T\rvert_{\mathrm{av.}}$ / K | $\lvert\Delta T\rvert_{\mathrm{max.}}$ / K | $\lvert\Delta T\rvert_{\mathrm{av.}}$ / K | $\lvert\Delta T\rvert_{\mathrm{max.}}$ / K |
| Dipropyl Caqrbonate (1) + DPC (2) | -3123.55 | 4189.61 | 0.2 | 0.65 | 1.49 | 3.42 | 11.92 |

N-vinylpyrrolidone + 2-pyrrolidone
Ao Su, Sifang Li, Measurement and correlation of solid–liquid phase equilibria for binary and ternary systems consisting of *N*-vinylpyrrolidone, 2-pyrrolidone and water, Chinese Journal of Chemical Engineering, Volume 26, Issue 4, April 2018, Pages 806-811

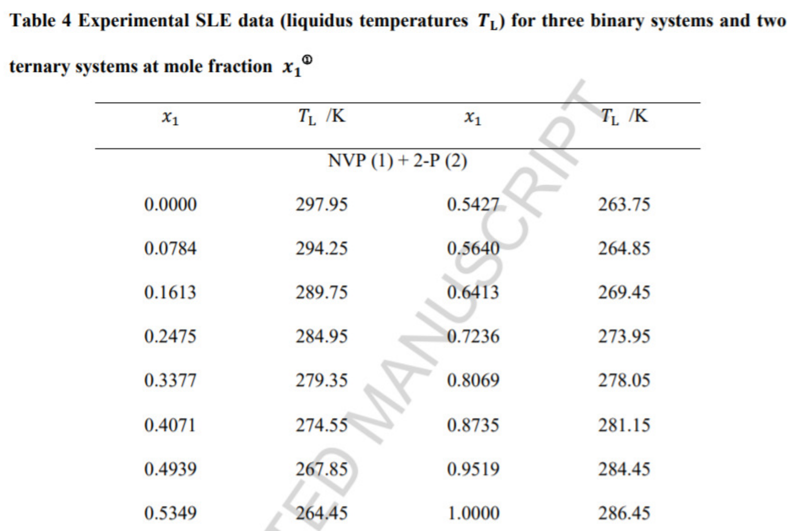


**Table 4 Experimental SLE data (liquidus temperatures $T_L$) for three binary systems and two ternary systems at mole fraction $x_1$①**

| $x_1$ | $T_L$ /K | $x_1$ | $T_L$ /K |
|---|---|---|---|
| NVP (1) + 2-P (2) | | | |
| 0.0000 | 297.95 | 0.5427 | 263.75 |
| 0.0784 | 294.25 | 0.5640 | 264.85 |
| 0.1613 | 289.75 | 0.6413 | 269.45 |
| 0.2475 | 284.95 | 0.7236 | 273.95 |
| 0.3377 | 279.35 | 0.8069 | 278.05 |
| 0.4071 | 274.55 | 0.8735 | 281.15 |
| 0.4939 | 267.85 | 0.9519 | 284.45 |
| 0.5349 | 264.45 | 1.0000 | 286.45 |

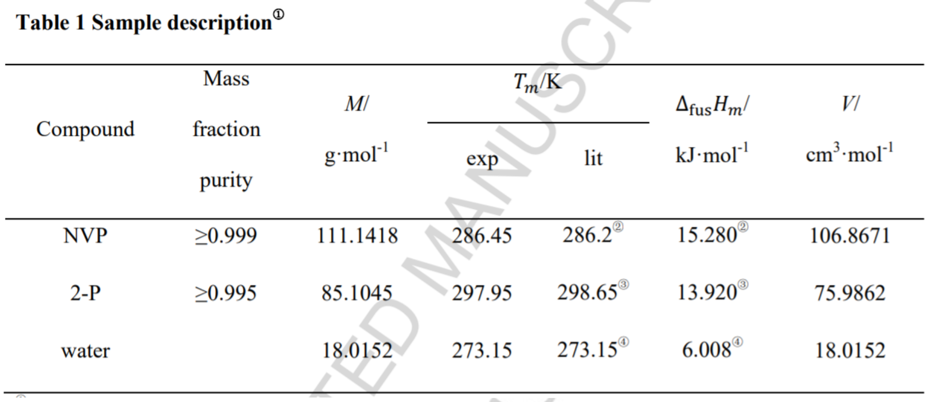


**Table 1 Sample description①**

| Compound | Mass fraction purity | $M$/ g·mol$^{-1}$ | $T_m$/K exp | $T_m$/K lit | $\Delta_{fus}H_m$/ kJ·mol$^{-1}$ | $V$/ cm$^3$·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| NVP | ≥0.999 | 111.1418 | 286.45 | 286.2② | 15.280② | 106.8671 |
| 2-P | ≥0.995 | 85.1045 | 297.95 | 298.65③ | 13.920③ | 75.9862 |
| water | | 18.0152 | 273.15 | 273.15④ | 6.008④ | 18.0152 |

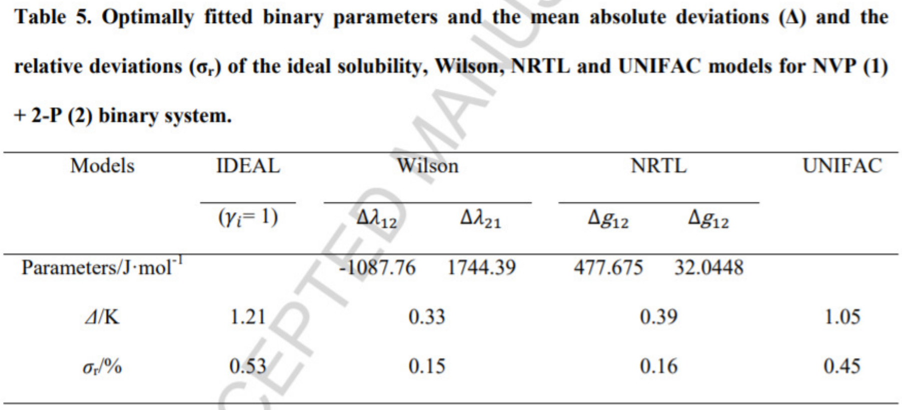


**Table 5. Optimally fitted binary parameters and the mean absolute deviations (Δ) and the relative deviations ($\sigma_r$) of the ideal solubility, Wilson, NRTL and UNIFAC models for NVP (1) + 2-P (2) binary system.**

| Models | IDEAL | Wilson | | NRTL | | UNIFAC |
|---|---|---|---|---|---|---|
| | ($\gamma_i$= 1) | $\Delta\lambda_{12}$ | $\Delta\lambda_{21}$ | $\Delta g_{12}$ | $\Delta g_{12}$ | |
| Parameters/J·mol$^{-1}$ | | -1087.76 | 1744.39 | 477.675 | 32.0448 | |
| $\Delta$/K | 1.21 | 0.33 | | 0.39 | | 1.05 |
| $\sigma_r$/% | 0.53 | 0.15 | | 0.16 | | 0.45 |

α = 0.3
ODABRATI JEDAN MODEL!

N-vinylpyrrolidone + water

Ao Su, Sifang Li, Measurement and correlation of solid–liquid phase equilibria for binary and ternary systems consisting of *N*-vinylpyrrolidone, 2-pyrrolidone and water, Chinese Journal of Chemical Engineering, Volume 26, Issue 4, April 2018, Pages 806-811

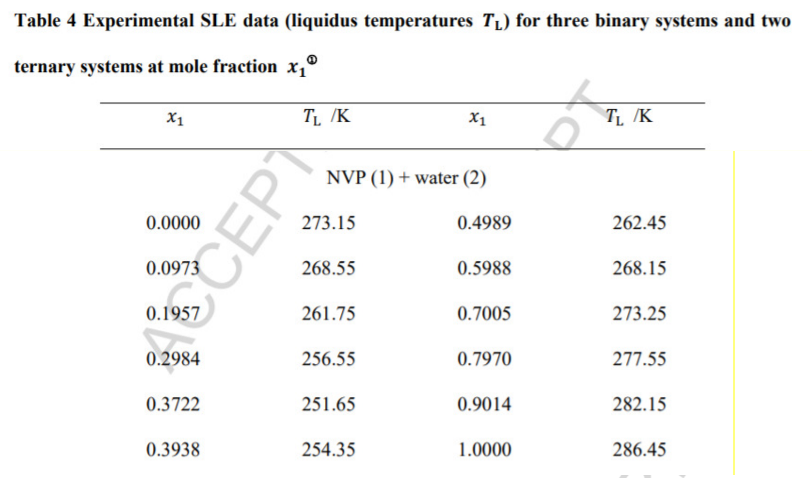


**Table 4 Experimental SLE data (liquidus temperatures $T_L$) for three binary systems and two ternary systems at mole fraction $x_1$①**

| $x_1$ | $T_L$ /K | $x_1$ | $T_L$ /K |
|---|---|---|---|
| NVP (1) + water (2) | | | |
| 0.0000 | 273.15 | 0.4989 | 262.45 |
| 0.0973 | 268.55 | 0.5988 | 268.15 |
| 0.1957 | 261.75 | 0.7005 | 273.25 |
| 0.2984 | 256.55 | 0.7970 | 277.55 |
| 0.3722 | 251.65 | 0.9014 | 282.15 |
| 0.3938 | 254.35 | 1.0000 | 286.45 |

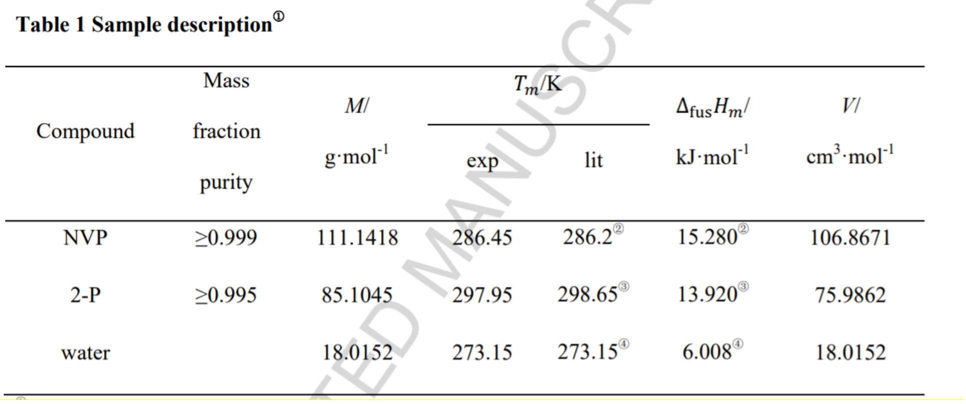


**Table 1 Sample description①**

| Compound | Mass fraction purity | $M$/ g·mol$^{-1}$ | $T_m$/K | | $\Delta_{fus}H_m$/ kJ·mol$^{-1}$ | $V$/ cm$^3$·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| | | | exp | lit | | |
| NVP | ≥0.999 | 111.1418 | 286.45 | 286.2② | 15.280② | 106.8671 |
| 2-P | ≥0.995 | 85.1045 | 297.95 | 298.65③ | 13.920③ | 75.9862 |
| water | | 18.0152 | 273.15 | 273.15④ | 6.008④ | 18.0152 |

2-pyrrolidone + water

Ao Su, Sifang Li, Measurement and correlation of solid–liquid phase equilibria for binary and ternary systems consisting of *N*-vinylpyrrolidone, 2-pyrrolidone and water, Chinese Journal of Chemical Engineering, Volume 26, Issue 4, April 2018, Pages 806-811

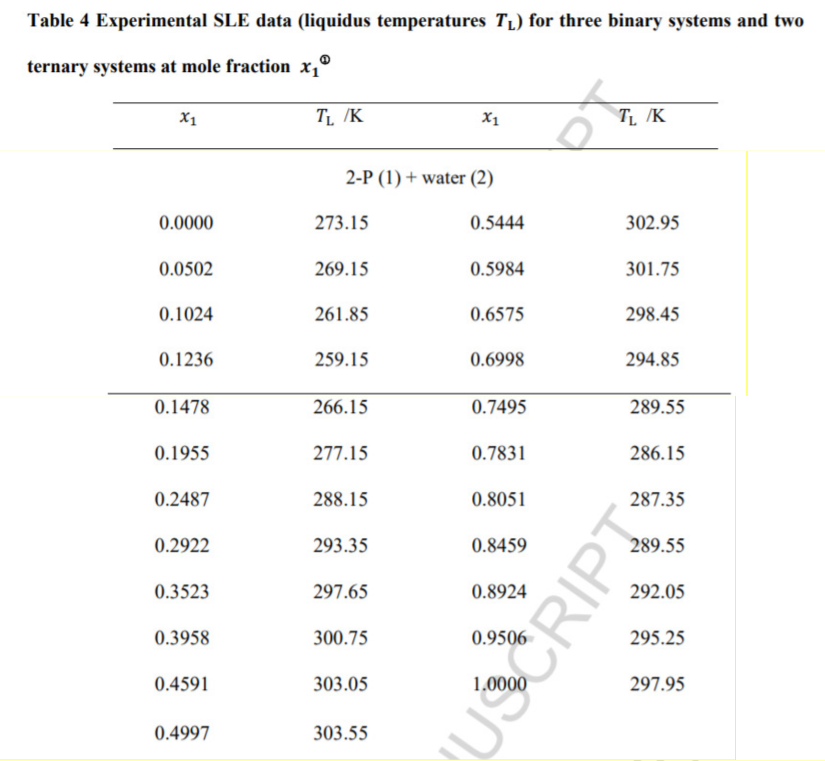


**Table 4 Experimental SLE data (liquidus temperatures $T_L$) for three binary systems and two ternary systems at mole fraction $x_1$①**

| $x_1$ | $T_L$ /K | $x_1$ | $T_L$ /K |
|---|---|---|---|
| 2-P (1) + water (2) | | | |
| 0.0000 | 273.15 | 0.5444 | 302.95 |
| 0.0502 | 269.15 | 0.5984 | 301.75 |
| 0.1024 | 261.85 | 0.6575 | 298.45 |
| 0.1236 | 259.15 | 0.6998 | 294.85 |
| 0.1478 | 266.15 | 0.7495 | 289.55 |
| 0.1955 | 277.15 | 0.7831 | 286.15 |
| 0.2487 | 288.15 | 0.8051 | 287.35 |
| 0.2922 | 293.35 | 0.8459 | 289.55 |
| 0.3523 | 297.65 | 0.8924 | 292.05 |
| 0.3958 | 300.75 | 0.9506 | 295.25 |
| 0.4591 | 303.05 | 1.0000 | 297.95 |
| 0.4997 | 303.55 | | |

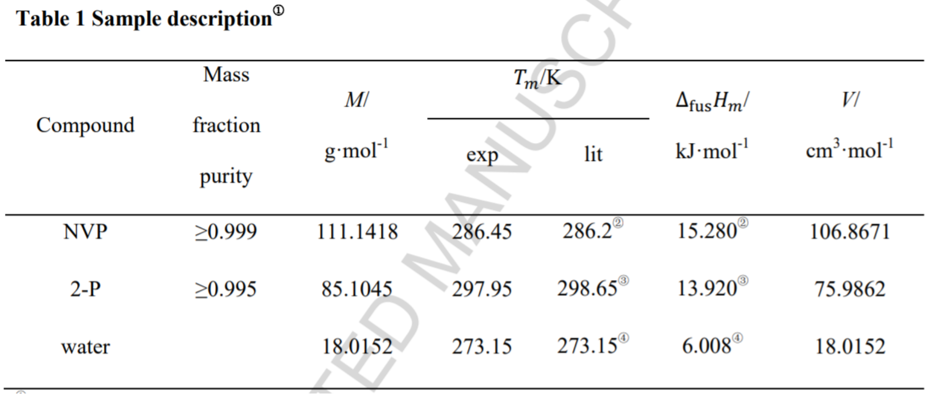


**Table 1 Sample description①**

| Compound | Mass fraction purity | $M$/ g·mol$^{-1}$ | $T_m$/K | | $\Delta_{fus}H_m$/ kJ·mol$^{-1}$ | $V$/ cm$^3$·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| | | | exp | lit | | |
| NVP | ≥0.999 | 111.1418 | 286.45 | 286.2② | 15.280② | 106.8671 |
| 2-P | ≥0.995 | 85.1045 | 297.95 | 298.65③ | 13.920③ | 75.9862 |
| water | | 18.0152 | 273.15 | 273.15④ | 6.008④ | 18.0152 |

anthracene + 2-phenylimidazole

Hocine Sifaoui, Marek Rogalski, Solid–liquid equilibria of three binary systems of anthracene with2-phenylimidazole, 4,5-diphenylimidazole and 2,4,5-triphenylimidazole, Thermochimica Acta 543 (2012) 32–36

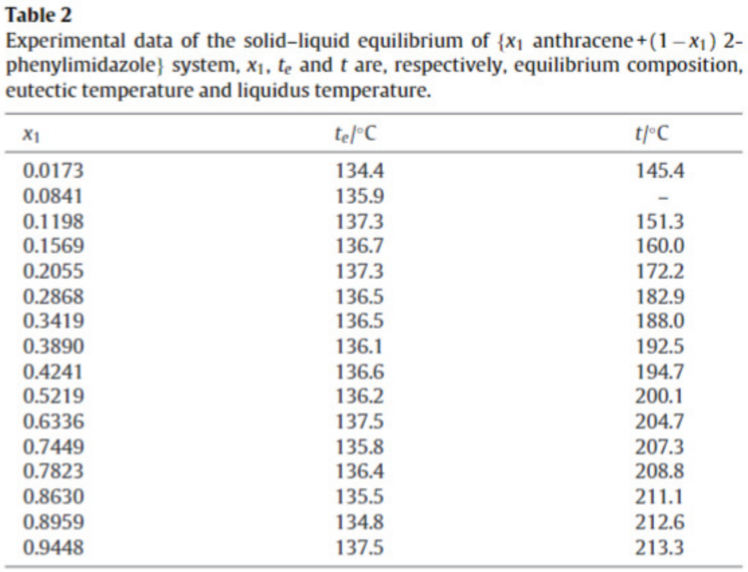


**Table 2**

Experimental data of the solid–liquid equilibrium of {$x_1$ anthracene + (1 − $x_1$) 2-phenylimidazole} system, $x_1$, $t_e$ and $t$ are, respectively, equilibrium composition, eutectic temperature and liquidus temperature.

| $x_1$ | $t_e$/°C | $t$/°C |
|---|---|---|
| 0.0173 | 134.4 | 145.4 |
| 0.0841 | 135.9 | – |
| 0.1198 | 137.3 | 151.3 |
| 0.1569 | 136.7 | 160.0 |
| 0.2055 | 137.3 | 172.2 |
| 0.2868 | 136.5 | 182.9 |
| 0.3419 | 136.5 | 188.0 |
| 0.3890 | 136.1 | 192.5 |
| 0.4241 | 136.6 | 194.7 |
| 0.5219 | 136.2 | 200.1 |
| 0.6336 | 137.5 | 204.7 |
| 0.7449 | 135.8 | 207.3 |
| 0.7823 | 136.4 | 208.8 |
| 0.8630 | 135.5 | 211.1 |
| 0.8959 | 134.8 | 212.6 |
| 0.9448 | 137.5 | 213.3 |

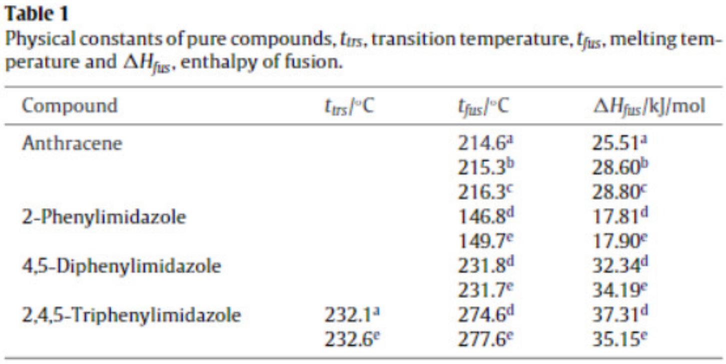


**Table 1**

Physical constants of pure compounds, $t_{trs}$, transition temperature, $t_{fus}$, melting temperature and $\Delta H_{fus}$, enthalpy of fusion.

| Compound | $t_{trs}$/°C | $t_{fus}$/°C | $\Delta H_{fus}$/kJ/mol |
|---|---|---|---|
| Anthracene | | 214.6[a] | 25.51[a] |
| | | 215.3[b] | 28.60[b] |
| | | 216.3[c] | 28.80[c] |
| 2-Phenylimidazole | | 146.8[d] | 17.81[d] |
| | | 149.7[e] | 17.90[e] |
| 4,5-Diphenylimidazole | | 231.8[d] | 32.34[d] |
| | | 231.7[e] | 34.19[e] |
| 2,4,5-Triphenylimidazole | 232.1[a] | 274.6[d] | 37.31[d] |
| | 232.6[e] | 277.6[e] | 35.15[e] |

anthracene + 4,5-diphenylimidazole

Hocine Sifaoui, Marek Rogalski, Solid–liquid equilibria of three binary systems of anthracene with2-phenylimidazole, 4,5-diphenylimidazole and 2,4,5-triphenylimidazole, Thermochimica Acta 543 (2012) 32–36

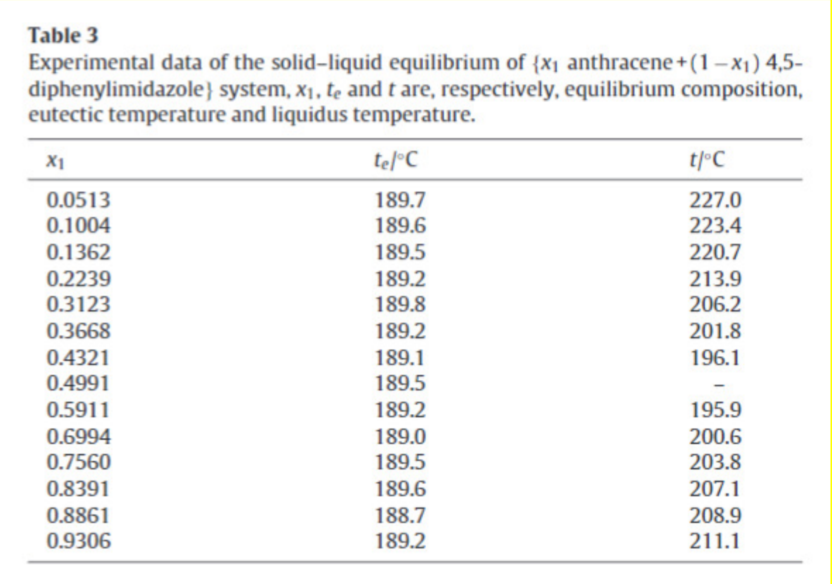


**Table 3**

Experimental data of the solid–liquid equilibrium of {$x_1$ anthracene + $(1-x_1)$ 4,5-diphenylimidazole} system, $x_1$, $t_e$ and $t$ are, respectively, equilibrium composition, eutectic temperature and liquidus temperature.

| $x_1$ | $t_e$/°C | $t$/°C |
|---|---|---|
| 0.0513 | 189.7 | 227.0 |
| 0.1004 | 189.6 | 223.4 |
| 0.1362 | 189.5 | 220.7 |
| 0.2239 | 189.2 | 213.9 |
| 0.3123 | 189.8 | 206.2 |
| 0.3668 | 189.2 | 201.8 |
| 0.4321 | 189.1 | 196.1 |
| 0.4991 | 189.5 | – |
| 0.5911 | 189.2 | 195.9 |
| 0.6994 | 189.0 | 200.6 |
| 0.7560 | 189.5 | 203.8 |
| 0.8391 | 189.6 | 207.1 |
| 0.8861 | 188.7 | 208.9 |
| 0.9306 | 189.2 | 211.1 |

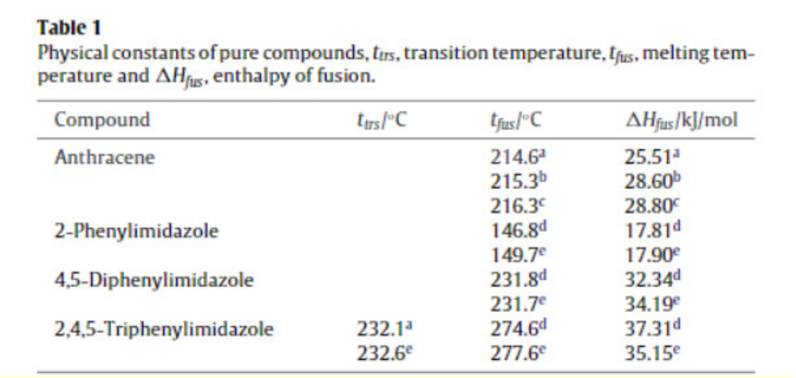


**Table 1**

Physical constants of pure compounds, $t_{trs}$, transition temperature, $t_{fus}$, melting temperature and $\Delta H_{fus}$, enthalpy of fusion.

| Compound | $t_{trs}$/°C | $t_{fus}$/°C | $\Delta H_{fus}$/kJ/mol |
|---|---|---|---|
| Anthracene | | 214.6[a] | 25.51[a] |
| | | 215.3[b] | 28.60[b] |
| | | 216.3[c] | 28.80[c] |
| 2-Phenylimidazole | | 146.8[d] | 17.81[d] |
| | | 149.7[e] | 17.90[e] |
| 4,5-Diphenylimidazole | | 231.8[d] | 32.34[d] |
| | | 231.7[e] | 34.19[e] |
| 2,4,5-Triphenylimidazole | 232.1[a] | 274.6[d] | 37.31[d] |
| | 232.6[e] | 277.6[e] | 35.15[e] |

anthracene + 2,4,5-triphenylimidazole

Hocine Sifaoui, Marek Rogalski, Solid–liquid equilibria of three binary systems of anthracene with2-phenylimidazole, 4,5-diphenylimidazole and 2,4,5-triphenylimidazole, Thermochimica Acta 543 (2012) 32–36

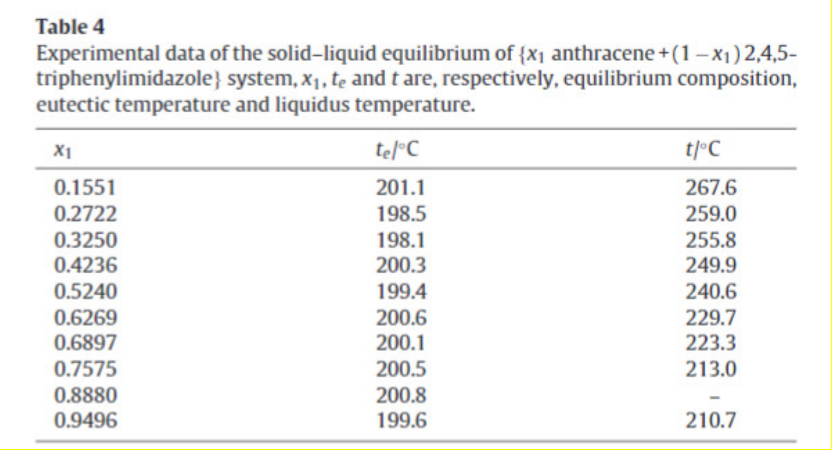


**Table 4**

Experimental data of the solid–liquid equilibrium of {$x_1$ anthracene + (1 − $x_1$) 2,4,5-triphenylimidazole} system, $x_1$, $t_e$ and $t$ are, respectively, equilibrium composition, eutectic temperature and liquidus temperature.

| $x_1$ | $t_e$/°C | $t$/°C |
|---|---|---|
| 0.1551 | 201.1 | 267.6 |
| 0.2722 | 198.5 | 259.0 |
| 0.3250 | 198.1 | 255.8 |
| 0.4236 | 200.3 | 249.9 |
| 0.5240 | 199.4 | 240.6 |
| 0.6269 | 200.6 | 229.7 |
| 0.6897 | 200.1 | 223.3 |
| 0.7575 | 200.5 | 213.0 |
| 0.8880 | 200.8 | – |
| 0.9496 | 199.6 | 210.7 |

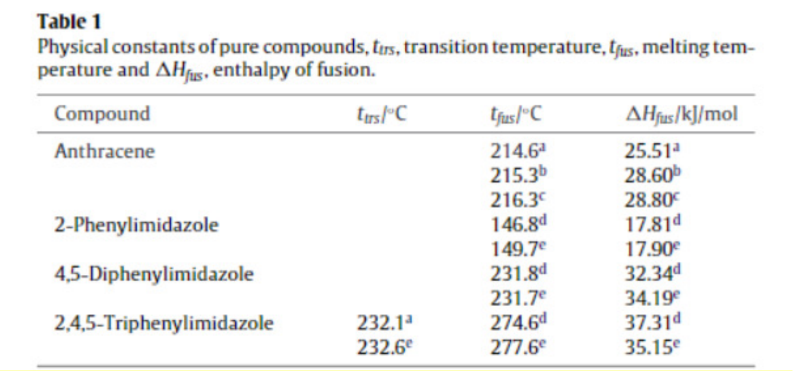


**Table 1**

Physical constants of pure compounds, $t_{trs}$, transition temperature, $t_{fus}$, melting temperature and $\Delta H_{fus}$, enthalpy of fusion.

| Compound | $t_{trs}$/°C | $t_{fus}$/°C | $\Delta H_{fus}$/kJ/mol |
|---|---|---|---|
| Anthracene | | 214.6[a] | 25.51[a] |
| | | 215.3[b] | 28.60[b] |
| | | 216.3[c] | 28.80[c] |
| 2-Phenylimidazole | | 146.8[d] | 17.81[d] |
| | | 149.7[e] | 17.90[e] |
| 4,5-Diphenylimidazole | | 231.8[d] | 32.34[d] |
| | | 231.7[e] | 34.19[e] |
| 2,4,5-Triphenylimidazole | 232.1[a] | 274.6[d] | 37.31[d] |
| | 232.6[e] | 277.6[e] | 35.15[e] |

*N*-hexyl-*N*-methylmorpholinium bromide + diethylene glycol

Marek Królikowski, Kinga Sankiewicz, New experimental data on (solid + liquid) phase equilibria of *N*-hexyl-*N*-methylmorholinium bromide with glycols and sulfolane. The use of these binary systems in a sulfur extraction, Journal of Molecular Liquids 263 (2018) 366–374

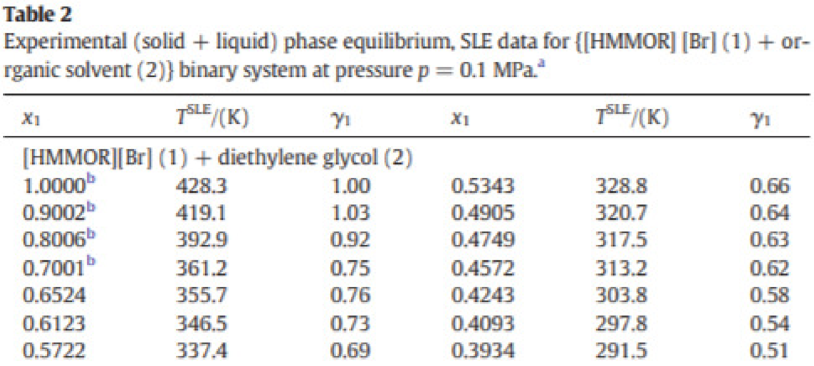


**Table 2**

Experimental (solid + liquid) phase equilibrium, SLE data for {[HMMOR] [Br] (1) + organic solvent (2)} binary system at pressure $p = 0.1$ MPa.[a]

| $x_1$ | $T^{SLE}/(K)$ | $\gamma_1$ | $x_1$ | $T^{SLE}/(K)$ | $\gamma_1$ |
|---|---|---|---|---|---|
| [HMMOR][Br] (1) + diethylene glycol (2) | | | | | |
| 1.0000[b] | 428.3 | 1.00 | 0.5343 | 328.8 | 0.66 |
| 0.9002[b] | 419.1 | 1.03 | 0.4905 | 320.7 | 0.64 |
| 0.8006[b] | 392.9 | 0.92 | 0.4749 | 317.5 | 0.63 |
| 0.7001[b] | 361.2 | 0.75 | 0.4572 | 313.2 | 0.62 |
| 0.6524 | 355.7 | 0.76 | 0.4243 | 303.8 | 0.58 |
| 0.6123 | 346.5 | 0.73 | 0.4093 | 297.8 | 0.54 |
| 0.5722 | 337.4 | 0.69 | 0.3934 | 291.5 | 0.51 |

[HMMOR][Br] Melting temperature $T_m$ is equal to 427.1 K with enthalpy $\Delta_m H = 12.24$ kJ mol$^{-1}$

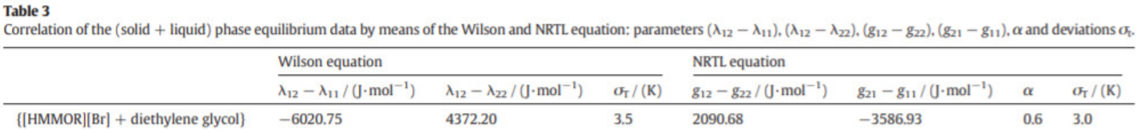


**Table 3**

Correlation of the (solid + liquid) phase equilibrium data by means of the Wilson and NRTL equation: parameters $(\lambda_{12} - \lambda_{11})$, $(\lambda_{12} - \lambda_{22})$, $(g_{12} - g_{22})$, $(g_{21} - g_{11})$, $\alpha$ and deviations $\sigma_T$.

| | Wilson equation | | | NRTL equation | | | |
|---|---|---|---|---|---|---|---|
| | $\lambda_{12} - \lambda_{11}$ / (J·mol$^{-1}$) | $\lambda_{12} - \lambda_{22}$ / (J·mol$^{-1}$) | $\sigma_T$ / (K) | $g_{12} - g_{22}$ / (J·mol$^{-1}$) | $g_{21} - g_{11}$ / (J·mol$^{-1}$) | $\alpha$ | $\sigma_T$ / (K) |
| {[HMMOR][Br] + diethylene glycol} | −6020.75 | 4372.20 | 3.5 | 2090.68 | −3586.93 | 0.6 | 3.0 |

ODABRATI JEDAN MODEL!

*N*-hexyl-*N*-methylmorpholinium bromide + triethylene glycol

Marek Królikowski, Kinga Sankiewicz, New experimental data on (solid + liquid) phase equilibria of *N*-hexyl-*N*-methylmorholinium bromide with glycols and sulfolane. The use of these binary systems in a sulfur extraction, Journal of Molecular Liquids 263 (2018) 366–374

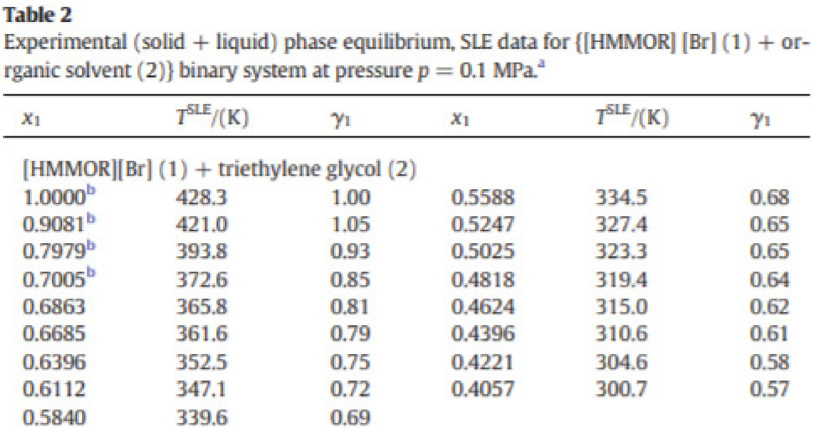


**Table 2**
Experimental (solid + liquid) phase equilibrium, SLE data for {[HMMOR] [Br] (1) + orrganic solvent (2)} binary system at pressure $p = 0.1$ MPa.[a]

| $x_1$ | $T^{SLE}/(K)$ | $\gamma_1$ | $x_1$ | $T^{SLE}/(K)$ | $\gamma_1$ |
|---|---|---|---|---|---|
| [HMMOR][Br] (1) + triethylene glycol (2) | | | | | |
| 1.0000[b] | 428.3 | 1.00 | 0.5588 | 334.5 | 0.68 |
| 0.9081[b] | 421.0 | 1.05 | 0.5247 | 327.4 | 0.65 |
| 0.7979[b] | 393.8 | 0.93 | 0.5025 | 323.3 | 0.65 |
| 0.7005[b] | 372.6 | 0.85 | 0.4818 | 319.4 | 0.64 |
| 0.6863 | 365.8 | 0.81 | 0.4624 | 315.0 | 0.62 |
| 0.6685 | 361.6 | 0.79 | 0.4396 | 310.6 | 0.61 |
| 0.6396 | 352.5 | 0.75 | 0.4221 | 304.6 | 0.58 |
| 0.6112 | 347.1 | 0.72 | 0.4057 | 300.7 | 0.57 |
| 0.5840 | 339.6 | 0.69 | | | |

[HMMOR][Br] Melting temperature $T_m$ is equal to 427.1 K with enthalpy $\Delta_m H = 12.24$ kJ mol$^{-1}$

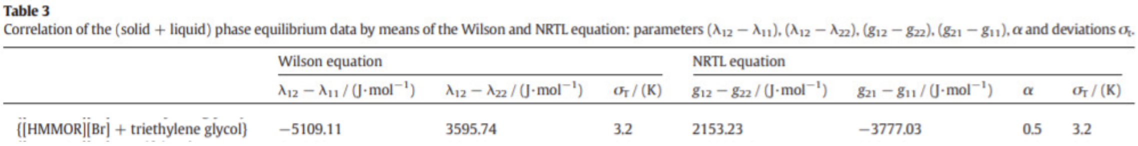


**Table 3**
Correlation of the (solid + liquid) phase equilibrium data by means of the Wilson and NRTL equation: parameters $(\lambda_{12}-\lambda_{11})$, $(\lambda_{12}-\lambda_{22})$, $(g_{12}-g_{22})$, $(g_{21}-g_{11})$, $\alpha$ and deviations $\sigma_T$.

| | Wilson equation | | | NRTL equation | | | |
|---|---|---|---|---|---|---|---|
| | $\lambda_{12}-\lambda_{11}$ / (J·mol$^{-1}$) | $\lambda_{12}-\lambda_{22}$ / (J·mol$^{-1}$) | $\sigma_T$ / (K) | $g_{12}-g_{22}$ / (J·mol$^{-1}$) | $g_{21}-g_{11}$ / (J·mol$^{-1}$) | $\alpha$ | $\sigma_T$ / (K) |
| {[HMMOR][Br] + triethylene glycol} | −5109.11 | 3595.74 | 3.2 | 2153.23 | −3777.03 | 0.5 | 3.2 |

ODABRATI JEDAN MODEL!

*N*-hexyl-*N*-methylmorpholinium bromide + sulfolane

Marek Królikowski, Kinga Sankiewicz, New experimental data on (solid + liquid) phase equilibria of *N*-hexyl-*N*-methylmorholinium bromide with glycols and sulfolane. The use of these binary systems in a sulfur extraction, Journal of Molecular Liquids 263 (2018) 366–374

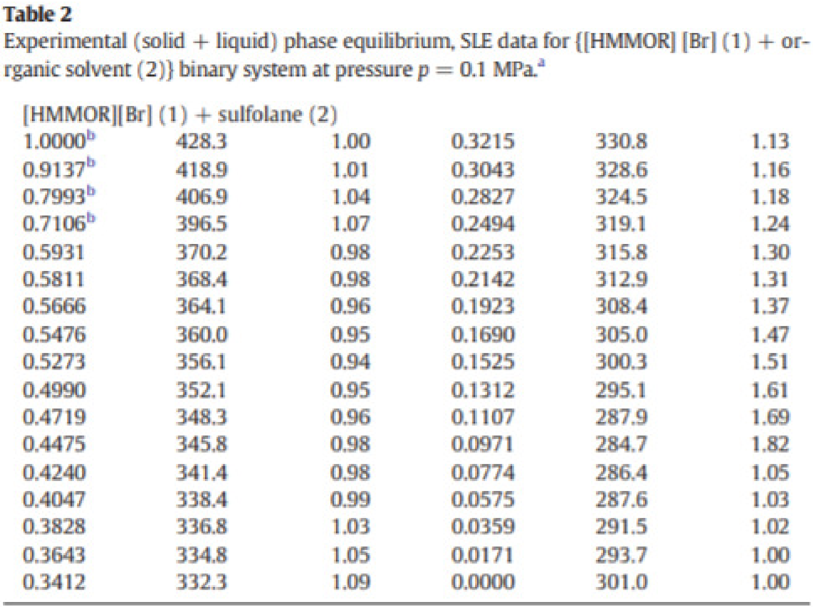


**Table 2**

Experimental (solid + liquid) phase equilibrium, SLE data for {[HMMOR] [Br] (1) + organic solvent (2)} binary system at pressure $p = 0.1$ MPa.[a]

| | | | | | |
|---|---|---|---|---|---|
| [HMMOR][Br] (1) + sulfolane (2) | | | | | |
| 1.0000[b] | 428.3 | 1.00 | 0.3215 | 330.8 | 1.13 |
| 0.9137[b] | 418.9 | 1.01 | 0.3043 | 328.6 | 1.16 |
| 0.7993[b] | 406.9 | 1.04 | 0.2827 | 324.5 | 1.18 |
| 0.7106[b] | 396.5 | 1.07 | 0.2494 | 319.1 | 1.24 |
| 0.5931 | 370.2 | 0.98 | 0.2253 | 315.8 | 1.30 |
| 0.5811 | 368.4 | 0.98 | 0.2142 | 312.9 | 1.31 |
| 0.5666 | 364.1 | 0.96 | 0.1923 | 308.4 | 1.37 |
| 0.5476 | 360.0 | 0.95 | 0.1690 | 305.0 | 1.47 |
| 0.5273 | 356.1 | 0.94 | 0.1525 | 300.3 | 1.51 |
| 0.4990 | 352.1 | 0.95 | 0.1312 | 295.1 | 1.61 |
| 0.4719 | 348.3 | 0.96 | 0.1107 | 287.9 | 1.69 |
| 0.4475 | 345.8 | 0.98 | 0.0971 | 284.7 | 1.82 |
| 0.4240 | 341.4 | 0.98 | 0.0774 | 286.4 | 1.05 |
| 0.4047 | 338.4 | 0.99 | 0.0575 | 287.6 | 1.03 |
| 0.3828 | 336.8 | 1.03 | 0.0359 | 291.5 | 1.02 |
| 0.3643 | 334.8 | 1.05 | 0.0171 | 293.7 | 1.00 |
| 0.3412 | 332.3 | 1.09 | 0.0000 | 301.0 | 1.00 |

[HMMOR][Br] Melting temperature $T_m$ is equal to 427.1 K with enthalpy $\Delta_m H = 12.24$ kJ mol$^{-1}$

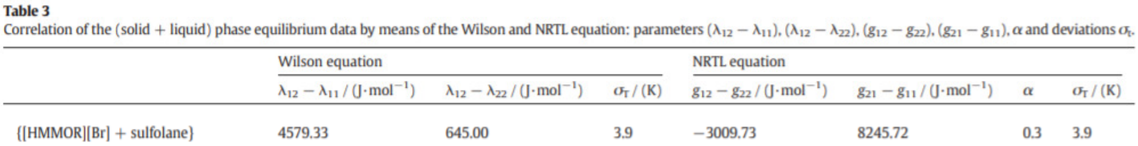


**Table 3**

Correlation of the (solid + liquid) phase equilibrium data by means of the Wilson and NRTL equation: parameters $(\lambda_{12} - \lambda_{11})$, $(\lambda_{12} - \lambda_{22})$, $(g_{12} - g_{22})$, $(g_{21} - g_{11})$, $\alpha$ and deviations $\sigma_T$.

| | Wilson equation | | | NRTL equation | | | |
|---|---|---|---|---|---|---|---|
| | $\lambda_{12} - \lambda_{11}$ / (J·mol$^{-1}$) | $\lambda_{12} - \lambda_{22}$ / (J·mol$^{-1}$) | $\sigma_T$ / (K) | $g_{12} - g_{22}$ / (J·mol$^{-1}$) | $g_{21} - g_{11}$ / (J·mol$^{-1}$) | $\alpha$ | $\sigma_T$ / (K) |
| {[HMMOR][Br] + sulfolane} | 4579.33 | 645.00 | 3.9 | −3009.73 | 8245.72 | 0.3 | 3.9 |

ODABRATI JEDAN MODEL!

naphthalene + *n*-eicosane

Kamel Khimeche, Yacine Boumrah, Mokhtar Benziane, Abdallah Dahmani, Solid–liquid equilibria and purity determination for binary *n*-alkane + naphthalene systems, Thermochimica Acta 444 (2006) 166–172

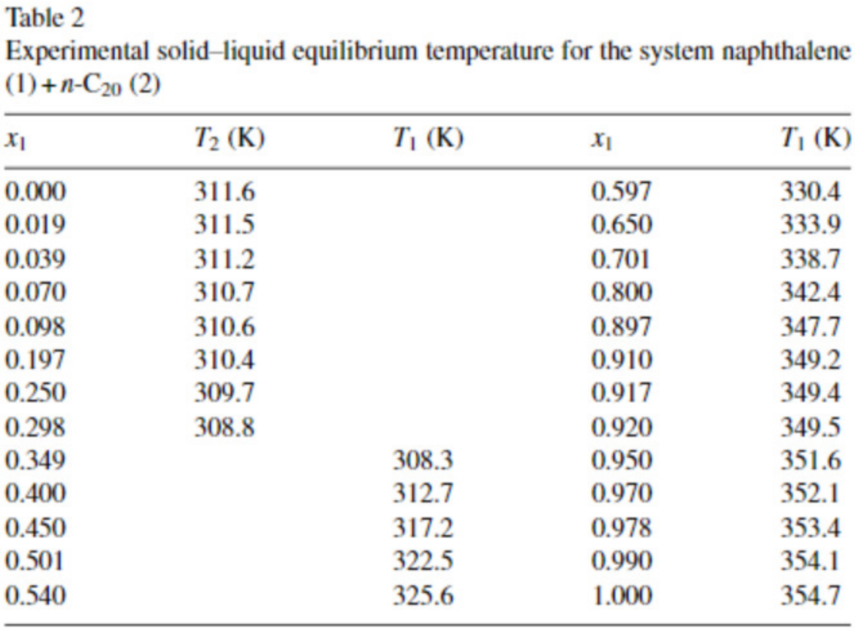


Table 2
Experimental solid–liquid equilibrium temperature for the system naphthalene (1) + *n*-$C_{20}$ (2)

| $x_1$ | $T_2$ (K) | $T_1$ (K) | $x_1$ | $T_1$ (K) |
|---|---|---|---|---|
| 0.000 | 311.6 | | 0.597 | 330.4 |
| 0.019 | 311.5 | | 0.650 | 333.9 |
| 0.039 | 311.2 | | 0.701 | 338.7 |
| 0.070 | 310.7 | | 0.800 | 342.4 |
| 0.098 | 310.6 | | 0.897 | 347.7 |
| 0.197 | 310.4 | | 0.910 | 349.2 |
| 0.250 | 309.7 | | 0.917 | 349.4 |
| 0.298 | 308.8 | | 0.920 | 349.5 |
| 0.349 | | 308.3 | 0.950 | 351.6 |
| 0.400 | | 312.7 | 0.970 | 352.1 |
| 0.450 | | 317.2 | 0.978 | 353.4 |
| 0.501 | | 322.5 | 0.990 | 354.1 |
| 0.540 | | 325.6 | 1.000 | 354.7 |

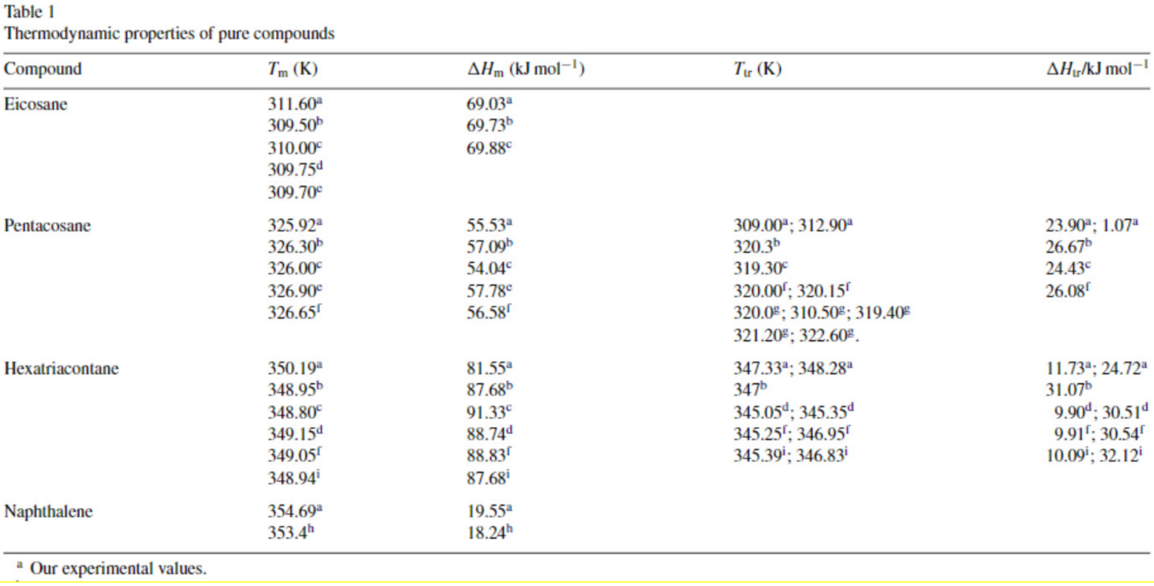


Table 1
Thermodynamic properties of pure compounds

| Compound | $T_m$ (K) | $\Delta H_m$ (kJ $mol^{-1}$) | $T_{tr}$ (K) | $\Delta H_{tr}$/kJ $mol^{-1}$ |
|---|---|---|---|---|
| Eicosane | $311.60^{a}$ | $69.03^{a}$ | | |
| | $309.50^{b}$ | $69.73^{b}$ | | |
| | $310.00^{c}$ | $69.88^{c}$ | | |
| | $309.75^{d}$ | | | |
| | $309.70^{e}$ | | | |
| Pentacosane | $325.92^{a}$ | $55.53^{a}$ | $309.00^{a}$; $312.90^{a}$ | $23.90^{a}$; $1.07^{a}$ |
| | $326.30^{b}$ | $57.09^{b}$ | $320.3^{b}$ | $26.67^{b}$ |
| | $326.00^{c}$ | $54.04^{c}$ | $319.30^{c}$ | $24.43^{c}$ |
| | $326.90^{e}$ | $57.78^{e}$ | $320.00^{f}$; $320.15^{f}$ | $26.08^{f}$ |
| | $326.65^{f}$ | $56.58^{f}$ | $320.0^{g}$; $310.50^{g}$; $319.40^{g}$ | |
| | | | $321.20^{g}$; $322.60^{g}$. | |
| Hexatriacontane | $350.19^{a}$ | $81.55^{a}$ | $347.33^{a}$; $348.28^{a}$ | $11.73^{a}$; $24.72^{a}$ |
| | $348.95^{b}$ | $87.68^{b}$ | $347^{b}$ | $31.07^{b}$ |
| | $348.80^{c}$ | $91.33^{c}$ | $345.05^{d}$; $345.35^{d}$ | $9.90^{d}$; $30.51^{d}$ |
| | $349.15^{d}$ | $88.74^{d}$ | $345.25^{f}$; $346.95^{f}$ | $9.91^{f}$; $30.54^{f}$ |
| | $349.05^{f}$ | $88.83^{f}$ | $345.39^{i}$; $346.83^{i}$ | $10.09^{i}$; $32.12^{i}$ |
| | $348.94^{i}$ | $87.68^{i}$ | | |
| Naphthalene | $354.69^{a}$ | $19.55^{a}$ | | |
| | $353.4^{h}$ | $18.24^{h}$ | | |

[a] Our experimental values.

naphthalene + *n*-pentacosane

Kamel Khimeche, Yacine Boumrah, Mokhtar Benziane, Abdallah Dahmani, Solid–liquid equilibria and purity determination for binary *n*-alkane + naphthalene systems, Thermochimica Acta 444 (2006) 166–172

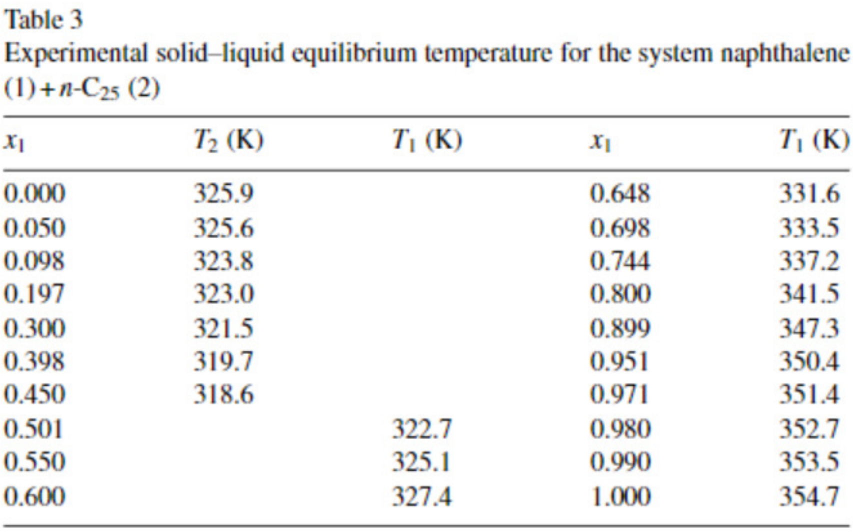


Table 3

Experimental solid–liquid equilibrium temperature for the system naphthalene (1) + $n$-$C_{25}$ (2)

| $x_1$ | $T_2$ (K) | $T_1$ (K) | $x_1$ | $T_1$ (K) |
|---|---|---|---|---|
| 0.000 | 325.9 | | 0.648 | 331.6 |
| 0.050 | 325.6 | | 0.698 | 333.5 |
| 0.098 | 323.8 | | 0.744 | 337.2 |
| 0.197 | 323.0 | | 0.800 | 341.5 |
| 0.300 | 321.5 | | 0.899 | 347.3 |
| 0.398 | 319.7 | | 0.951 | 350.4 |
| 0.450 | 318.6 | | 0.971 | 351.4 |
| 0.501 | | 322.7 | 0.980 | 352.7 |
| 0.550 | | 325.1 | 0.990 | 353.5 |
| 0.600 | | 327.4 | 1.000 | 354.7 |

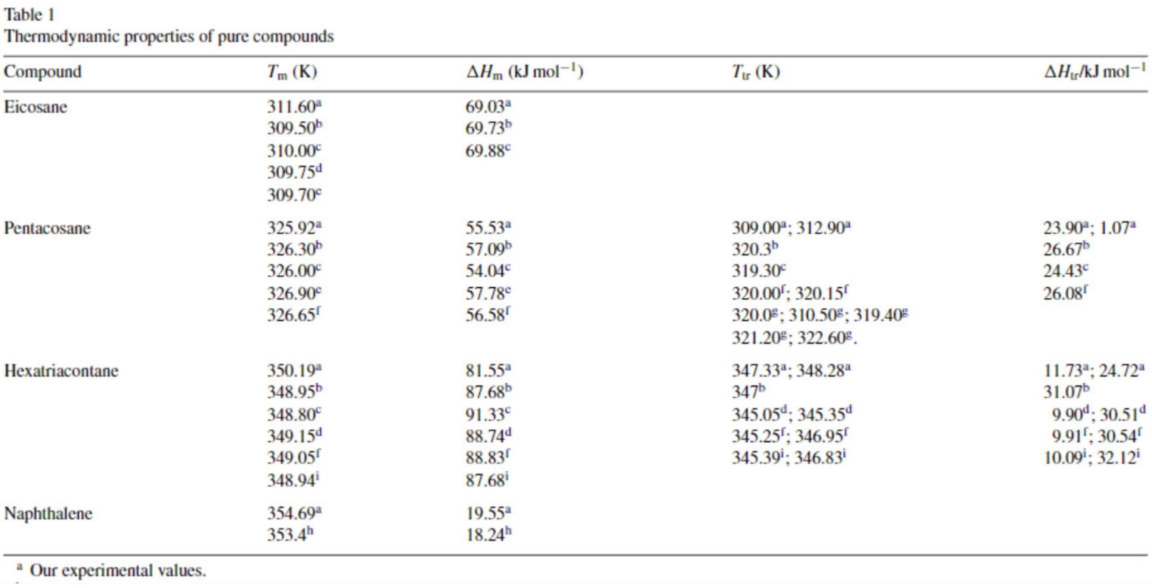


Table 1

Thermodynamic properties of pure compounds

| Compound | $T_m$ (K) | $\Delta H_m$ (kJ mol$^{-1}$) | $T_{tr}$ (K) | $\Delta H_{tr}$/kJ mol$^{-1}$ |
|---|---|---|---|---|
| Eicosane | 311.60[a]<br>309.50[b]<br>310.00[c]<br>309.75[d]<br>309.70[e] | 69.03[a]<br>69.73[b]<br>69.88[c] | | |
| Pentacosane | 325.92[a]<br>326.30[b]<br>326.00[c]<br>326.90[e]<br>326.65[f] | 55.53[a]<br>57.09[b]<br>54.04[c]<br>57.78[e]<br>56.58[f] | 309.00[a]; 312.90[a]<br>320.3[b]<br>319.30[c]<br>320.00[f]; 320.15[f]<br>320.0[g]; 310.50[g]; 319.40[g]<br>321.20[g]; 322.60[g]. | 23.90[a]; 1.07[a]<br>26.67[b]<br>24.43[c]<br>26.08[f] |
| Hexatriacontane | 350.19[a]<br>348.95[b]<br>348.80[c]<br>349.15[d]<br>349.05[f]<br>348.94[i] | 81.55[a]<br>87.68[b]<br>91.33[c]<br>88.74[d]<br>88.83[f]<br>87.68[i] | 347.33[a]; 348.28[a]<br>347[b]<br>345.05[d]; 345.35[d]<br>345.25[f]; 346.95[f]<br>345.39[i]; 346.83[i] | 11.73[a]; 24.72[a]<br>31.07[b]<br>9.90[d]; 30.51[d]<br>9.91[f]; 30.54[f]<br>10.09[i]; 32.12[i] |
| Naphthalene | 354.69[a]<br>353.4[h] | 19.55[a]<br>18.24[h] | | |

[a] Our experimental values.

naphthalene + *n*-hexatriacontane

Kamel Khimeche, Yacine Boumrah, Mokhtar Benziane, Abdallah Dahmani, Solid–liquid equilibria and purity determination for binary *n*-alkane + naphthalene systems, Thermochimica Acta 444 (2006) 166–172

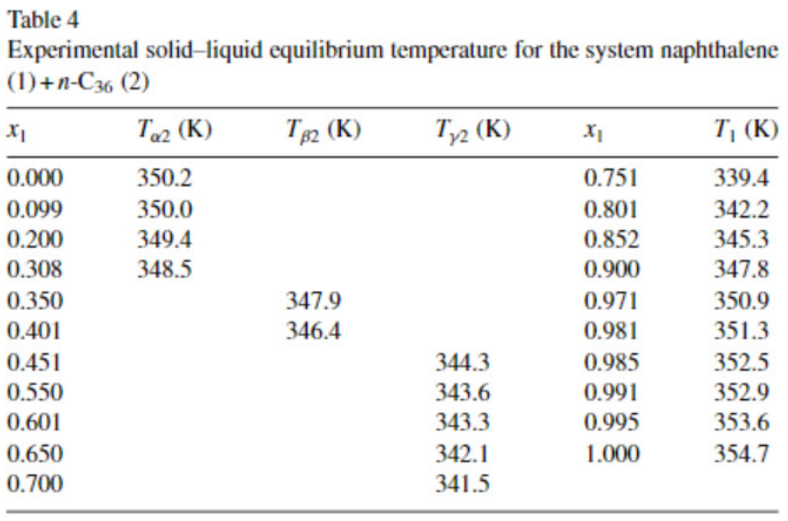


Table 4
Experimental solid–liquid equilibrium temperature for the system naphthalene (1) + $n$-$C_{36}$ (2)

| $x_1$ | $T_{\alpha 2}$ (K) | $T_{\beta 2}$ (K) | $T_{\gamma 2}$ (K) | $x_1$ | $T_1$ (K) |
|---|---|---|---|---|---|
| 0.000 | 350.2 | | | 0.751 | 339.4 |
| 0.099 | 350.0 | | | 0.801 | 342.2 |
| 0.200 | 349.4 | | | 0.852 | 345.3 |
| 0.308 | 348.5 | | | 0.900 | 347.8 |
| 0.350 | | 347.9 | | 0.971 | 350.9 |
| 0.401 | | 346.4 | | 0.981 | 351.3 |
| 0.451 | | | 344.3 | 0.985 | 352.5 |
| 0.550 | | | 343.6 | 0.991 | 352.9 |
| 0.601 | | | 343.3 | 0.995 | 353.6 |
| 0.650 | | | 342.1 | 1.000 | 354.7 |
| 0.700 | | | 341.5 | | |

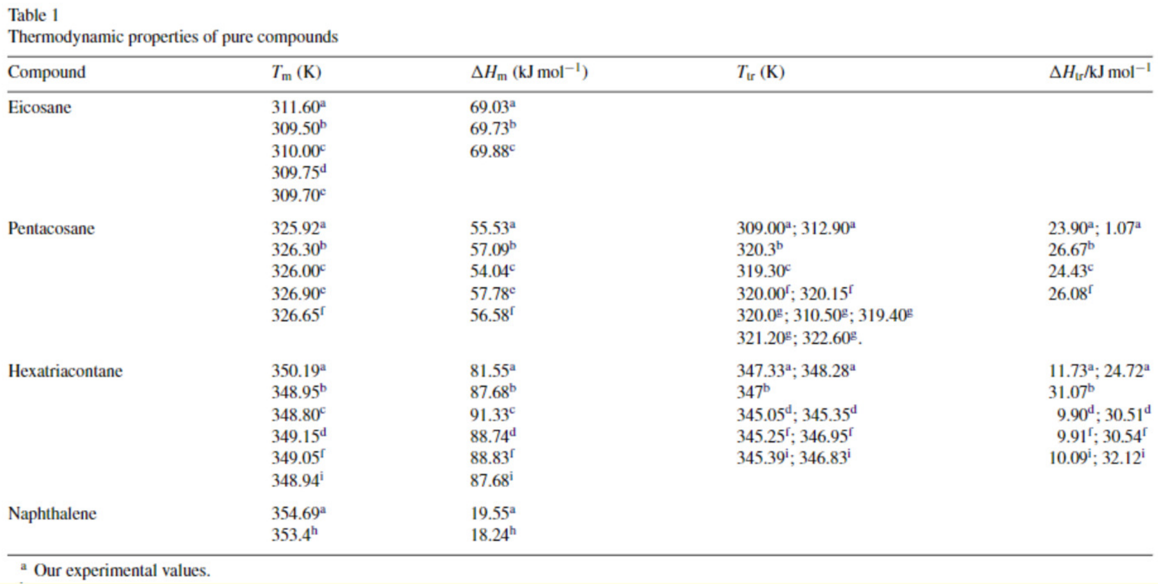


Table 1
Thermodynamic properties of pure compounds

| Compound | $T_m$ (K) | $\Delta H_m$ (kJ mol$^{-1}$) | $T_{tr}$ (K) | $\Delta H_{tr}$/kJ mol$^{-1}$ |
|---|---|---|---|---|
| Eicosane | 311.60[a]<br>309.50[b]<br>310.00[c]<br>309.75[d]<br>309.70[e] | 69.03[a]<br>69.73[b]<br>69.88[c] | | |
| Pentacosane | 325.92[a]<br>326.30[b]<br>326.00[c]<br>326.90[e]<br>326.65[f] | 55.53[a]<br>57.09[b]<br>54.04[c]<br>57.78[e]<br>56.58[f] | 309.00[a]; 312.90[a]<br>320.3[b]<br>319.30[c]<br>320.00[f]; 320.15[f]<br>320.0[g]; 310.50[g]; 319.40[g]<br>321.20[g]; 322.60[g]. | 23.90[a]; 1.07[a]<br>26.67[b]<br>24.43[c]<br>26.08[f] |
| Hexatriacontane | 350.19[a]<br>348.95[b]<br>348.80[c]<br>349.15[d]<br>349.05[f]<br>348.94[i] | 81.55[a]<br>87.68[b]<br>91.33[c]<br>88.74[d]<br>88.83[f]<br>87.68[i] | 347.33[a]; 348.28[a]<br>347[b]<br>345.05[d]; 345.35[d]<br>345.25[f]; 346.95[f]<br>345.39[i]; 346.83[i] | 11.73[a]; 24.72[a]<br>31.07[b]<br>9.90[d]; 30.51[d]<br>9.91[f]; 30.54[f]<br>10.09[i]; 32.12[i] |
| Naphthalene | 354.69[a]<br>353.4[h] | 19.55[a]<br>18.24[h] | | |

[a] Our experimental values.

*N*-nitrosodiphenylamine + diphenylamine

Ahmed Mekki, Kamel Khimeche, Abdallah Dahmani, Measurement and prediction of (solid + liquid) equilibria of gun powder's andpropellant's stabilizers mixtures, J. Chem. Thermodynamics 42 (2010) 1050–1055

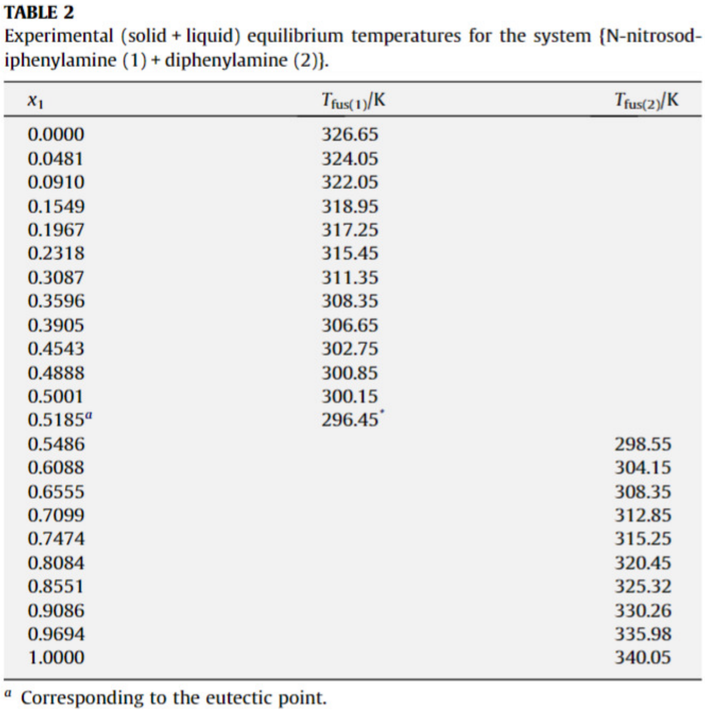


**TABLE 2**

Experimental (solid + liquid) equilibrium temperatures for the system {N-nitrosodiphenylamine (1) + diphenylamine (2)}.

| $x_1$ | $T_{fus(1)}$/K | $T_{fus(2)}$/K |
|---|---|---|
| 0.0000 | 326.65 | |
| 0.0481 | 324.05 | |
| 0.0910 | 322.05 | |
| 0.1549 | 318.95 | |
| 0.1967 | 317.25 | |
| 0.2318 | 315.45 | |
| 0.3087 | 311.35 | |
| 0.3596 | 308.35 | |
| 0.3905 | 306.65 | |
| 0.4543 | 302.75 | |
| 0.4888 | 300.85 | |
| 0.5001 | 300.15 | |
| 0.5185[a] | 296.45[*] | |
| 0.5486 | | 298.55 |
| 0.6088 | | 304.15 |
| 0.6555 | | 308.35 |
| 0.7099 | | 312.85 |
| 0.7474 | | 315.25 |
| 0.8084 | | 320.45 |
| 0.8551 | | 325.32 |
| 0.9086 | | 330.26 |
| 0.9694 | | 335.98 |
| 1.0000 | | 340.05 |

[a] Corresponding to the eutectic point.

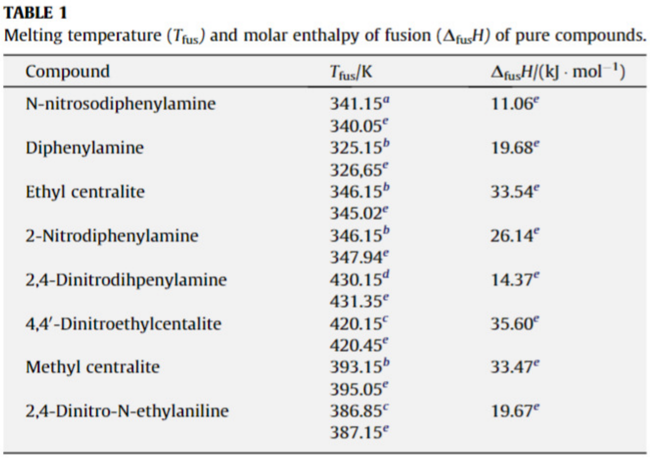


**TABLE 1**

Melting temperature ($T_{fus}$) and molar enthalpy of fusion ($\Delta_{fus}H$) of pure compounds.

| Compound | $T_{fus}$/K | $\Delta_{fus}H/(\mathrm{kJ \cdot mol^{-1}})$ |
|---|---|---|
| N-nitrosodiphenylamine | 341.15[a]<br>340.05[e] | 11.06[e] |
| Diphenylamine | 325.15[b]<br>326,65[e] | 19.68[e] |
| Ethyl centralite | 346.15[b]<br>345.02[e] | 33.54[e] |
| 2-Nitrodiphenylamine | 346.15[b]<br>347.94[e] | 26.14[e] |
| 2,4-Dinitrodihpenylamine | 430.15[d]<br>431.35[e] | 14.37[e] |
| 4,4′-Dinitroethylcentalite | 420.15[c]<br>420.45[e] | 35.60[e] |
| Methyl centralite | 393.15[b]<br>395.05[e] | 33.47[e] |
| 2,4-Dinitro-N-ethylaniline | 386.85[c]<br>387.15[e] | 19.67[e] |

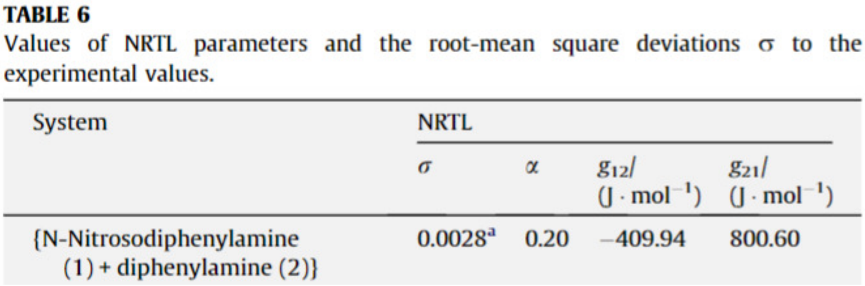


**TABLE 6**

Values of NRTL parameters and the root-mean square deviations σ to the experimental values.

| System | NRTL | | | |
|---|---|---|---|---|
| | σ | α | $g_{12}$/(J · mol$^{-1}$) | $g_{21}$/(J · mol$^{-1}$) |
| {N-Nitrosodiphenylamine (1) + diphenylamine (2)} | 0.0028[a] | 0.20 | −409.94 | 800.60 |

2-nitrodiphenyl-amine + ethyl centralite

Ahmed Mekki, Kamel Khimeche, Abdallah Dahmani, Measurement and prediction of (solid + liquid) equilibria of gun powder’s andpropellant’s stabilizers mixtures, J. Chem. Thermodynamics 42 (2010) 1050–1055

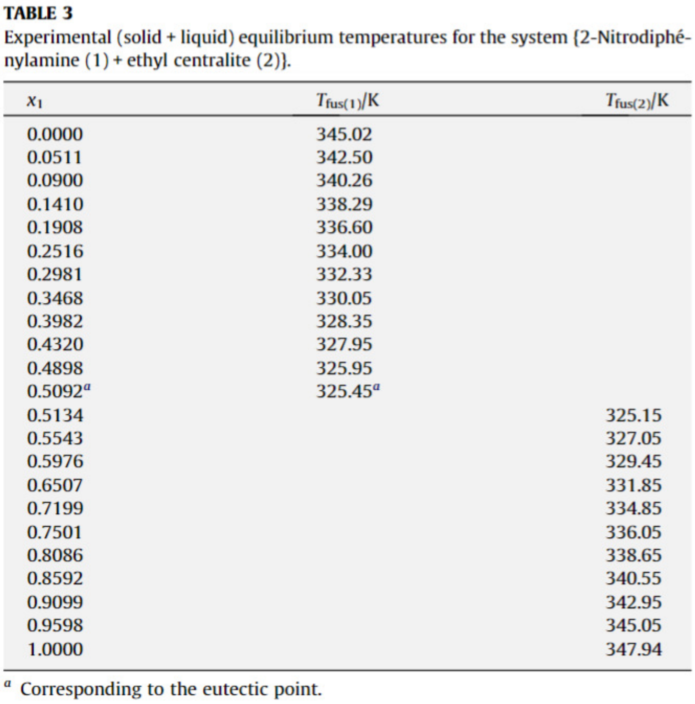


**TABLE 3**

Experimental (solid + liquid) equilibrium temperatures for the system {2-Nitrodiphénylamine (1) + ethyl centralite (2)}.

| $x_1$ | $T_{fus(1)}$/K | $T_{fus(2)}$/K |
|---|---|---|
| 0.0000 | 345.02 | |
| 0.0511 | 342.50 | |
| 0.0900 | 340.26 | |
| 0.1410 | 338.29 | |
| 0.1908 | 336.60 | |
| 0.2516 | 334.00 | |
| 0.2981 | 332.33 | |
| 0.3468 | 330.05 | |
| 0.3982 | 328.35 | |
| 0.4320 | 327.95 | |
| 0.4898 | 325.95 | |
| 0.5092[a] | 325.45[a] | |
| 0.5134 | | 325.15 |
| 0.5543 | | 327.05 |
| 0.5976 | | 329.45 |
| 0.6507 | | 331.85 |
| 0.7199 | | 334.85 |
| 0.7501 | | 336.05 |
| 0.8086 | | 338.65 |
| 0.8592 | | 340.55 |
| 0.9099 | | 342.95 |
| 0.9598 | | 345.05 |
| 1.0000 | | 347.94 |

[a] Corresponding to the eutectic point.

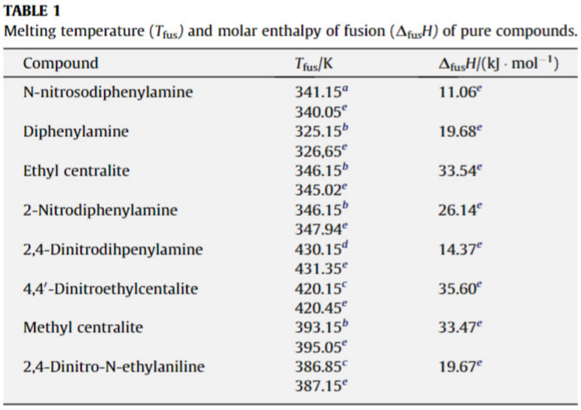


**TABLE 1**

Melting temperature ($T_{fus}$) and molar enthalpy of fusion ($\Delta_{fus}H$) of pure compounds.

| Compound | $T_{fus}$/K | $\Delta_{fus}H/(kJ \cdot mol^{-1})$ |
|---|---|---|
| N-nitrosodiphenylamine | 341.15[a]<br>340.05[e] | 11.06[e] |
| Diphenylamine | 325.15[b]<br>326,65[e] | 19.68[e] |
| Ethyl centralite | 346.15[b]<br>345.02[e] | 33.54[e] |
| 2-Nitrodiphenylamine | 346.15[b]<br>347.94[e] | 26.14[e] |
| 2,4-Dinitrodihpenylamine | 430.15[d]<br>431.35[e] | 14.37[e] |
| 4,4′-Dinitroethylcentalite | 420.15[c]<br>420.45[e] | 35.60[e] |
| Methyl centralite | 393.15[b]<br>395.05[e] | 33.47[e] |
| 2,4-Dinitro-N-ethylaniline | 386.85[c]<br>387.15[e] | 19.67[e] |

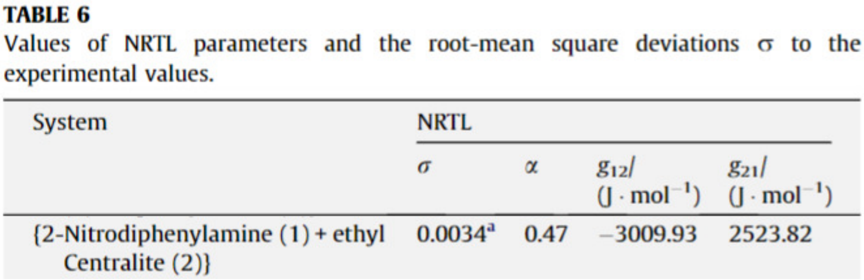


**TABLE 6**

Values of NRTL parameters and the root-mean square deviations σ to the experimental values.

| System | NRTL | | | |
|---|---|---|---|---|
| | $\sigma$ | $\alpha$ | $g_{12}/(J \cdot mol^{-1})$ | $g_{21}/(J \cdot mol^{-1})$ |
| {2-Nitrodiphenylamine (1) + ethyl Centralite (2)} | 0.0034[a] | 0.47 | −3009.93 | 2523.82 |

2,4-dinitro-*N*-ethylaniline + methyl centralite

Ahmed Mekki, Kamel Khimeche, Abdallah Dahmani, Measurement and prediction of (solid + liquid) equilibria of gun powder's andpropellant's stabilizers mixtures, J. Chem. Thermodynamics 42 (2010) 1050–1055

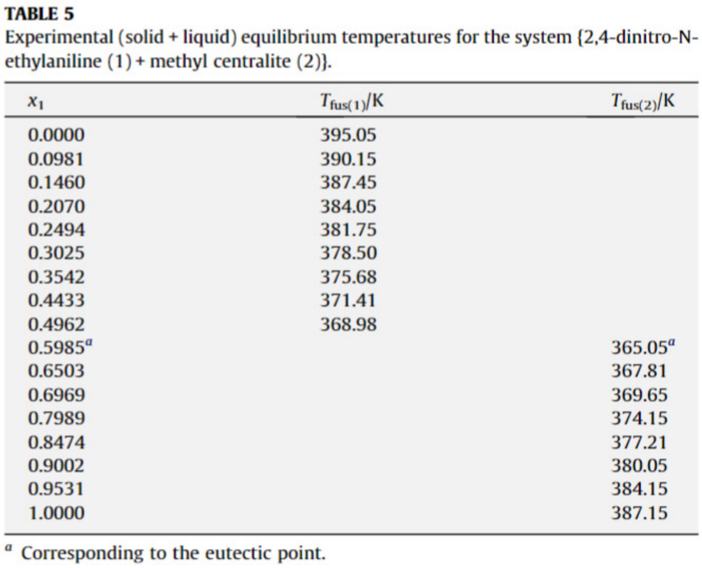


**TABLE 5**

Experimental (solid + liquid) equilibrium temperatures for the system {2,4-dinitro-N-ethylaniline (1) + methyl centralite (2)}.

| $x_1$ | $T_{fus(1)}$/K | $T_{fus(2)}$/K |
|---|---|---|
| 0.0000 | 395.05 | |
| 0.0981 | 390.15 | |
| 0.1460 | 387.45 | |
| 0.2070 | 384.05 | |
| 0.2494 | 381.75 | |
| 0.3025 | 378.50 | |
| 0.3542 | 375.68 | |
| 0.4433 | 371.41 | |
| 0.4962 | 368.98 | |
| 0.5985[a] | | 365.05[a] |
| 0.6503 | | 367.81 |
| 0.6969 | | 369.65 |
| 0.7989 | | 374.15 |
| 0.8474 | | 377.21 |
| 0.9002 | | 380.05 |
| 0.9531 | | 384.15 |
| 1.0000 | | 387.15 |

[a] Corresponding to the eutectic point.

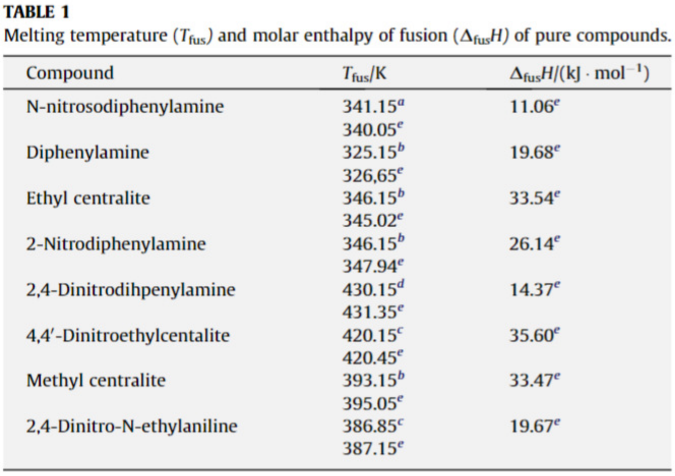


**TABLE 1**

Melting temperature ($T_{fus}$) and molar enthalpy of fusion ($\Delta_{fus}H$) of pure compounds.

| Compound | $T_{fus}$/K | $\Delta_{fus}H$/(kJ · mol$^{-1}$) |
|---|---|---|
| N-nitrosodiphenylamine | 341.15[a]<br>340.05[e] | 11.06[e] |
| Diphenylamine | 325.15[b]<br>326,65[e] | 19.68[e] |
| Ethyl centralite | 346.15[b]<br>345.02[e] | 33.54[e] |
| 2-Nitrodiphenylamine | 346.15[b]<br>347.94[e] | 26.14[e] |
| 2,4-Dinitrodihpenylamine | 430.15[d]<br>431.35[e] | 14.37[e] |
| 4,4′-Dinitroethylcentalite | 420.15[c]<br>420.45[e] | 35.60[e] |
| Methyl centralite | 393.15[b]<br>395.05[e] | 33.47[e] |
| 2,4-Dinitro-N-ethylaniline | 386.85[c]<br>387.15[e] | 19.67[e] |

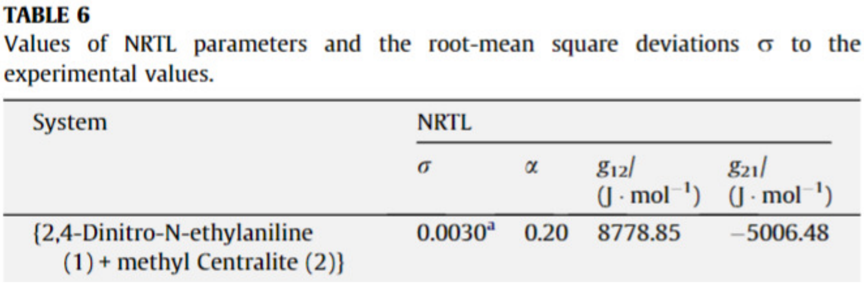


**TABLE 6**

Values of NRTL parameters and the root-mean square deviations σ to the experimental values.

| System | NRTL | | | |
|---|---|---|---|---|
| | σ | α | $g_{12}$/(J · mol$^{-1}$) | $g_{21}$/(J · mol$^{-1}$) |
| {2,4-Dinitro-N-ethylaniline (1) + methyl Centralite (2)} | 0.0030[a] | 0.20 | 8778.85 | −5006.48 |

2,4-dinitrodiphenylamine + 4,4'-dinitroethylcentralite
Ahmed Mekki, Kamel Khimeche, Abdallah Dahmani, Measurement and prediction of (solid + liquid) equilibria of gun powder’s andpropellant’s stabilizers mixtures, J. Chem. Thermodynamics 42 (2010) 1050–1055

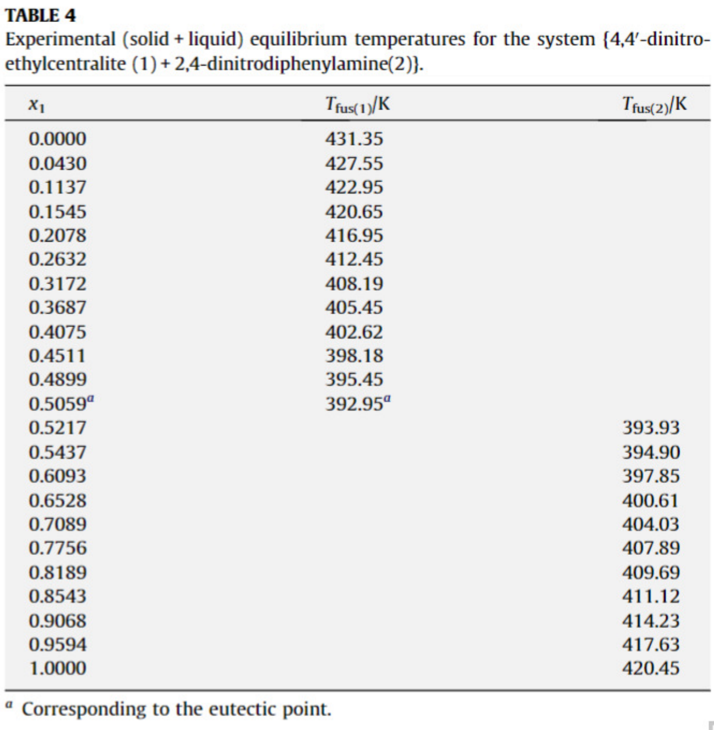


**TABLE 4**

Experimental (solid + liquid) equilibrium temperatures for the system {4,4′-dinitroethylcentralite (1) + 2,4-dinitrodiphenylamine(2)}.

| $x_1$ | $T_{fus(1)}$/K | $T_{fus(2)}$/K |
|---|---|---|
| 0.0000 | 431.35 | |
| 0.0430 | 427.55 | |
| 0.1137 | 422.95 | |
| 0.1545 | 420.65 | |
| 0.2078 | 416.95 | |
| 0.2632 | 412.45 | |
| 0.3172 | 408.19 | |
| 0.3687 | 405.45 | |
| 0.4075 | 402.62 | |
| 0.4511 | 398.18 | |
| 0.4899 | 395.45 | |
| 0.5059[a] | 392.95[a] | |
| 0.5217 | | 393.93 |
| 0.5437 | | 394.90 |
| 0.6093 | | 397.85 |
| 0.6528 | | 400.61 |
| 0.7089 | | 404.03 |
| 0.7756 | | 407.89 |
| 0.8189 | | 409.69 |
| 0.8543 | | 411.12 |
| 0.9068 | | 414.23 |
| 0.9594 | | 417.63 |
| 1.0000 | | 420.45 |

[a] Corresponding to the eutectic point.

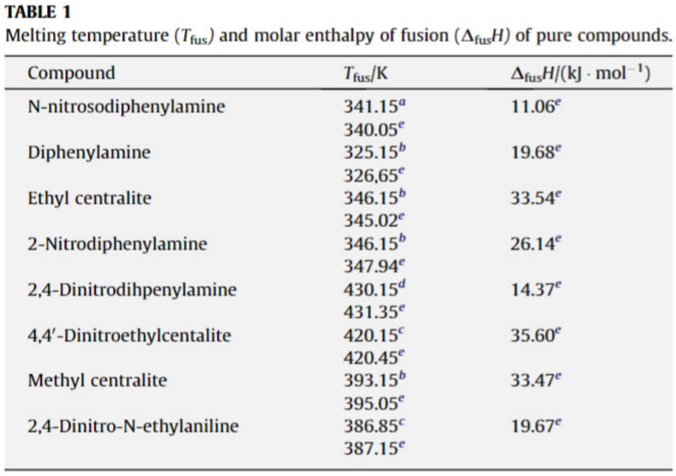


**TABLE 1**

Melting temperature ($T_{fus}$) and molar enthalpy of fusion ($\Delta_{fus}H$) of pure compounds.

| Compound | $T_{fus}$/K | $\Delta_{fus}H$/(kJ · mol$^{-1}$) |
|---|---|---|
| N-nitrosodiphenylamine | 341.15[a]<br>340.05[e] | 11.06[e] |
| Diphenylamine | 325.15[b]<br>326,65[e] | 19.68[e] |
| Ethyl centralite | 346.15[b]<br>345.02[e] | 33.54[e] |
| 2-Nitrodiphenylamine | 346.15[b]<br>347.94[e] | 26.14[e] |
| 2,4-Dinitrodihpenylamine | 430.15[d]<br>431.35[e] | 14.37[e] |
| 4,4′-Dinitroethylcentalite | 420.15[c]<br>420.45[e] | 35.60[e] |
| Methyl centralite | 393.15[b]<br>395.05[e] | 33.47[e] |
| 2,4-Dinitro-N-ethylaniline | 386.85[c]<br>387.15[e] | 19.67[e] |

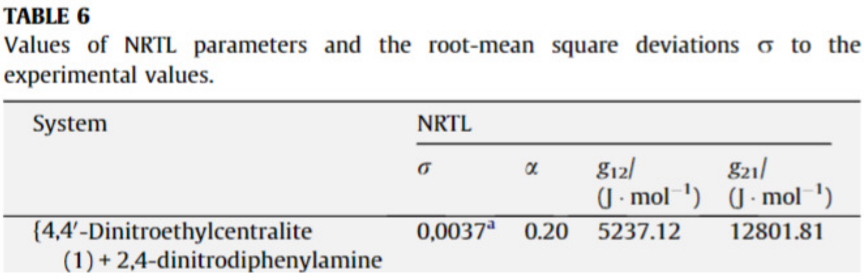


**TABLE 6**

Values of NRTL parameters and the root-mean square deviations σ to the experimental values.

| System | NRTL | | | |
|---|---|---|---|---|
| | σ | α | $g_{12}$/(J · mol$^{-1}$) | $g_{21}$/(J · mol$^{-1}$) |
| {4,4′-Dinitroethylcentralite (1) + 2,4-dinitrodiphenylamine | 0,0037[a] | 0.20 | 5237.12 | 12801.81 |

docosane + dibenzofuran
A. Chikh Baelhadj, O. Dahmani, R. Mahmoud, N. Foudil Cherif, Solid–liquid equilibria of binary and ternary systems consisting of docosane, dibenzofuran and biphenyl: Experimental data and prediction with DISQUAC model, Journal of Molecular Liquids 198 (2014) 134–138

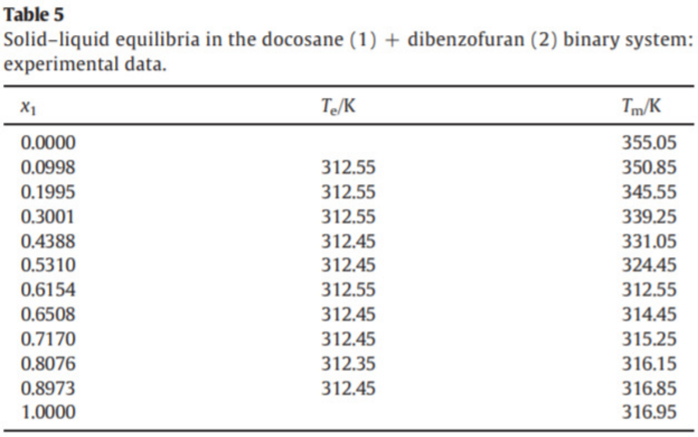


**Table 5**
Solid–liquid equilibria in the docosane (1) + dibenzofuran (2) binary system: experimental data.

| $x_1$ | $T_e$/K | $T_m$/K |
|---|---|---|
| 0.0000 | | 355.05 |
| 0.0998 | 312.55 | 350.85 |
| 0.1995 | 312.55 | 345.55 |
| 0.3001 | 312.55 | 339.25 |
| 0.4388 | 312.45 | 331.05 |
| 0.5310 | 312.45 | 324.45 |
| 0.6154 | 312.55 | 312.55 |
| 0.6508 | 312.45 | 314.45 |
| 0.7170 | 312.45 | 315.25 |
| 0.8076 | 312.35 | 316.15 |
| 0.8973 | 312.45 | 316.85 |
| 1.0000 | | 316.95 |

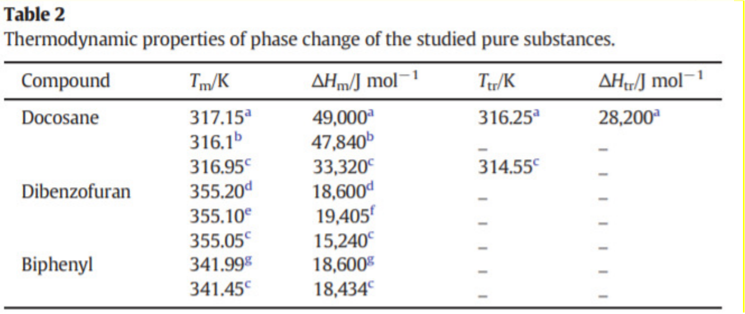


**Table 2**
Thermodynamic properties of phase change of the studied pure substances.

| Compound | $T_m$/K | $\Delta H_m$/J mol$^{-1}$ | $T_{tr}$/K | $\Delta H_{tr}$/J mol$^{-1}$ |
|---|---|---|---|---|
| Docosane | 317.15[a] | 49,000[a] | 316.25[a] | 28,200[a] |
| | 316.1[b] | 47,840[b] | – | – |
| | 316.95[c] | 33,320[c] | 314.55[c] | – |
| Dibenzofuran | 355.20[d] | 18,600[d] | – | – |
| | 355.10[e] | 19,405[f] | – | – |
| | 355.05[c] | 15,240[c] | – | – |
| Biphenyl | 341.99[g] | 18,600[g] | – | – |
| | 341.45[c] | 18,434[c] | – | – |

docosane + biphenyl

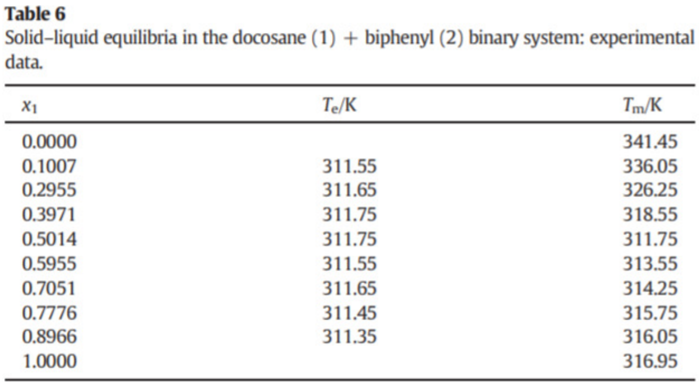


**Table 6**

Solid–liquid equilibria in the docosane (1) + biphenyl (2) binary system: experimental data.

| $x_1$ | $T_e$/K | $T_m$/K |
|---|---|---|
| 0.0000 | | 341.45 |
| 0.1007 | 311.55 | 336.05 |
| 0.2955 | 311.65 | 326.25 |
| 0.3971 | 311.75 | 318.55 |
| 0.5014 | 311.75 | 311.75 |
| 0.5955 | 311.55 | 313.55 |
| 0.7051 | 311.65 | 314.25 |
| 0.7776 | 311.45 | 315.75 |
| 0.8966 | 311.35 | 316.05 |
| 1.0000 | | 316.95 |

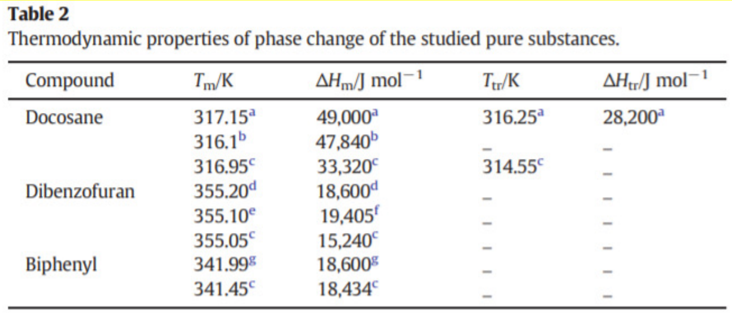


**Table 2**

Thermodynamic properties of phase change of the studied pure substances.

| Compound | $T_m$/K | $\Delta H_m$/J mol$^{-1}$ | $T_{tr}$/K | $\Delta H_{tr}$/J mol$^{-1}$ |
|---|---|---|---|---|
| Docosane | 317.15[a] | 49,000[a] | 316.25[a] | 28,200[a] |
| | 316.1[b] | 47,840[b] | – | – |
| | 316.95[c] | 33,320[c] | 314.55[c] | – |
| Dibenzofuran | 355.20[d] | 18,600[d] | – | – |
| | 355.10[e] | 19,405[f] | – | – |
| | 355.05[c] | 15,240[c] | – | – |
| Biphenyl | 341.99[g] | 18,600[g] | – | – |
| | 341.45[c] | 18,434[c] | – | – |

dibenzofuran + biphenyl

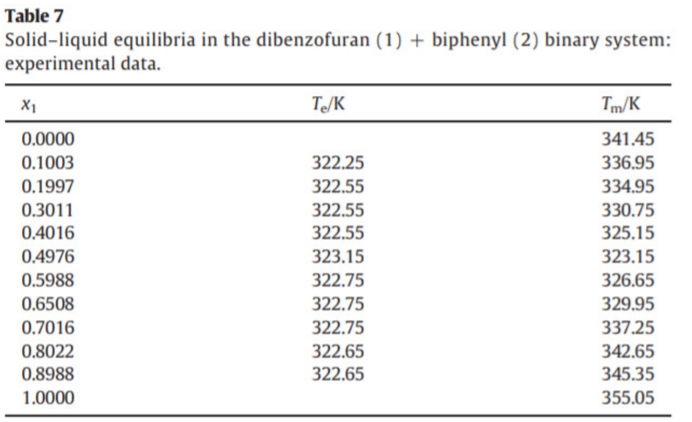


**Table 7**
Solid–liquid equilibria in the dibenzofuran (1) + biphenyl (2) binary system: experimental data.

| $x_1$ | $T_e$/K | $T_m$/K |
|---|---|---|
| 0.0000 | | 341.45 |
| 0.1003 | 322.25 | 336.95 |
| 0.1997 | 322.55 | 334.95 |
| 0.3011 | 322.55 | 330.75 |
| 0.4016 | 322.55 | 325.15 |
| 0.4976 | 323.15 | 323.15 |
| 0.5988 | 322.75 | 326.65 |
| 0.6508 | 322.75 | 329.95 |
| 0.7016 | 322.75 | 337.25 |
| 0.8022 | 322.65 | 342.65 |
| 0.8988 | 322.65 | 345.35 |
| 1.0000 | | 355.05 |

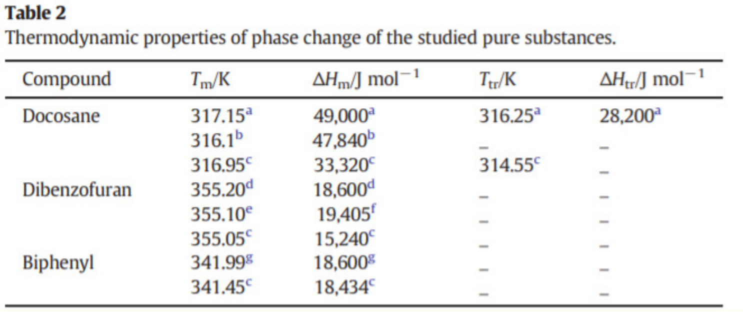


**Table 2**
Thermodynamic properties of phase change of the studied pure substances.

| Compound | $T_m$/K | $\Delta H_m$/J mol$^{-1}$ | $T_{tr}$/K | $\Delta H_{tr}$/J mol$^{-1}$ |
|---|---|---|---|---|
| Docosane | 317.15[a] | 49,000[a] | 316.25[a] | 28,200[a] |
| | 316.1[b] | 47,840[b] | – | – |
| | 316.95[c] | 33,320[c] | 314.55[c] | – |
| Dibenzofuran | 355.20[d] | 18,600[d] | – | – |
| | 355.10[e] | 19,405[f] | – | – |
| | 355.05[c] | 15,240[c] | – | – |
| Biphenyl | 341.99[g] | 18,600[g] | – | – |
| | 341.45[c] | 18,434[c] | – | – |

*N*-phenylacetamide + 4-aminoacetophenone

Yan-Ping Chen, Muoi Tang, Ju-Chia Kuo, Solid–liquid equilibria for binary mixtures of *N*-phenylacetamide with 4-aminoacetophenone, 3-hydroxyacetophenone and 4-hydroxyacetophenone, Fluid Phase Equilibria 232 (2005) 182–188

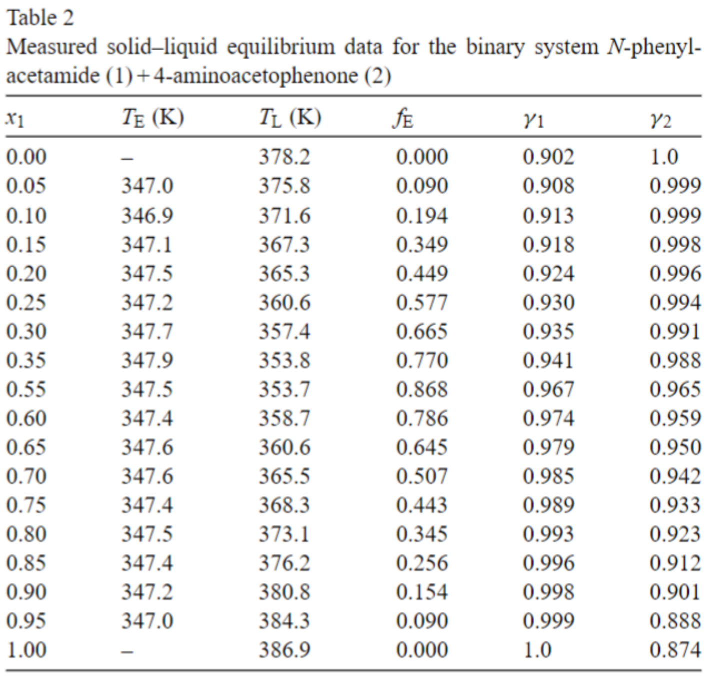


Table 2
Measured solid–liquid equilibrium data for the binary system *N*-phenylacetamide (1) + 4-aminoacetophenone (2)

| $x_1$ | $T_E$ (K) | $T_L$ (K) | $f_E$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|---|
| 0.00 | – | 378.2 | 0.000 | 0.902 | 1.0 |
| 0.05 | 347.0 | 375.8 | 0.090 | 0.908 | 0.999 |
| 0.10 | 346.9 | 371.6 | 0.194 | 0.913 | 0.999 |
| 0.15 | 347.1 | 367.3 | 0.349 | 0.918 | 0.998 |
| 0.20 | 347.5 | 365.3 | 0.449 | 0.924 | 0.996 |
| 0.25 | 347.2 | 360.6 | 0.577 | 0.930 | 0.994 |
| 0.30 | 347.7 | 357.4 | 0.665 | 0.935 | 0.991 |
| 0.35 | 347.9 | 353.8 | 0.770 | 0.941 | 0.988 |
| 0.55 | 347.5 | 353.7 | 0.868 | 0.967 | 0.965 |
| 0.60 | 347.4 | 358.7 | 0.786 | 0.974 | 0.959 |
| 0.65 | 347.6 | 360.6 | 0.645 | 0.979 | 0.950 |
| 0.70 | 347.6 | 365.5 | 0.507 | 0.985 | 0.942 |
| 0.75 | 347.4 | 368.3 | 0.443 | 0.989 | 0.933 |
| 0.80 | 347.5 | 373.1 | 0.345 | 0.993 | 0.923 |
| 0.85 | 347.4 | 376.2 | 0.256 | 0.996 | 0.912 |
| 0.90 | 347.2 | 380.8 | 0.154 | 0.998 | 0.901 |
| 0.95 | 347.0 | 384.3 | 0.090 | 0.999 | 0.888 |
| 1.00 | – | 386.9 | 0.000 | 1.0 | 0.874 |

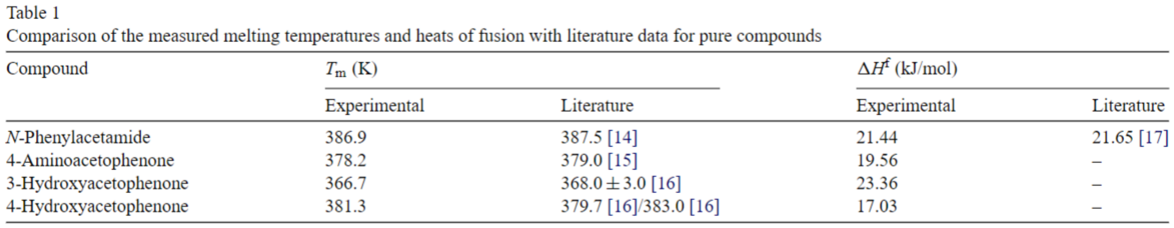


Table 1
Comparison of the measured melting temperatures and heats of fusion with literature data for pure compounds

| Compound | $T_m$ (K) | | $\Delta H^f$ (kJ/mol) | |
|---|---|---|---|---|
| | Experimental | Literature | Experimental | Literature |
| *N*-Phenylacetamide | 386.9 | 387.5 [14] | 21.44 | 21.65 [17] |
| 4-Aminoacetophenone | 378.2 | 379.0 [15] | 19.56 | – |
| 3-Hydroxyacetophenone | 366.7 | 368.0 ± 3.0 [16] | 23.36 | – |
| 4-Hydroxyacetophenone | 381.3 | 379.7 [16]/383.0 [16] | 17.03 | – |

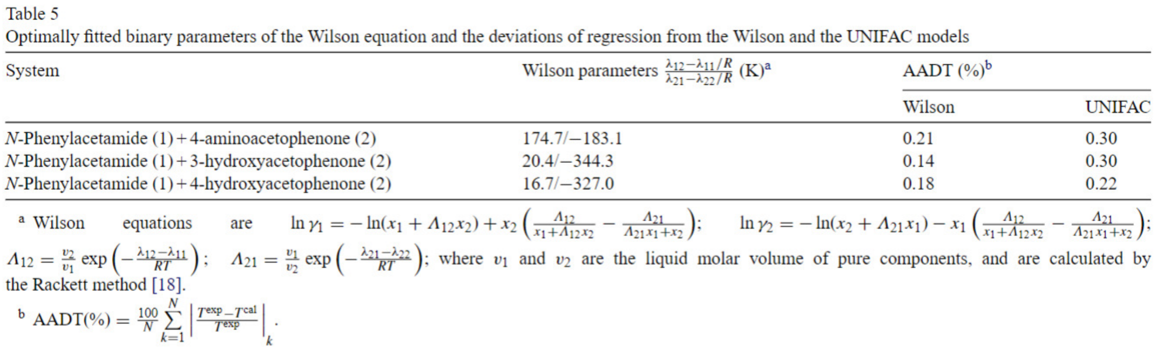


Table 5
Optimally fitted binary parameters of the Wilson equation and the deviations of regression from the Wilson and the UNIFAC models

| System | Wilson parameters $\frac{\lambda_{12}-\lambda_{11}/R}{\lambda_{21}-\lambda_{22}/R}$ (K)[a] | AADT (%)[b] | |
|---|---|---|---|
| | | Wilson | UNIFAC |
| *N*-Phenylacetamide (1) + 4-aminoacetophenone (2) | 174.7/−183.1 | 0.21 | 0.30 |
| *N*-Phenylacetamide (1) + 3-hydroxyacetophenone (2) | 20.4/−344.3 | 0.14 | 0.30 |
| *N*-Phenylacetamide (1) + 4-hydroxyacetophenone (2) | 16.7/−327.0 | 0.18 | 0.22 |

[a] Wilson equations are $\ln\gamma_1 = -\ln(x_1 + \Lambda_{12}x_2) + x_2\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1+x_2}\right)$; $\ln\gamma_2 = -\ln(x_2 + \Lambda_{21}x_1) - x_1\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1+x_2}\right)$; $\Lambda_{12} = \frac{v_2}{v_1}\exp\left(-\frac{\lambda_{12}-\lambda_{11}}{RT}\right)$; $\Lambda_{21} = \frac{v_1}{v_2}\exp\left(-\frac{\lambda_{21}-\lambda_{22}}{RT}\right)$; where $v_1$ and $v_2$ are the liquid molar volume of pure components, and are calculated by the Rackett method [18].

[b] $\mathrm{AADT}(\%) = \frac{100}{N}\sum_{k=1}^{N}\left|\frac{T^{\exp}-T^{\mathrm{cal}}}{T^{\exp}}\right|_k$.

*N*-phenylacetamide + 3-hydroxyacetophenone

Yan-Ping Chen, Muoi Tang, Ju-Chia Kuo, Solid–liquid equilibria for binary mixtures of *N*-phenylacetamide with 4-aminoacetophenone, 3-hydroxyacetophenone and 4-hydroxyacetophenone, Fluid Phase Equilibria 232 (2005) 182–188

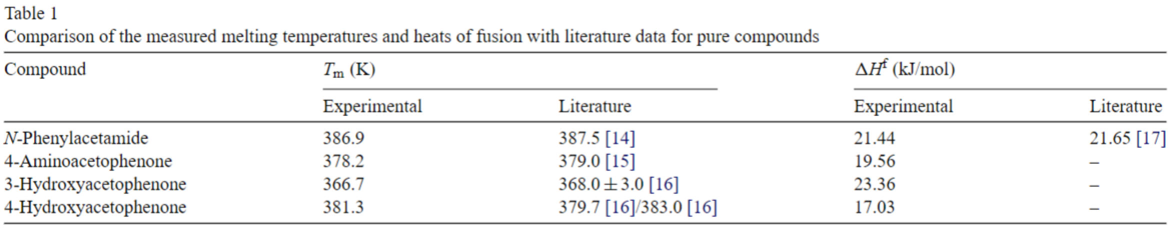


Table 1
Comparison of the measured melting temperatures and heats of fusion with literature data for pure compounds

| Compound | $T_m$ (K) | | $\Delta H^f$ (kJ/mol) | |
|---|---|---|---|---|
| | Experimental | Literature | Experimental | Literature |
| *N*-Phenylacetamide | 386.9 | 387.5 [14] | 21.44 | 21.65 [17] |
| 4-Aminoacetophenone | 378.2 | 379.0 [15] | 19.56 | – |
| 3-Hydroxyacetophenone | 366.7 | 368.0 ± 3.0 [16] | 23.36 | – |
| 4-Hydroxyacetophenone | 381.3 | 379.7 [16]/383.0 [16] | 17.03 | – |

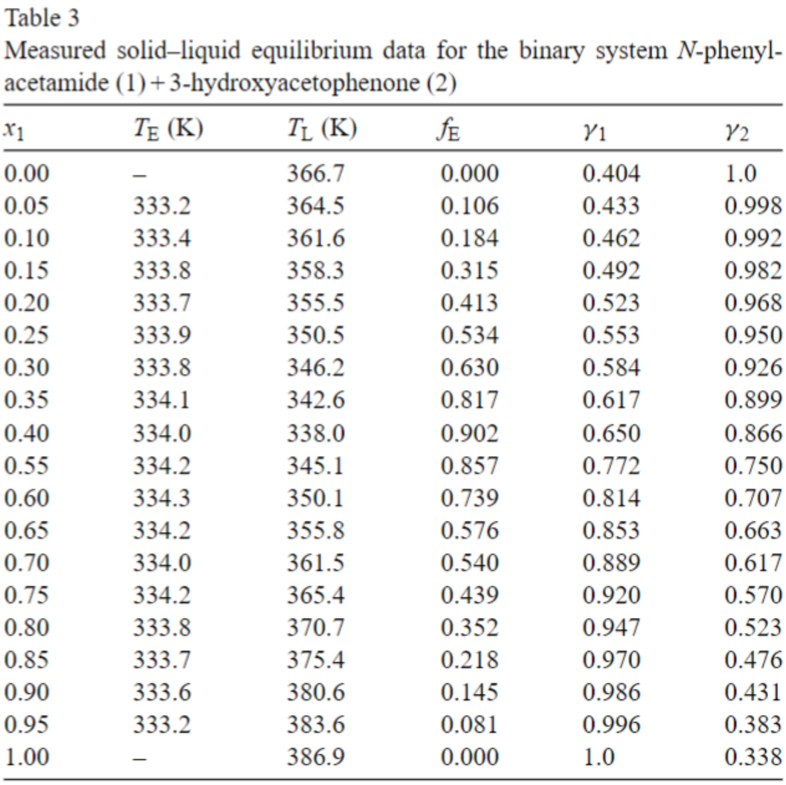


Table 3
Measured solid–liquid equilibrium data for the binary system *N*-phenylacetamide (1) + 3-hydroxyacetophenone (2)

| $x_1$ | $T_E$ (K) | $T_L$ (K) | $f_E$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|---|
| 0.00 | – | 366.7 | 0.000 | 0.404 | 1.0 |
| 0.05 | 333.2 | 364.5 | 0.106 | 0.433 | 0.998 |
| 0.10 | 333.4 | 361.6 | 0.184 | 0.462 | 0.992 |
| 0.15 | 333.8 | 358.3 | 0.315 | 0.492 | 0.982 |
| 0.20 | 333.7 | 355.5 | 0.413 | 0.523 | 0.968 |
| 0.25 | 333.9 | 350.5 | 0.534 | 0.553 | 0.950 |
| 0.30 | 333.8 | 346.2 | 0.630 | 0.584 | 0.926 |
| 0.35 | 334.1 | 342.6 | 0.817 | 0.617 | 0.899 |
| 0.40 | 334.0 | 338.0 | 0.902 | 0.650 | 0.866 |
| 0.55 | 334.2 | 345.1 | 0.857 | 0.772 | 0.750 |
| 0.60 | 334.3 | 350.1 | 0.739 | 0.814 | 0.707 |
| 0.65 | 334.2 | 355.8 | 0.576 | 0.853 | 0.663 |
| 0.70 | 334.0 | 361.5 | 0.540 | 0.889 | 0.617 |
| 0.75 | 334.2 | 365.4 | 0.439 | 0.920 | 0.570 |
| 0.80 | 333.8 | 370.7 | 0.352 | 0.947 | 0.523 |
| 0.85 | 333.7 | 375.4 | 0.218 | 0.970 | 0.476 |
| 0.90 | 333.6 | 380.6 | 0.145 | 0.986 | 0.431 |
| 0.95 | 333.2 | 383.6 | 0.081 | 0.996 | 0.383 |
| 1.00 | – | 386.9 | 0.000 | 1.0 | 0.338 |

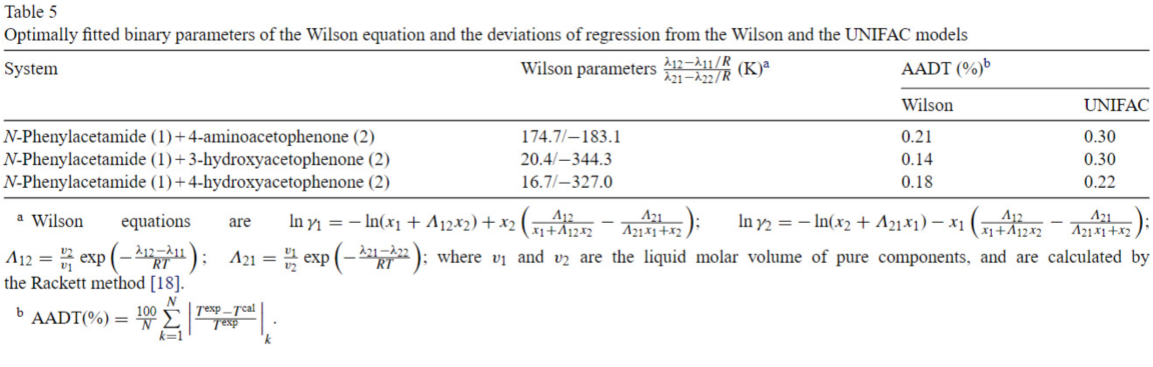


Table 5
Optimally fitted binary parameters of the Wilson equation and the deviations of regression from the Wilson and the UNIFAC models

| System | Wilson parameters $\frac{\lambda_{12}-\lambda_{11}/R}{\lambda_{21}-\lambda_{22}/R}$ (K)[a] | AADT (%)[b] | |
|---|---|---|---|
| | | Wilson | UNIFAC |
| *N*-Phenylacetamide (1) + 4-aminoacetophenone (2) | 174.7/−183.1 | 0.21 | 0.30 |
| *N*-Phenylacetamide (1) + 3-hydroxyacetophenone (2) | 20.4/−344.3 | 0.14 | 0.30 |
| *N*-Phenylacetamide (1) + 4-hydroxyacetophenone (2) | 16.7/−327.0 | 0.18 | 0.22 |

[a] Wilson equations are $\ln\gamma_1 = -\ln(x_1 + \Lambda_{12}x_2) + x_2\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1+x_2}\right)$; $\ln\gamma_2 = -\ln(x_2 + \Lambda_{21}x_1) - x_1\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1+x_2}\right)$; $\Lambda_{12} = \frac{v_2}{v_1}\exp\left(-\frac{\lambda_{12}-\lambda_{11}}{RT}\right)$; $\Lambda_{21} = \frac{v_1}{v_2}\exp\left(-\frac{\lambda_{21}-\lambda_{22}}{RT}\right)$; where $v_1$ and $v_2$ are the liquid molar volume of pure components, and are calculated by the Rackett method [18].

[b] $\mathrm{AADT}(\%) = \frac{100}{N}\sum_{k=1}^{N}\left|\frac{T^{\exp}-T^{\mathrm{cal}}}{T^{\exp}}\right|_k$.

*N*-phenylacetamide + 4-hydroxyacetophenone

Yan-Ping Chen, Muoi Tang, Ju-Chia Kuo, Solid–liquid equilibria for binary mixtures of *N*-phenylacetamide with 4-aminoacetophenone, 3-hydroxyacetophenone and 4-hydroxyacetophenone, Fluid Phase Equilibria 232 (2005) 182–188

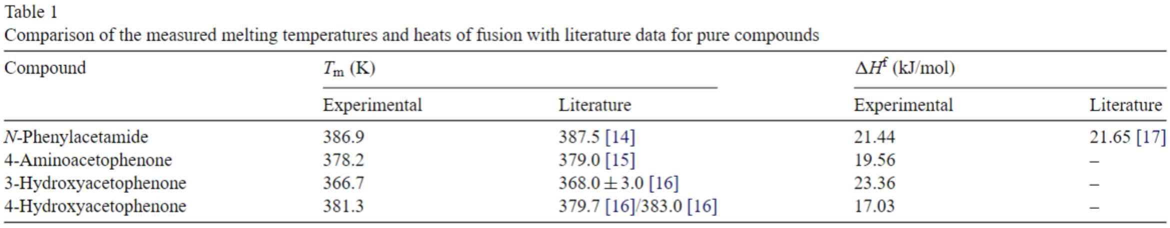


Table 1

Comparison of the measured melting temperatures and heats of fusion with literature data for pure compounds

| Compound | $T_m$ (K) |  | $\Delta H^f$ (kJ/mol) |  |
|---|---|---|---|---|
|  | Experimental | Literature | Experimental | Literature |
| *N*-Phenylacetamide | 386.9 | 387.5 [14] | 21.44 | 21.65 [17] |
| 4-Aminoacetophenone | 378.2 | 379.0 [15] | 19.56 | – |
| 3-Hydroxyacetophenone | 366.7 | 368.0 ± 3.0 [16] | 23.36 | – |
| 4-Hydroxyacetophenone | 381.3 | 379.7 [16]/383.0 [16] | 17.03 | – |

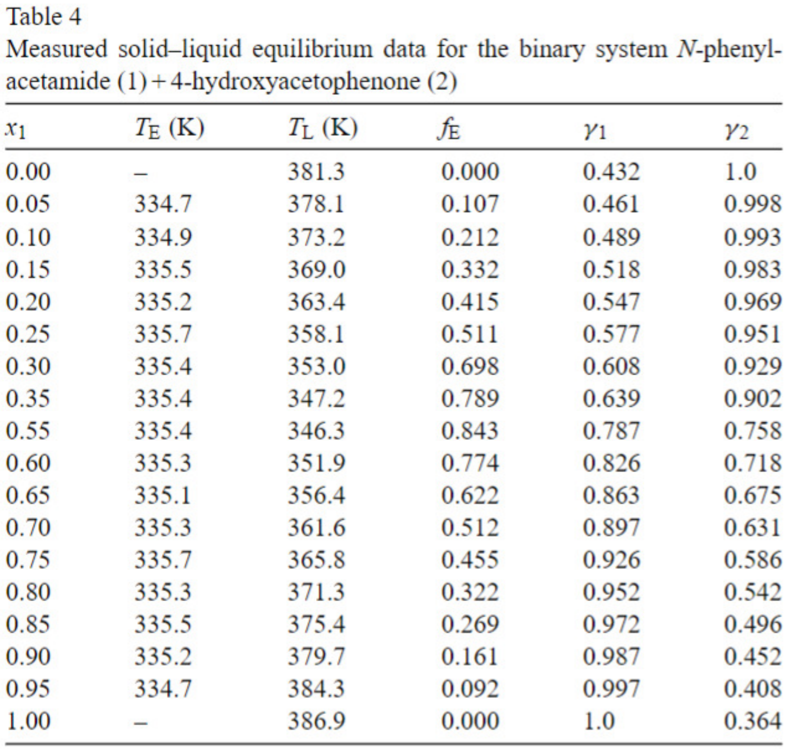


Table 4

Measured solid–liquid equilibrium data for the binary system *N*-phenylacetamide (1) + 4-hydroxyacetophenone (2)

| $x_1$ | $T_E$ (K) | $T_L$ (K) | $f_E$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|---|
| 0.00 | – | 381.3 | 0.000 | 0.432 | 1.0 |
| 0.05 | 334.7 | 378.1 | 0.107 | 0.461 | 0.998 |
| 0.10 | 334.9 | 373.2 | 0.212 | 0.489 | 0.993 |
| 0.15 | 335.5 | 369.0 | 0.332 | 0.518 | 0.983 |
| 0.20 | 335.2 | 363.4 | 0.415 | 0.547 | 0.969 |
| 0.25 | 335.7 | 358.1 | 0.511 | 0.577 | 0.951 |
| 0.30 | 335.4 | 353.0 | 0.698 | 0.608 | 0.929 |
| 0.35 | 335.4 | 347.2 | 0.789 | 0.639 | 0.902 |
| 0.55 | 335.4 | 346.3 | 0.843 | 0.787 | 0.758 |
| 0.60 | 335.3 | 351.9 | 0.774 | 0.826 | 0.718 |
| 0.65 | 335.1 | 356.4 | 0.622 | 0.863 | 0.675 |
| 0.70 | 335.3 | 361.6 | 0.512 | 0.897 | 0.631 |
| 0.75 | 335.7 | 365.8 | 0.455 | 0.926 | 0.586 |
| 0.80 | 335.3 | 371.3 | 0.322 | 0.952 | 0.542 |
| 0.85 | 335.5 | 375.4 | 0.269 | 0.972 | 0.496 |
| 0.90 | 335.2 | 379.7 | 0.161 | 0.987 | 0.452 |
| 0.95 | 334.7 | 384.3 | 0.092 | 0.997 | 0.408 |
| 1.00 | – | 386.9 | 0.000 | 1.0 | 0.364 |

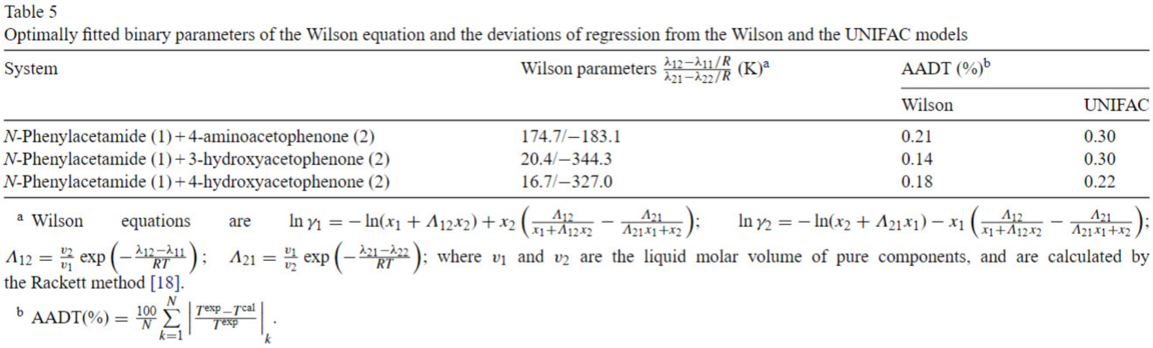


Table 5

Optimally fitted binary parameters of the Wilson equation and the deviations of regression from the Wilson and the UNIFAC models

| System | Wilson parameters $\frac{\lambda_{12}-\lambda_{11}/R}{\lambda_{21}-\lambda_{22}/R}$ (K)[a] | AADT (%)[b] |  |
|---|---|---|---|
|  |  | Wilson | UNIFAC |
| *N*-Phenylacetamide (1) + 4-aminoacetophenone (2) | 174.7/−183.1 | 0.21 | 0.30 |
| *N*-Phenylacetamide (1) + 3-hydroxyacetophenone (2) | 20.4/−344.3 | 0.14 | 0.30 |
| *N*-Phenylacetamide (1) + 4-hydroxyacetophenone (2) | 16.7/−327.0 | 0.18 | 0.22 |

[a] Wilson equations are $\ln \gamma_1 = -\ln(x_1 + \Lambda_{12}x_2) + x_2\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1+x_2}\right)$; $\ln \gamma_2 = -\ln(x_2 + \Lambda_{21}x_1) - x_1\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1+x_2}\right)$; $\Lambda_{12} = \frac{v_2}{v_1}\exp\left(-\frac{\lambda_{12}-\lambda_{11}}{RT}\right)$; $\Lambda_{21} = \frac{v_1}{v_2}\exp\left(-\frac{\lambda_{21}-\lambda_{22}}{RT}\right)$; where $v_1$ and $v_2$ are the liquid molar volume of pure components, and are calculated by the Rackett method [18].

[b] $\mathrm{AADT}(\%) = \frac{100}{N}\sum_{k=1}^{N}\left|\frac{T^{\exp}-T^{\mathrm{cal}}}{T^{\exp}}\right|_k$.

benzene + ethyl myristate

Eileen Collinet, Jürgen Gmehling, Activity coefficient at infinite dilution, azeotropic data,excess enthalpies and solid–liquid-equilibria for binarysystems of alkanes and aromatics with esters, Fluid Phase Equilibria 230 (2005) 131–142

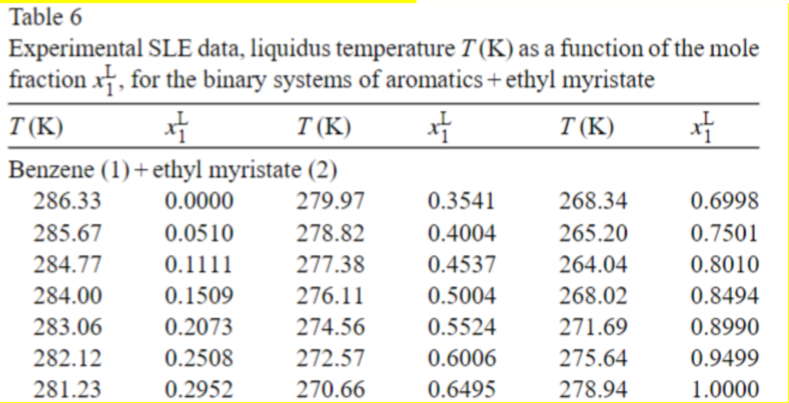


Table 6

Experimental SLE data, liquidus temperature $T$ (K) as a function of the mole fraction $x_1^L$, for the binary systems of aromatics + ethyl myristate

| $T$ (K) | $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) | $x_1^L$ |
|---|---|---|---|---|---|
| Benzene (1) + ethyl myristate (2) | | | | | |
| 286.33 | 0.0000 | 279.97 | 0.3541 | 268.34 | 0.6998 |
| 285.67 | 0.0510 | 278.82 | 0.4004 | 265.20 | 0.7501 |
| 284.77 | 0.1111 | 277.38 | 0.4537 | 264.04 | 0.8010 |
| 284.00 | 0.1509 | 276.11 | 0.5004 | 268.02 | 0.8494 |
| 283.06 | 0.2073 | 274.56 | 0.5524 | 271.69 | 0.8990 |
| 282.12 | 0.2508 | 272.57 | 0.6006 | 275.64 | 0.9499 |
| 281.23 | 0.2952 | 270.66 | 0.6495 | 278.94 | 1.0000 |

ethyl myristate + *p*-xylene

Eileen Collinet, Jürgen Gmehling, Activity coefficient at infinite dilution, azeotropic data,excess enthalpies and solid–liquid-equilibria for binarysystems of alkanes and aromatics with esters, Fluid Phase Equilibria 230 (2005) 131–142

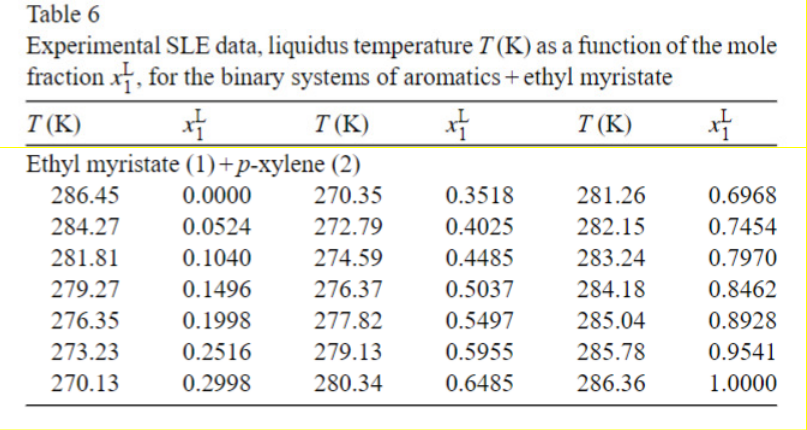


Table 6

Experimental SLE data, liquidus temperature $T$ (K) as a function of the mole fraction $x_1^L$, for the binary systems of aromatics + ethyl myristate

| $T$ (K) | $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) | $x_1^L$ |
|---|---|---|---|---|---|
| Ethyl myristate (1) + *p*-xylene (2) | | | | | |
| 286.45 | 0.0000 | 270.35 | 0.3518 | 281.26 | 0.6968 |
| 284.27 | 0.0524 | 272.79 | 0.4025 | 282.15 | 0.7454 |
| 281.81 | 0.1040 | 274.59 | 0.4485 | 283.24 | 0.7970 |
| 279.27 | 0.1496 | 276.37 | 0.5037 | 284.18 | 0.8462 |
| 276.35 | 0.1998 | 277.82 | 0.5497 | 285.04 | 0.8928 |
| 273.23 | 0.2516 | 279.13 | 0.5955 | 285.78 | 0.9541 |
| 270.13 | 0.2998 | 280.34 | 0.6485 | 286.36 | 1.0000 |

butyl-3-methylpyridinium tosylate + water
Trevor M. Letcher, Deresh Ramjugernath, Kaniki Tumba, Marek Królikowski, Urszula Domanska, (Solid + liquid) and (liquid + liquid) phase equilibria study and correlationof the binary systems {*N*-butyl-3-methylpyridinium tosylate + water,or + an alcohol, or + a hydrocarbon}, Fluid Phase Equilibria 294 (2010) 89–97

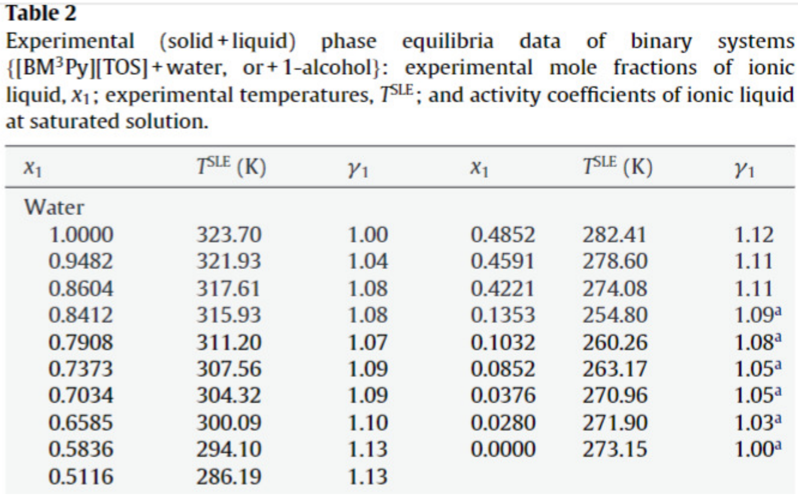


**Table 2**

Experimental (solid + liquid) phase equilibria data of binary systems {[BM$^3$Py][TOS] + water, or + 1-alcohol}: experimental mole fractions of ionic liquid, $x_1$; experimental temperatures, $T^{SLE}$; and activity coefficients of ionic liquid at saturated solution.

| $x_1$ | $T^{SLE}$ (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| Water | | | | | |
| 1.0000 | 323.70 | 1.00 | 0.4852 | 282.41 | 1.12 |
| 0.9482 | 321.93 | 1.04 | 0.4591 | 278.60 | 1.11 |
| 0.8604 | 317.61 | 1.08 | 0.4221 | 274.08 | 1.11 |
| 0.8412 | 315.93 | 1.08 | 0.1353 | 254.80 | 1.09[a] |
| 0.7908 | 311.20 | 1.07 | 0.1032 | 260.26 | 1.08[a] |
| 0.7373 | 307.56 | 1.09 | 0.0852 | 263.17 | 1.05[a] |
| 0.7034 | 304.32 | 1.09 | 0.0376 | 270.96 | 1.05[a] |
| 0.6585 | 300.09 | 1.10 | 0.0280 | 271.90 | 1.03[a] |
| 0.5836 | 294.10 | 1.13 | 0.0000 | 273.15 | 1.00[a] |
| 0.5116 | 286.19 | 1.13 | | | |

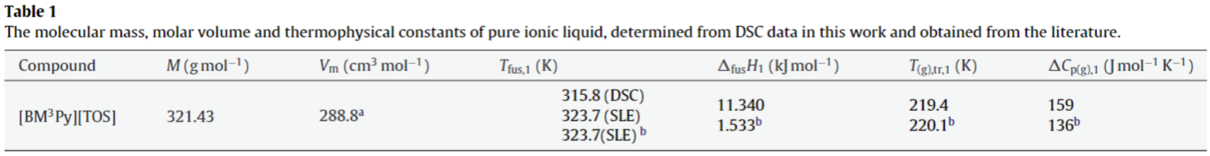


**Table 1**

The molecular mass, molar volume and thermophysical constants of pure ionic liquid, determined from DSC data in this work and obtained from the literature.

| Compound | $M$ (g mol$^{-1}$) | $V_m$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $T_{(g),tr,1}$ (K) | $\Delta C_{p(g),1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| [BM$^3$Py][TOS] | 321.43 | 288.8[a] | 315.8 (DSC)<br>323.7 (SLE)<br>323.7(SLE) [b] | 11.340<br>1.533[b] | 219.4<br>220.1[b] | 159<br>136[b] |

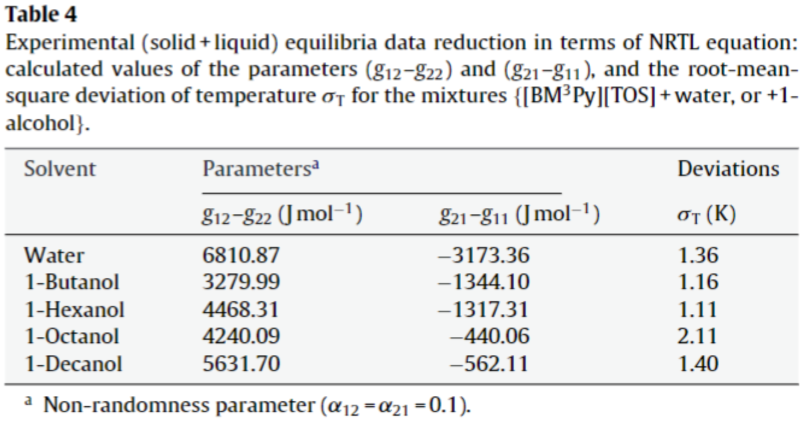


**Table 4**

Experimental (solid + liquid) equilibria data reduction in terms of NRTL equation: calculated values of the parameters ($g_{12}$–$g_{22}$) and ($g_{21}$–$g_{11}$), and the root-mean-square deviation of temperature $\sigma_T$ for the mixtures {[BM$^3$Py][TOS] + water, or + 1-alcohol}.

| Solvent | Parameters[a] | | Deviations |
|---|---|---|---|
| | $g_{12}$–$g_{22}$ (J mol$^{-1}$) | $g_{21}$–$g_{11}$ (J mol$^{-1}$) | $\sigma_T$ (K) |
| Water | 6810.87 | −3173.36 | 1.36 |
| 1-Butanol | 3279.99 | −1344.10 | 1.16 |
| 1-Hexanol | 4468.31 | −1317.31 | 1.11 |
| 1-Octanol | 4240.09 | −440.06 | 2.11 |
| 1-Decanol | 5631.70 | −562.11 | 1.40 |

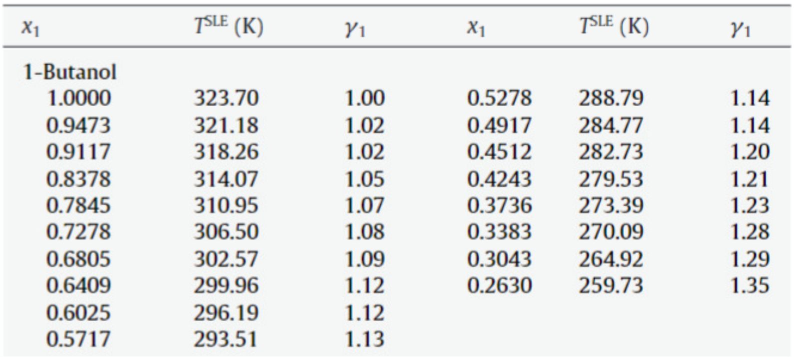
[a] Non-randomness parameter ($\alpha_{12} = \alpha_{21} = 0.1$).

butyl-3-methylpyridinium tosylate + 1-butanol

Trevor M. Letcher, Deresh Ramjugernath, Kaniki Tumba, Marek Królikowski, Urszula Domanska, (Solid + liquid) and (liquid + liquid) phase equilibria study and correlationof the binary systems {*N*-butyl-3-methylpyridinium tosylate + water,or + an alcohol, or + a hydrocarbon}, Fluid Phase Equilibria 294 (2010) 89–97

**Table 2**

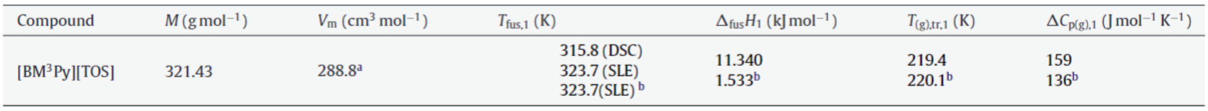
Experimental (solid + liquid) phase equilibria data of binary systems {[BM$^3$Py][TOS] + water, or + 1-alcohol}: experimental mole fractions of ionic liquid, $x_1$; experimental temperatures, $T^{SLE}$; and activity coefficients of ionic liquid at saturated solution.



| $x_1$ | $T^{SLE}$ (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| 1-Butanol | | | | | |
| 1.0000 | 323.70 | 1.00 | 0.5278 | 288.79 | 1.14 |
| 0.9473 | 321.18 | 1.02 | 0.4917 | 284.77 | 1.14 |
| 0.9117 | 318.26 | 1.02 | 0.4512 | 282.73 | 1.20 |
| 0.8378 | 314.07 | 1.05 | 0.4243 | 279.53 | 1.21 |
| 0.7845 | 310.95 | 1.07 | 0.3736 | 273.39 | 1.23 |
| 0.7278 | 306.50 | 1.08 | 0.3383 | 270.09 | 1.28 |
| 0.6805 | 302.57 | 1.09 | 0.3043 | 264.92 | 1.29 |
| 0.6409 | 299.96 | 1.12 | 0.2630 | 259.73 | 1.35 |
| 0.6025 | 296.19 | 1.12 | | | |
| 0.5717 | 293.51 | 1.13 | | | |

**Table 1**

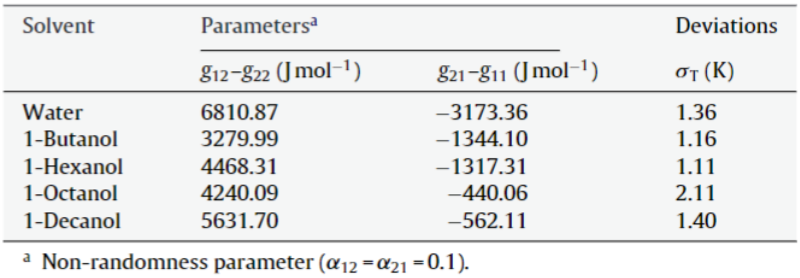
The molecular mass, molar volume and thermophysical constants of pure ionic liquid, determined from DSC data in this work and obtained from the literature.



| Compound | $M$ (g mol$^{-1}$) | $V_m$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $T_{(g),tr,1}$ (K) | $\Delta C_{p(g),1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| [BM$^3$Py][TOS] | 321.43 | 288.8$^a$ | 315.8 (DSC)<br>323.7 (SLE)<br>323.7(SLE)$^b$ | 11.340<br>1.533$^b$ | 219.4<br>220.1$^b$ | 159<br>136$^b$ |

**Table 4**

Experimental (solid + liquid) equilibria data reduction in terms of NRTL equation: calculated values of the parameters ($g_{12}$–$g_{22}$) and ($g_{21}$–$g_{11}$), and the root-mean-square deviation of temperature $\sigma_T$ for the mixtures {[BM$^3$Py][TOS] + water, or +1-alcohol}.



| Solvent | Parameters$^a$ | | Deviations |
|---|---|---|---|
| | $g_{12}$–$g_{22}$ (J mol$^{-1}$) | $g_{21}$–$g_{11}$ (J mol$^{-1}$) | $\sigma_T$ (K) |
| Water | 6810.87 | −3173.36 | 1.36 |
| 1-Butanol | 3279.99 | −1344.10 | 1.16 |
| 1-Hexanol | 4468.31 | −1317.31 | 1.11 |
| 1-Octanol | 4240.09 | −440.06 | 2.11 |
| 1-Decanol | 5631.70 | −562.11 | 1.40 |

[a] Non-randomness parameter ($\alpha_{12} = \alpha_{21} = 0.1$).

butyl-3-methylpyridinium tosylate + 1-hexanol

Trevor M. Letcher, Deresh Ramjugernath, Kaniki Tumba, Marek Królikowski, Urszula Domanska, (Solid + liquid) and (liquid + liquid) phase equilibria study and correlationof the binary systems {*N*-butyl-3-methylpyridinium tosylate + water,or + an alcohol, or + a hydrocarbon}, Fluid Phase Equilibria 294 (2010) 89–97

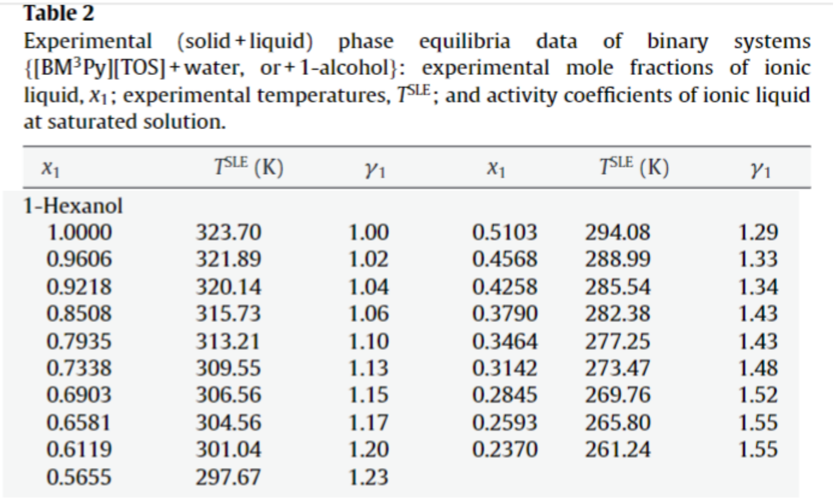


**Table 2**

Experimental (solid + liquid) phase equilibria data of binary systems {[BM$^3$Py][TOS] + water, or + 1-alcohol}: experimental mole fractions of ionic liquid, $x_1$; experimental temperatures, $T^{SLE}$; and activity coefficients of ionic liquid at saturated solution.

| $x_1$ | $T^{SLE}$ (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| 1-Hexanol | | | | | |
| 1.0000 | 323.70 | 1.00 | 0.5103 | 294.08 | 1.29 |
| 0.9606 | 321.89 | 1.02 | 0.4568 | 288.99 | 1.33 |
| 0.9218 | 320.14 | 1.04 | 0.4258 | 285.54 | 1.34 |
| 0.8508 | 315.73 | 1.06 | 0.3790 | 282.38 | 1.43 |
| 0.7935 | 313.21 | 1.10 | 0.3464 | 277.25 | 1.43 |
| 0.7338 | 309.55 | 1.13 | 0.3142 | 273.47 | 1.48 |
| 0.6903 | 306.56 | 1.15 | 0.2845 | 269.76 | 1.52 |
| 0.6581 | 304.56 | 1.17 | 0.2593 | 265.80 | 1.55 |
| 0.6119 | 301.04 | 1.20 | 0.2370 | 261.24 | 1.55 |
| 0.5655 | 297.67 | 1.23 | | | |

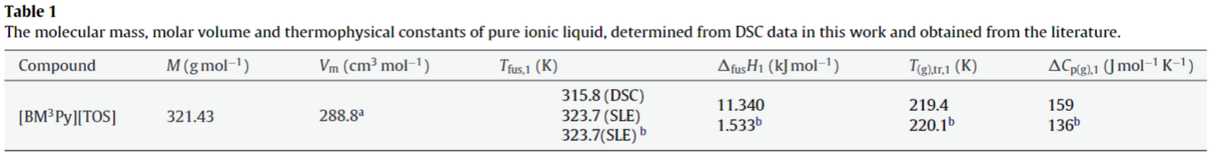


**Table 1**

The molecular mass, molar volume and thermophysical constants of pure ionic liquid, determined from DSC data in this work and obtained from the literature.

| Compound | $M$ (g mol$^{-1}$) | $V_m$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $T_{(g),tr,1}$ (K) | $\Delta C_{p(g),1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| [BM$^3$Py][TOS] | 321.43 | 288.8[a] | 315.8 (DSC)<br>323.7 (SLE)<br>323.7(SLE) [b] | 11.340<br>1.533[b] | 219.4<br>220.1[b] | 159<br>136[b] |

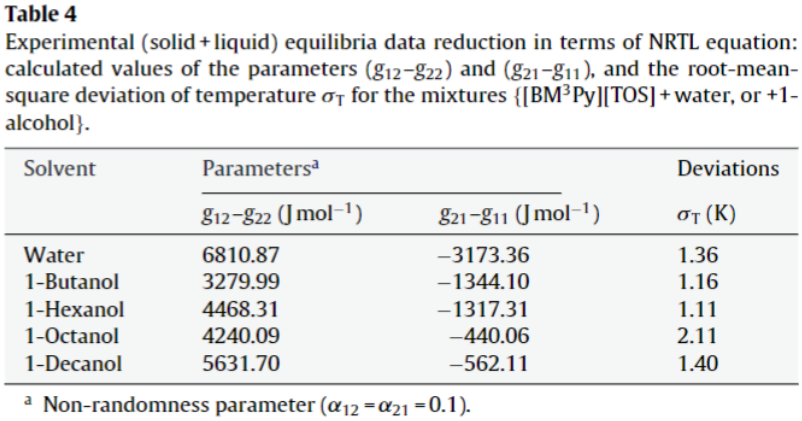


**Table 4**

Experimental (solid + liquid) equilibria data reduction in terms of NRTL equation: calculated values of the parameters ($g_{12}-g_{22}$) and ($g_{21}-g_{11}$), and the root-mean-square deviation of temperature $\sigma_T$ for the mixtures {[BM$^3$Py][TOS] + water, or +1-alcohol}.

| Solvent | Parameters[a] | | Deviations |
|---|---|---|---|
| | $g_{12}-g_{22}$ (J mol$^{-1}$) | $g_{21}-g_{11}$ (J mol$^{-1}$) | $\sigma_T$ (K) |
| Water | 6810.87 | −3173.36 | 1.36 |
| 1-Butanol | 3279.99 | −1344.10 | 1.16 |
| 1-Hexanol | 4468.31 | −1317.31 | 1.11 |
| 1-Octanol | 4240.09 | −440.06 | 2.11 |
| 1-Decanol | 5631.70 | −562.11 | 1.40 |

[a] Non-randomness parameter ($\alpha_{12} = \alpha_{21} = 0.1$).

butyl-3-methylpyridinium tosylate + 1-octanol

Trevor M. Letcher, Deresh Ramjugernath, Kaniki Tumba, Marek Królikowski, Urszula Domanska, (Solid + liquid) and (liquid + liquid) phase equilibria study and correlationof the binary systems {*N*-butyl-3-methylpyridinium tosylate + water,or + an alcohol, or + a hydrocarbon}, Fluid Phase Equilibria 294 (2010) 89–97

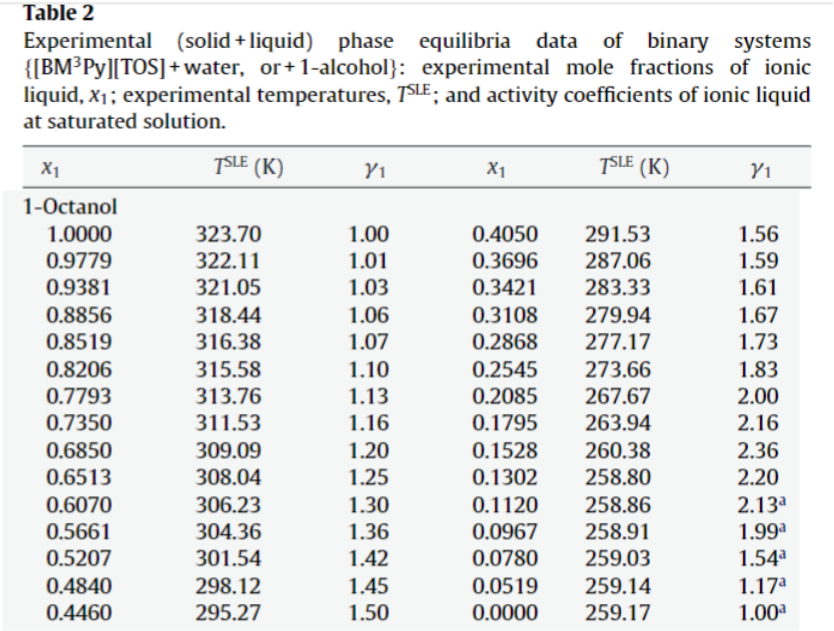


**Table 2**

Experimental (solid + liquid) phase equilibria data of binary systems {[BM$^3$Py][TOS] + water, or + 1-alcohol}: experimental mole fractions of ionic liquid, $x_1$; experimental temperatures, $T^{SLE}$; and activity coefficients of ionic liquid at saturated solution.

| $x_1$ | $T^{SLE}$ (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| 1-Octanol | | | | | |
| 1.0000 | 323.70 | 1.00 | 0.4050 | 291.53 | 1.56 |
| 0.9779 | 322.11 | 1.01 | 0.3696 | 287.06 | 1.59 |
| 0.9381 | 321.05 | 1.03 | 0.3421 | 283.33 | 1.61 |
| 0.8856 | 318.44 | 1.06 | 0.3108 | 279.94 | 1.67 |
| 0.8519 | 316.38 | 1.07 | 0.2868 | 277.17 | 1.73 |
| 0.8206 | 315.58 | 1.10 | 0.2545 | 273.66 | 1.83 |
| 0.7793 | 313.76 | 1.13 | 0.2085 | 267.67 | 2.00 |
| 0.7350 | 311.53 | 1.16 | 0.1795 | 263.94 | 2.16 |
| 0.6850 | 309.09 | 1.20 | 0.1528 | 260.38 | 2.36 |
| 0.6513 | 308.04 | 1.25 | 0.1302 | 258.80 | 2.20 |
| 0.6070 | 306.23 | 1.30 | 0.1120 | 258.86 | 2.13[a] |
| 0.5661 | 304.36 | 1.36 | 0.0967 | 258.91 | 1.99[a] |
| 0.5207 | 301.54 | 1.42 | 0.0780 | 259.03 | 1.54[a] |
| 0.4840 | 298.12 | 1.45 | 0.0519 | 259.14 | 1.17[a] |
| 0.4460 | 295.27 | 1.50 | 0.0000 | 259.17 | 1.00[a] |

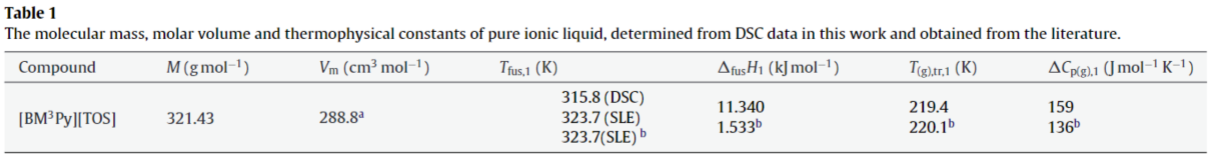


**Table 1**

The molecular mass, molar volume and thermophysical constants of pure ionic liquid, determined from DSC data in this work and obtained from the literature.

| Compound | $M$ (g mol$^{-1}$) | $V_m$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $T_{(g),tr,1}$ (K) | $\Delta C_{p(g),1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| [BM$^3$Py][TOS] | 321.43 | 288.8[a] | 315.8 (DSC)<br>323.7 (SLE)<br>323.7(SLE)[b] | 11.340<br>1.533[b] | 219.4<br>220.1[b] | 159<br>136[b] |

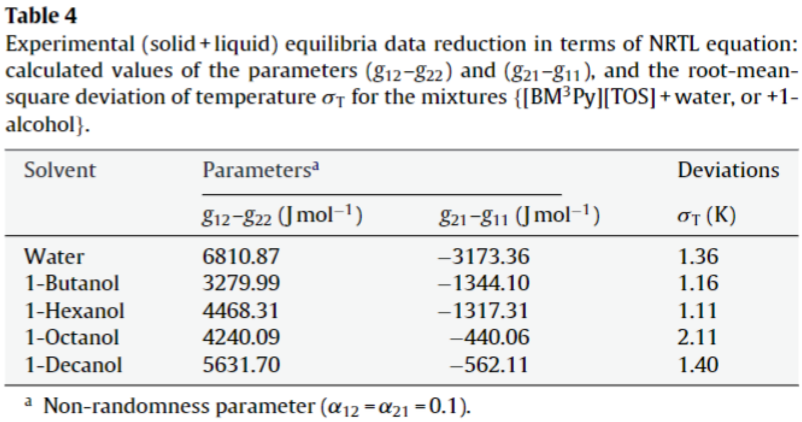


**Table 4**

Experimental (solid + liquid) equilibria data reduction in terms of NRTL equation: calculated values of the parameters ($g_{12}$–$g_{22}$) and ($g_{21}$–$g_{11}$), and the root-mean-square deviation of temperature $\sigma_T$ for the mixtures {[BM$^3$Py][TOS] + water, or +1-alcohol}.

| Solvent | Parameters[a] | | Deviations |
|---|---|---|---|
| | $g_{12}$–$g_{22}$ (J mol$^{-1}$) | $g_{21}$–$g_{11}$ (J mol$^{-1}$) | $\sigma_T$ (K) |
| Water | 6810.87 | −3173.36 | 1.36 |
| 1-Butanol | 3279.99 | −1344.10 | 1.16 |
| 1-Hexanol | 4468.31 | −1317.31 | 1.11 |
| 1-Octanol | 4240.09 | −440.06 | 2.11 |
| 1-Decanol | 5631.70 | −562.11 | 1.40 |

[a] Non-randomness parameter ($\alpha_{12} = \alpha_{21} = 0.1$).

butyl-3-methylpyridinium tosylate + 1-decanol
Trevor M. Letcher, Deresh Ramjugernath, Kaniki Tumba, Marek Królikowski, Urszula Domanska, (Solid + liquid) and (liquid + liquid) phase equilibria study and correlationof the binary systems {*N*-butyl-3-methylpyridinium tosylate + water,or + an alcohol, or + a hydrocarbon}, Fluid Phase Equilibria 294 (2010) 89–97

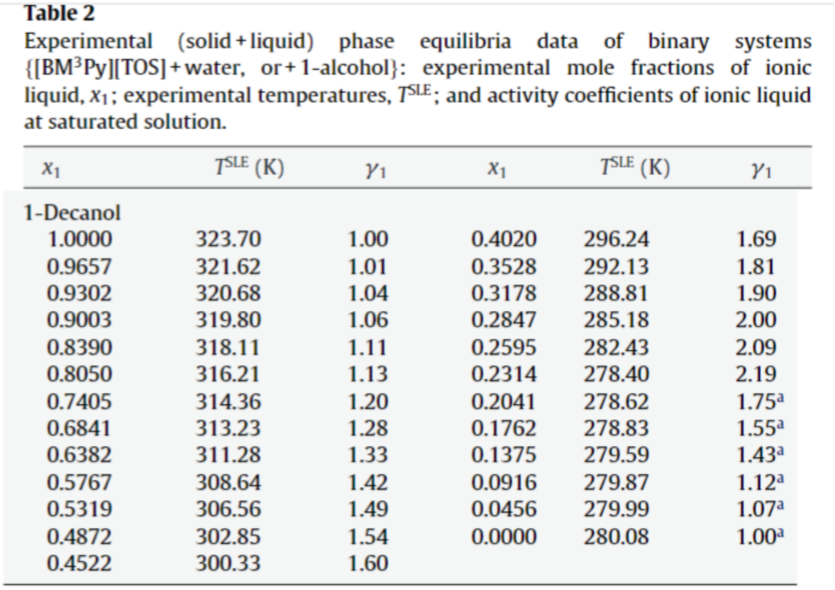


**Table 2**
Experimental (solid + liquid) phase equilibria data of binary systems {[BM$^3$Py][TOS] + water, or + 1-alcohol}: experimental mole fractions of ionic liquid, $x_1$; experimental temperatures, $T^{SLE}$; and activity coefficients of ionic liquid at saturated solution.

| $x_1$ | $T^{SLE}$ (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| 1-Decanol | | | | | |
| 1.0000 | 323.70 | 1.00 | 0.4020 | 296.24 | 1.69 |
| 0.9657 | 321.62 | 1.01 | 0.3528 | 292.13 | 1.81 |
| 0.9302 | 320.68 | 1.04 | 0.3178 | 288.81 | 1.90 |
| 0.9003 | 319.80 | 1.06 | 0.2847 | 285.18 | 2.00 |
| 0.8390 | 318.11 | 1.11 | 0.2595 | 282.43 | 2.09 |
| 0.8050 | 316.21 | 1.13 | 0.2314 | 278.40 | 2.19 |
| 0.7405 | 314.36 | 1.20 | 0.2041 | 278.62 | 1.75[a] |
| 0.6841 | 313.23 | 1.28 | 0.1762 | 278.83 | 1.55[a] |
| 0.6382 | 311.28 | 1.33 | 0.1375 | 279.59 | 1.43[a] |
| 0.5767 | 308.64 | 1.42 | 0.0916 | 279.87 | 1.12[a] |
| 0.5319 | 306.56 | 1.49 | 0.0456 | 279.99 | 1.07[a] |
| 0.4872 | 302.85 | 1.54 | 0.0000 | 280.08 | 1.00[a] |
| 0.4522 | 300.33 | 1.60 | | | |

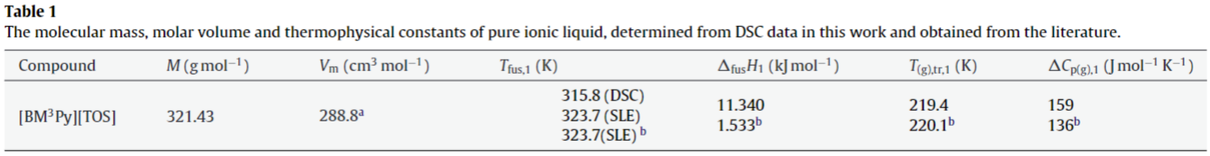


**Table 1**
The molecular mass, molar volume and thermophysical constants of pure ionic liquid, determined from DSC data in this work and obtained from the literature.

| Compound | $M$ (g mol$^{-1}$) | $V_m$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $T_{(g),tr,1}$ (K) | $\Delta C_{p(g),1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| [BM$^3$Py][TOS] | 321.43 | 288.8[a] | 315.8 (DSC)<br>323.7 (SLE)<br>323.7(SLE)[b] | 11.340<br>1.533[b] | 219.4<br>220.1[b] | 159<br>136[b] |

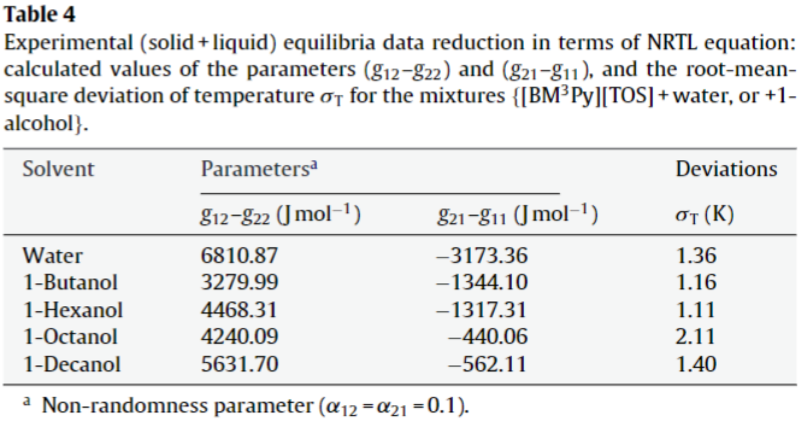


**Table 4**
Experimental (solid + liquid) equilibria data reduction in terms of NRTL equation: calculated values of the parameters ($g_{12}-g_{22}$) and ($g_{21}-g_{11}$), and the root-mean-square deviation of temperature $\sigma_T$ for the mixtures {[BM$^3$Py][TOS] + water, or +1-alcohol}.

| Solvent | Parameters[a] | | Deviations |
|---|---|---|---|
| | $g_{12}-g_{22}$ (J mol$^{-1}$) | $g_{21}-g_{11}$ (J mol$^{-1}$) | $\sigma_T$ (K) |
| Water | 6810.87 | −3173.36 | 1.36 |
| 1-Butanol | 3279.99 | −1344.10 | 1.16 |
| 1-Hexanol | 4468.31 | −1317.31 | 1.11 |
| 1-Octanol | 4240.09 | −440.06 | 2.11 |
| 1-Decanol | 5631.70 | −562.11 | 1.40 |

[a] Non-randomness parameter ($\alpha_{12} = \alpha_{21} = 0.1$).

benzene + diethoxymethane

Mariana Teodorescu, Michael Wilken, Roland Wittig, Jürgen Gmehling, Azeotropic and solid–liquid equilibria data for several binaryorganic systems containing one acetal compound, Fluid Phase Equilibria 204 (2003) 267–280

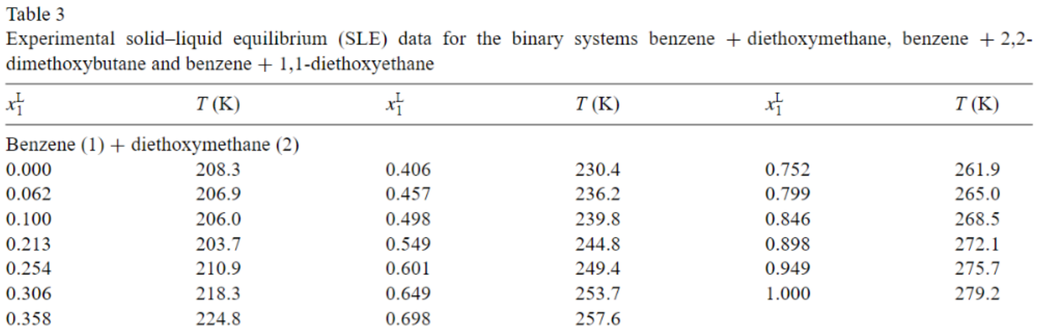


Table 3

Experimental solid–liquid equilibrium (SLE) data for the binary systems benzene + diethoxymethane, benzene + 2,2-dimethoxybutane and benzene + 1,1-diethoxyethane

| $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) |
|---|---|---|---|---|---|
| Benzene (1) + diethoxymethane (2) | | | | | |
| 0.000 | 208.3 | 0.406 | 230.4 | 0.752 | 261.9 |
| 0.062 | 206.9 | 0.457 | 236.2 | 0.799 | 265.0 |
| 0.100 | 206.0 | 0.498 | 239.8 | 0.846 | 268.5 |
| 0.213 | 203.7 | 0.549 | 244.8 | 0.898 | 272.1 |
| 0.254 | 210.9 | 0.601 | 249.4 | 0.949 | 275.7 |
| 0.306 | 218.3 | 0.649 | 253.7 | 1.000 | 279.2 |
| 0.358 | 224.8 | 0.698 | 257.6 | | |

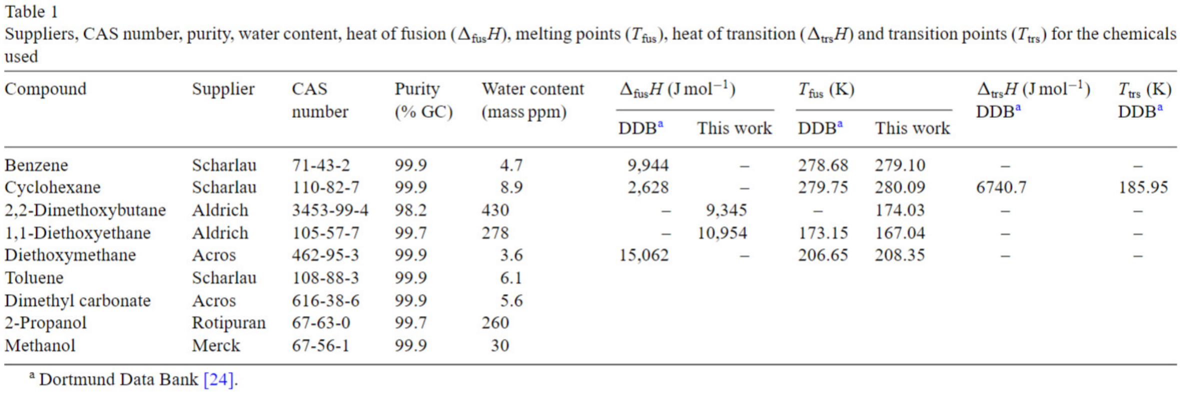


Table 1

Suppliers, CAS number, purity, water content, heat of fusion ($\Delta_{fus}H$), melting points ($T_{fus}$), heat of transition ($\Delta_{trs}H$) and transition points ($T_{trs}$) for the chemicals used

| Compound | Supplier | CAS number | Purity (% GC) | Water content (mass ppm) | $\Delta_{fus}H$ (J mol$^{-1}$) | | $T_{fus}$ (K) | | $\Delta_{trs}H$ (J mol$^{-1}$) DDB[a] | $T_{trs}$ (K) DDB[a] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | DDB[a] | This work | DDB[a] | This work | | |
| Benzene | Scharlau | 71-43-2 | 99.9 | 4.7 | 9,944 | – | 278.68 | 279.10 | – | – |
| Cyclohexane | Scharlau | 110-82-7 | 99.9 | 8.9 | 2,628 | – | 279.75 | 280.09 | 6740.7 | 185.95 |
| 2,2-Dimethoxybutane | Aldrich | 3453-99-4 | 98.2 | 430 | – | 9,345 | – | 174.03 | – | – |
| 1,1-Diethoxyethane | Aldrich | 105-57-7 | 99.7 | 278 | – | 10,954 | 173.15 | 167.04 | – | – |
| Diethoxymethane | Acros | 462-95-3 | 99.9 | 3.6 | 15,062 | – | 206.65 | 208.35 | – | – |
| Toluene | Scharlau | 108-88-3 | 99.9 | 6.1 | | | | | | |
| Dimethyl carbonate | Acros | 616-38-6 | 99.9 | 5.6 | | | | | | |
| 2-Propanol | Rotipuran | 67-63-0 | 99.7 | 260 | | | | | | |
| Methanol | Merck | 67-56-1 | 99.9 | 30 | | | | | | |

[a] Dortmund Data Bank [24].

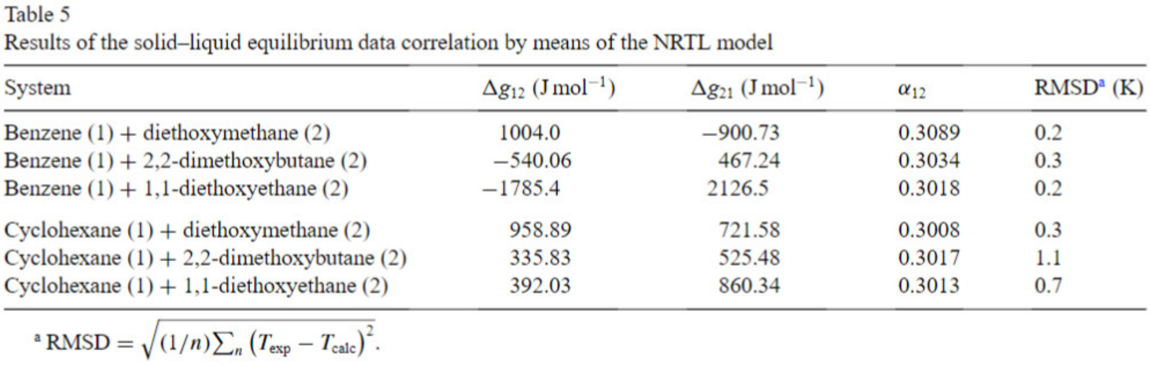


Table 5

Results of the solid–liquid equilibrium data correlation by means of the NRTL model

| System | $\Delta g_{12}$ (J mol$^{-1}$) | $\Delta g_{21}$ (J mol$^{-1}$) | $\alpha_{12}$ | RMSD[a] (K) |
|---|---|---|---|---|
| Benzene (1) + diethoxymethane (2) | 1004.0 | −900.73 | 0.3089 | 0.2 |
| Benzene (1) + 2,2-dimethoxybutane (2) | −540.06 | 467.24 | 0.3034 | 0.3 |
| Benzene (1) + 1,1-diethoxyethane (2) | −1785.4 | 2126.5 | 0.3018 | 0.2 |
| Cyclohexane (1) + diethoxymethane (2) | 958.89 | 721.58 | 0.3008 | 0.3 |
| Cyclohexane (1) + 2,2-dimethoxybutane (2) | 335.83 | 525.48 | 0.3017 | 1.1 |
| Cyclohexane (1) + 1,1-diethoxyethane (2) | 392.03 | 860.34 | 0.3013 | 0.7 |

[a] $\mathrm{RMSD} = \sqrt{(1/n)\sum_n \left(T_{exp} - T_{calc}\right)^2}$.

benzene + 2,2-dimethoxybutane
Mariana Teodorescu, Michael Wilken, Roland Wittig, Jürgen Gmehling, Azeotropic and solid–liquid equilibria data for several binaryorganic systems containing one acetal compound, Fluid Phase Equilibria 204 (2003) 267–280

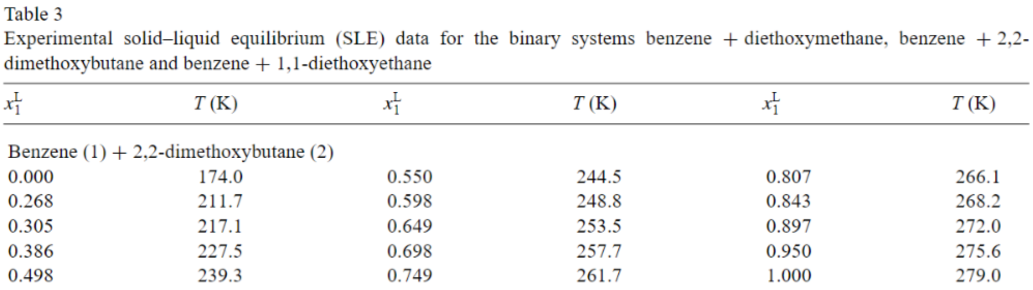


Table 3
Experimental solid–liquid equilibrium (SLE) data for the binary systems benzene + diethoxymethane, benzene + 2,2-dimethoxybutane and benzene + 1,1-diethoxyethane

| $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) |
|---|---|---|---|---|---|
| Benzene (1) + 2,2-dimethoxybutane (2) | | | | | |
| 0.000 | 174.0 | 0.550 | 244.5 | 0.807 | 266.1 |
| 0.268 | 211.7 | 0.598 | 248.8 | 0.843 | 268.2 |
| 0.305 | 217.1 | 0.649 | 253.5 | 0.897 | 272.0 |
| 0.386 | 227.5 | 0.698 | 257.7 | 0.950 | 275.6 |
| 0.498 | 239.3 | 0.749 | 261.7 | 1.000 | 279.0 |

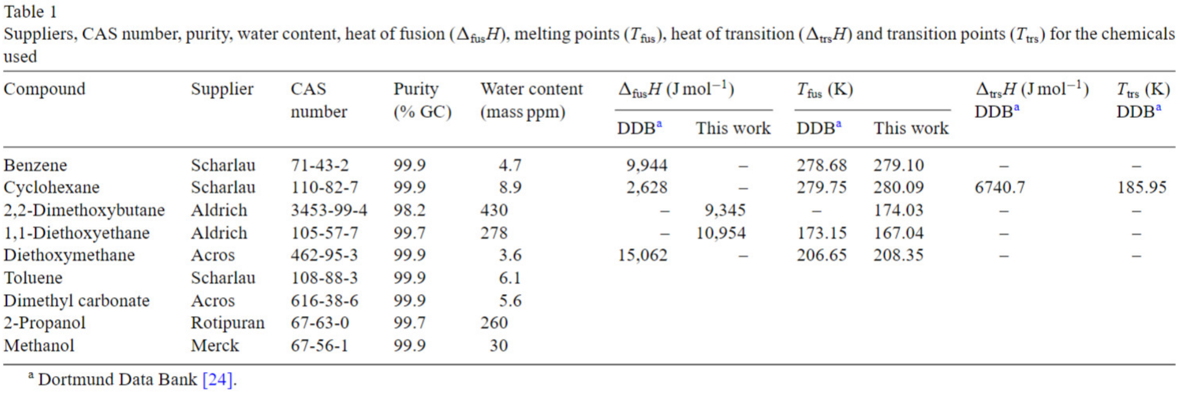


Table 1
Suppliers, CAS number, purity, water content, heat of fusion ($\Delta_{fus}H$), melting points ($T_{fus}$), heat of transition ($\Delta_{trs}H$) and transition points ($T_{trs}$) for the chemicals used

| Compound | Supplier | CAS number | Purity (% GC) | Water content (mass ppm) | $\Delta_{fus}H$ (J mol$^{-1}$) | | $T_{fus}$ (K) | | $\Delta_{trs}H$ (J mol$^{-1}$) DDB[a] | $T_{trs}$ (K) DDB[a] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | DDB[a] | This work | DDB[a] | This work | | |
| Benzene | Scharlau | 71-43-2 | 99.9 | 4.7 | 9,944 | – | 278.68 | 279.10 | – | – |
| Cyclohexane | Scharlau | 110-82-7 | 99.9 | 8.9 | 2,628 | – | 279.75 | 280.09 | 6740.7 | 185.95 |
| 2,2-Dimethoxybutane | Aldrich | 3453-99-4 | 98.2 | 430 | – | 9,345 | – | 174.03 | – | – |
| 1,1-Diethoxyethane | Aldrich | 105-57-7 | 99.7 | 278 | – | 10,954 | 173.15 | 167.04 | – | – |
| Diethoxymethane | Acros | 462-95-3 | 99.9 | 3.6 | 15,062 | – | 206.65 | 208.35 | – | – |
| Toluene | Scharlau | 108-88-3 | 99.9 | 6.1 | | | | | | |
| Dimethyl carbonate | Acros | 616-38-6 | 99.9 | 5.6 | | | | | | |
| 2-Propanol | Rotipuran | 67-63-0 | 99.7 | 260 | | | | | | |
| Methanol | Merck | 67-56-1 | 99.9 | 30 | | | | | | |

[a] Dortmund Data Bank [24].

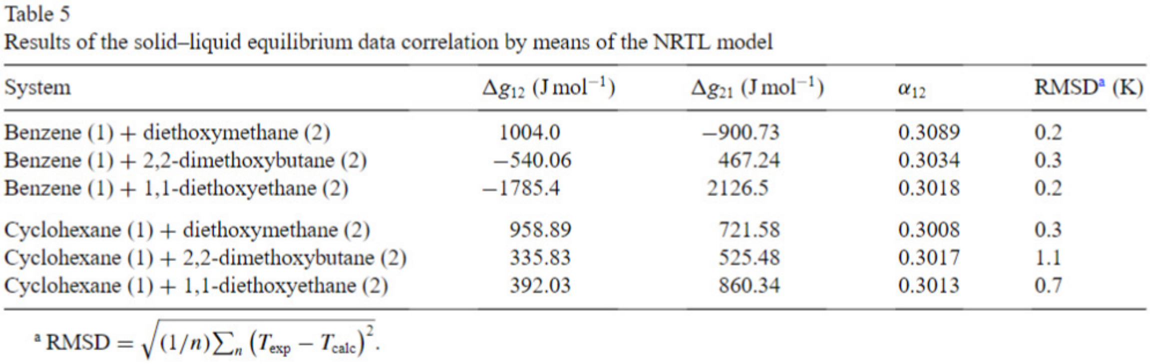


Table 5
Results of the solid–liquid equilibrium data correlation by means of the NRTL model

| System | $\Delta g_{12}$ (J mol$^{-1}$) | $\Delta g_{21}$ (J mol$^{-1}$) | $\alpha_{12}$ | RMSD[a] (K) |
|---|---|---|---|---|
| Benzene (1) + diethoxymethane (2) | 1004.0 | −900.73 | 0.3089 | 0.2 |
| Benzene (1) + 2,2-dimethoxybutane (2) | −540.06 | 467.24 | 0.3034 | 0.3 |
| Benzene (1) + 1,1-diethoxyethane (2) | −1785.4 | 2126.5 | 0.3018 | 0.2 |
| Cyclohexane (1) + diethoxymethane (2) | 958.89 | 721.58 | 0.3008 | 0.3 |
| Cyclohexane (1) + 2,2-dimethoxybutane (2) | 335.83 | 525.48 | 0.3017 | 1.1 |
| Cyclohexane (1) + 1,1-diethoxyethane (2) | 392.03 | 860.34 | 0.3013 | 0.7 |

[a] $\mathrm{RMSD} = \sqrt{(1/n)\sum_n \left(T_{exp} - T_{calc}\right)^2}$.

benzene + 1,1-diethoxyethane

Mariana Teodorescu, Michael Wilken, Roland Wittig, Jürgen Gmehling, Azeotropic and solid–liquid equilibria data for several binaryorganic systems containing one acetal compound, Fluid Phase Equilibria 204 (2003) 267–280

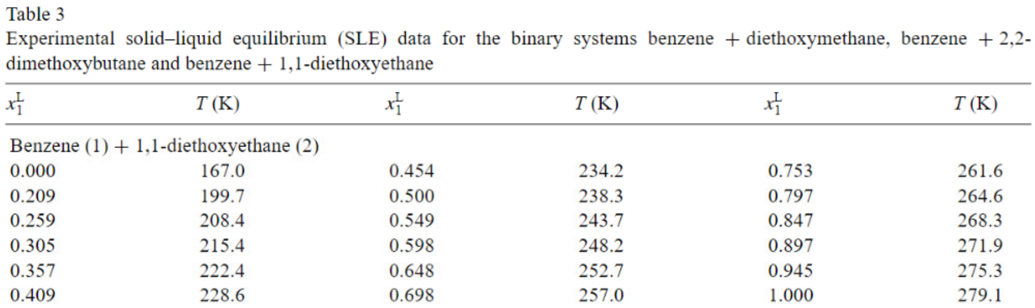


Table 3

Experimental solid–liquid equilibrium (SLE) data for the binary systems benzene + diethoxymethane, benzene + 2,2-dimethoxybutane and benzene + 1,1-diethoxyethane

| $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) |
|---|---|---|---|---|---|
| Benzene (1) + 1,1-diethoxyethane (2) | | | | | |
| 0.000 | 167.0 | 0.454 | 234.2 | 0.753 | 261.6 |
| 0.209 | 199.7 | 0.500 | 238.3 | 0.797 | 264.6 |
| 0.259 | 208.4 | 0.549 | 243.7 | 0.847 | 268.3 |
| 0.305 | 215.4 | 0.598 | 248.2 | 0.897 | 271.9 |
| 0.357 | 222.4 | 0.648 | 252.7 | 0.945 | 275.3 |
| 0.409 | 228.6 | 0.698 | 257.0 | 1.000 | 279.1 |

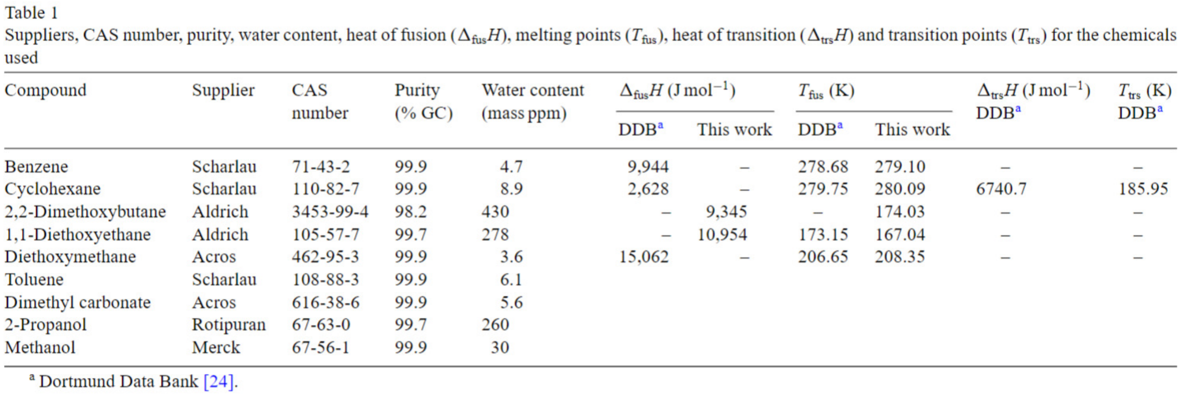


Table 1

Suppliers, CAS number, purity, water content, heat of fusion ($\Delta_{fus}H$), melting points ($T_{fus}$), heat of transition ($\Delta_{trs}H$) and transition points ($T_{trs}$) for the chemicals used

| Compound | Supplier | CAS number | Purity (% GC) | Water content (mass ppm) | $\Delta_{fus}H$ (J mol$^{-1}$) | | $T_{fus}$ (K) | | $\Delta_{trs}H$ (J mol$^{-1}$) DDB[a] | $T_{trs}$ (K) DDB[a] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | DDB[a] | This work | DDB[a] | This work | | |
| Benzene | Scharlau | 71-43-2 | 99.9 | 4.7 | 9,944 | – | 278.68 | 279.10 | – | – |
| Cyclohexane | Scharlau | 110-82-7 | 99.9 | 8.9 | 2,628 | – | 279.75 | 280.09 | 6740.7 | 185.95 |
| 2,2-Dimethoxybutane | Aldrich | 3453-99-4 | 98.2 | 430 | – | 9,345 | – | 174.03 | – | – |
| 1,1-Diethoxyethane | Aldrich | 105-57-7 | 99.7 | 278 | – | 10,954 | 173.15 | 167.04 | – | – |
| Diethoxymethane | Acros | 462-95-3 | 99.9 | 3.6 | 15,062 | – | 206.65 | 208.35 | – | – |
| Toluene | Scharlau | 108-88-3 | 99.9 | 6.1 | | | | | | |
| Dimethyl carbonate | Acros | 616-38-6 | 99.9 | 5.6 | | | | | | |
| 2-Propanol | Rotipuran | 67-63-0 | 99.7 | 260 | | | | | | |
| Methanol | Merck | 67-56-1 | 99.9 | 30 | | | | | | |

[a] Dortmund Data Bank [24].

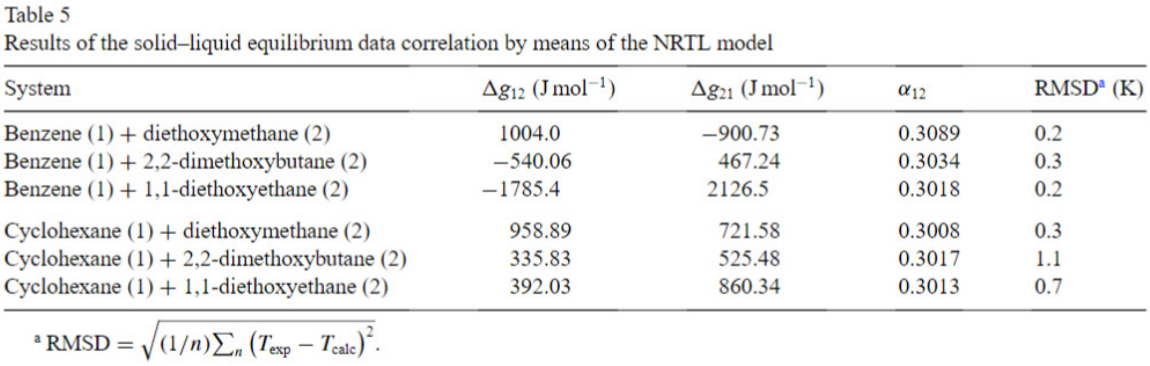


Table 5

Results of the solid–liquid equilibrium data correlation by means of the NRTL model

| System | $\Delta g_{12}$ (J mol$^{-1}$) | $\Delta g_{21}$ (J mol$^{-1}$) | $\alpha_{12}$ | RMSD[a] (K) |
|---|---|---|---|---|
| Benzene (1) + diethoxymethane (2) | 1004.0 | −900.73 | 0.3089 | 0.2 |
| Benzene (1) + 2,2-dimethoxybutane (2) | −540.06 | 467.24 | 0.3034 | 0.3 |
| Benzene (1) + 1,1-diethoxyethane (2) | −1785.4 | 2126.5 | 0.3018 | 0.2 |
| Cyclohexane (1) + diethoxymethane (2) | 958.89 | 721.58 | 0.3008 | 0.3 |
| Cyclohexane (1) + 2,2-dimethoxybutane (2) | 335.83 | 525.48 | 0.3017 | 1.1 |
| Cyclohexane (1) + 1,1-diethoxyethane (2) | 392.03 | 860.34 | 0.3013 | 0.7 |

[a] $\mathrm{RMSD} = \sqrt{(1/n)\sum_n (T_{exp} - T_{calc})^2}$.

cyclohexane + diethoxymethane

Mariana Teodorescu, Michael Wilken, Roland Wittig, Jürgen Gmehling, Azeotropic and solid–liquid equilibria data for several binaryorganic systems containing one acetal compound, Fluid Phase Equilibria 204 (2003) 267–280

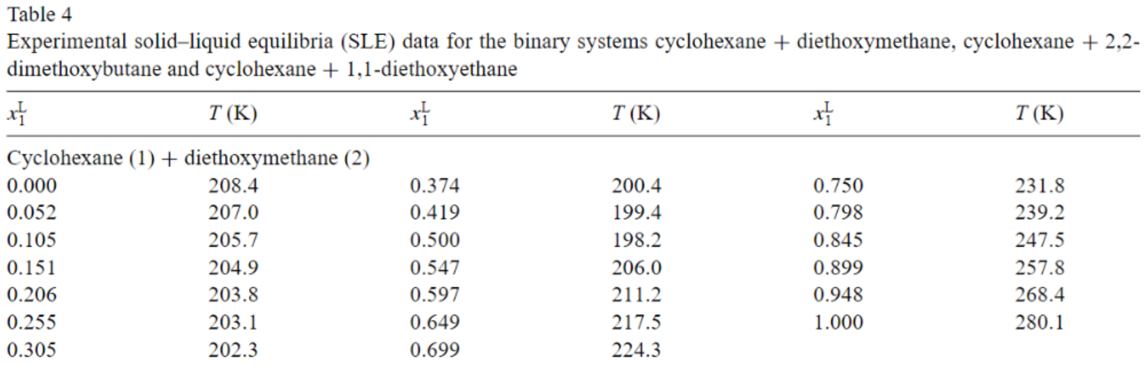


Table 4

Experimental solid–liquid equilibria (SLE) data for the binary systems cyclohexane + diethoxymethane, cyclohexane + 2,2-dimethoxybutane and cyclohexane + 1,1-diethoxyethane

| $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) |
|---|---|---|---|---|---|
| Cyclohexane (1) + diethoxymethane (2) | | | | | |
| 0.000 | 208.4 | 0.374 | 200.4 | 0.750 | 231.8 |
| 0.052 | 207.0 | 0.419 | 199.4 | 0.798 | 239.2 |
| 0.105 | 205.7 | 0.500 | 198.2 | 0.845 | 247.5 |
| 0.151 | 204.9 | 0.547 | 206.0 | 0.899 | 257.8 |
| 0.206 | 203.8 | 0.597 | 211.2 | 0.948 | 268.4 |
| 0.255 | 203.1 | 0.649 | 217.5 | 1.000 | 280.1 |
| 0.305 | 202.3 | 0.699 | 224.3 | | |

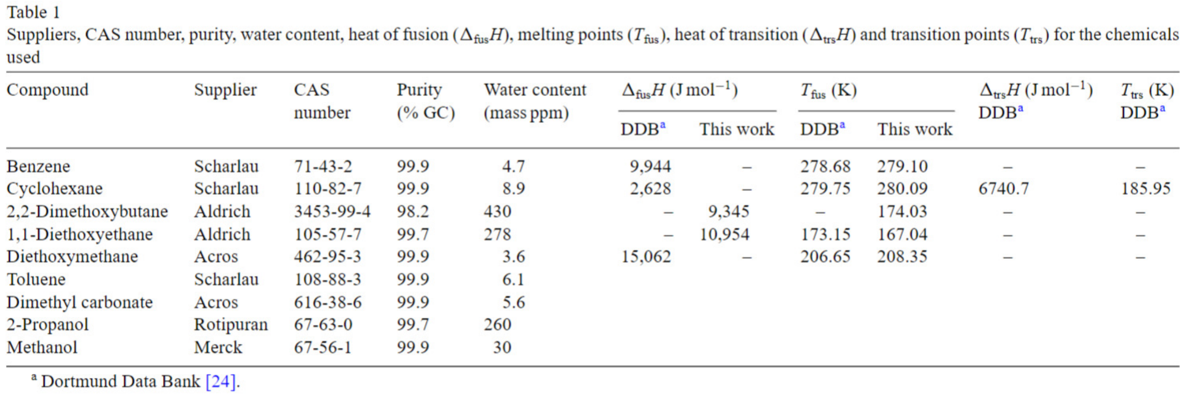


Table 1

Suppliers, CAS number, purity, water content, heat of fusion ($\Delta_{fus}H$), melting points ($T_{fus}$), heat of transition ($\Delta_{trs}H$) and transition points ($T_{trs}$) for the chemicals used

| Compound | Supplier | CAS number | Purity (% GC) | Water content (mass ppm) | $\Delta_{fus}H$ (J mol$^{-1}$) | | $T_{fus}$ (K) | | $\Delta_{trs}H$ (J mol$^{-1}$) DDB[a] | $T_{trs}$ (K) DDB[a] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | DDB[a] | This work | DDB[a] | This work | | |
| Benzene | Scharlau | 71-43-2 | 99.9 | 4.7 | 9,944 | – | 278.68 | 279.10 | – | – |
| Cyclohexane | Scharlau | 110-82-7 | 99.9 | 8.9 | 2,628 | – | 279.75 | 280.09 | 6740.7 | 185.95 |
| 2,2-Dimethoxybutane | Aldrich | 3453-99-4 | 98.2 | 430 | – | 9,345 | – | 174.03 | – | – |
| 1,1-Diethoxyethane | Aldrich | 105-57-7 | 99.7 | 278 | – | 10,954 | 173.15 | 167.04 | – | – |
| Diethoxymethane | Acros | 462-95-3 | 99.9 | 3.6 | 15,062 | – | 206.65 | 208.35 | – | – |
| Toluene | Scharlau | 108-88-3 | 99.9 | 6.1 | | | | | | |
| Dimethyl carbonate | Acros | 616-38-6 | 99.9 | 5.6 | | | | | | |
| 2-Propanol | Rotipuran | 67-63-0 | 99.7 | 260 | | | | | | |
| Methanol | Merck | 67-56-1 | 99.9 | 30 | | | | | | |

[a] Dortmund Data Bank [24].

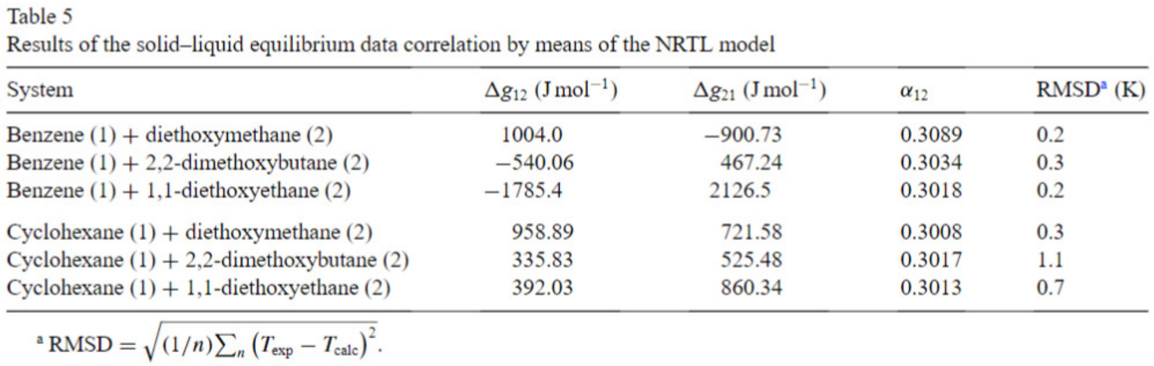


Table 5

Results of the solid–liquid equilibrium data correlation by means of the NRTL model

| System | $\Delta g_{12}$ (J mol$^{-1}$) | $\Delta g_{21}$ (J mol$^{-1}$) | $\alpha_{12}$ | RMSD[a] (K) |
|---|---|---|---|---|
| Benzene (1) + diethoxymethane (2) | 1004.0 | −900.73 | 0.3089 | 0.2 |
| Benzene (1) + 2,2-dimethoxybutane (2) | −540.06 | 467.24 | 0.3034 | 0.3 |
| Benzene (1) + 1,1-diethoxyethane (2) | −1785.4 | 2126.5 | 0.3018 | 0.2 |
| Cyclohexane (1) + diethoxymethane (2) | 958.89 | 721.58 | 0.3008 | 0.3 |
| Cyclohexane (1) + 2,2-dimethoxybutane (2) | 335.83 | 525.48 | 0.3017 | 1.1 |
| Cyclohexane (1) + 1,1-diethoxyethane (2) | 392.03 | 860.34 | 0.3013 | 0.7 |

[a] $\mathrm{RMSD} = \sqrt{(1/n)\sum_n \left(T_{exp} - T_{calc}\right)^2}$.

cyclohexane + 2,2-dimethoxybutane
Mariana Teodorescu, Michael Wilken, Roland Wittig, Jürgen Gmehling, Azeotropic and solid–liquid equilibria data for several binaryorganic systems containing one acetal compound, Fluid Phase Equilibria 204 (2003) 267–280

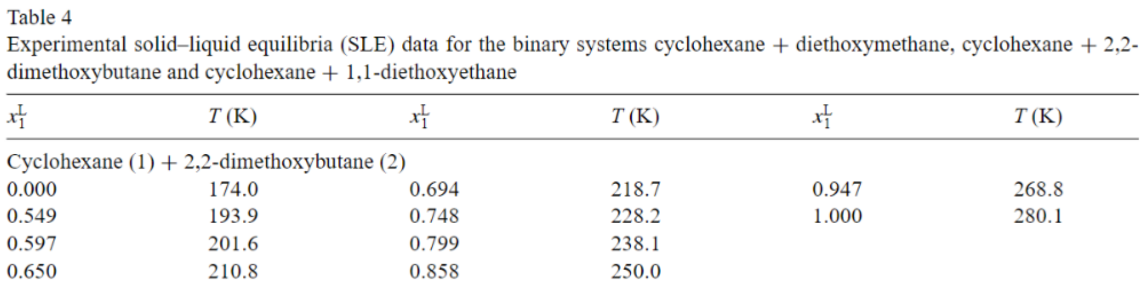


Table 4
Experimental solid–liquid equilibria (SLE) data for the binary systems cyclohexane + diethoxymethane, cyclohexane + 2,2-dimethoxybutane and cyclohexane + 1,1-diethoxyethane

| $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) |
|---|---|---|---|---|---|
| Cyclohexane (1) + 2,2-dimethoxybutane (2) | | | | | |
| 0.000 | 174.0 | 0.694 | 218.7 | 0.947 | 268.8 |
| 0.549 | 193.9 | 0.748 | 228.2 | 1.000 | 280.1 |
| 0.597 | 201.6 | 0.799 | 238.1 | | |
| 0.650 | 210.8 | 0.858 | 250.0 | | |

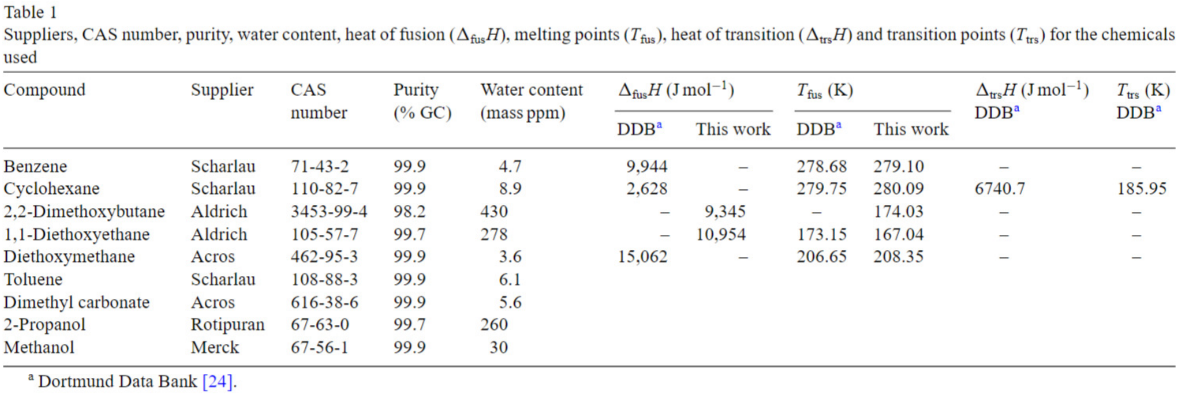


Table 1
Suppliers, CAS number, purity, water content, heat of fusion ($\Delta_{fus}H$), melting points ($T_{fus}$), heat of transition ($\Delta_{trs}H$) and transition points ($T_{trs}$) for the chemicals used

| Compound | Supplier | CAS number | Purity (% GC) | Water content (mass ppm) | $\Delta_{fus}H$ (J mol$^{-1}$) | | $T_{fus}$ (K) | | $\Delta_{trs}H$ (J mol$^{-1}$) DDB[a] | $T_{trs}$ (K) DDB[a] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | DDB[a] | This work | DDB[a] | This work | | |
| Benzene | Scharlau | 71-43-2 | 99.9 | 4.7 | 9,944 | – | 278.68 | 279.10 | – | – |
| Cyclohexane | Scharlau | 110-82-7 | 99.9 | 8.9 | 2,628 | – | 279.75 | 280.09 | 6740.7 | 185.95 |
| 2,2-Dimethoxybutane | Aldrich | 3453-99-4 | 98.2 | 430 | – | 9,345 | – | 174.03 | – | – |
| 1,1-Diethoxyethane | Aldrich | 105-57-7 | 99.7 | 278 | – | 10,954 | 173.15 | 167.04 | – | – |
| Diethoxymethane | Acros | 462-95-3 | 99.9 | 3.6 | 15,062 | – | 206.65 | 208.35 | – | – |
| Toluene | Scharlau | 108-88-3 | 99.9 | 6.1 | | | | | | |
| Dimethyl carbonate | Acros | 616-38-6 | 99.9 | 5.6 | | | | | | |
| 2-Propanol | Rotipuran | 67-63-0 | 99.7 | 260 | | | | | | |
| Methanol | Merck | 67-56-1 | 99.9 | 30 | | | | | | |

[a] Dortmund Data Bank [24].

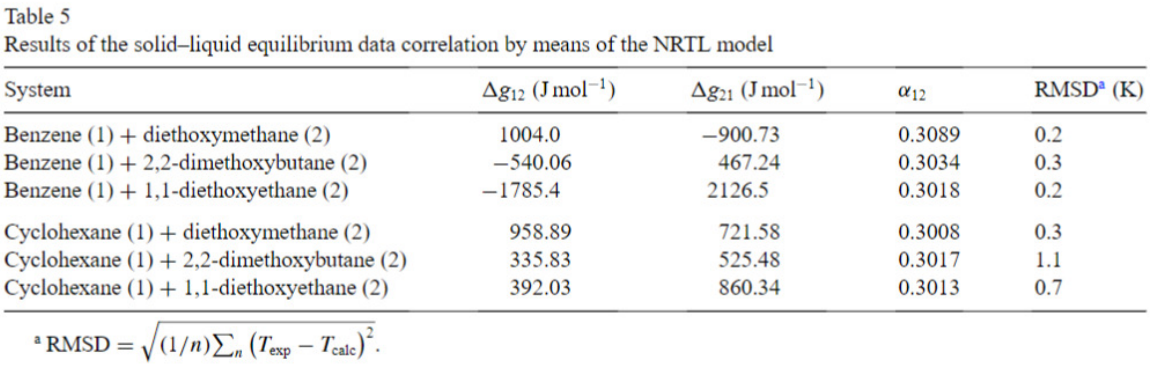


Table 5
Results of the solid–liquid equilibrium data correlation by means of the NRTL model

| System | $\Delta g_{12}$ (J mol$^{-1}$) | $\Delta g_{21}$ (J mol$^{-1}$) | $\alpha_{12}$ | RMSD[a] (K) |
|---|---|---|---|---|
| Benzene (1) + diethoxymethane (2) | 1004.0 | −900.73 | 0.3089 | 0.2 |
| Benzene (1) + 2,2-dimethoxybutane (2) | −540.06 | 467.24 | 0.3034 | 0.3 |
| Benzene (1) + 1,1-diethoxyethane (2) | −1785.4 | 2126.5 | 0.3018 | 0.2 |
| Cyclohexane (1) + diethoxymethane (2) | 958.89 | 721.58 | 0.3008 | 0.3 |
| Cyclohexane (1) + 2,2-dimethoxybutane (2) | 335.83 | 525.48 | 0.3017 | 1.1 |
| Cyclohexane (1) + 1,1-diethoxyethane (2) | 392.03 | 860.34 | 0.3013 | 0.7 |

[a] $\mathrm{RMSD} = \sqrt{(1/n)\sum_n \left(T_{exp} - T_{calc}\right)^2}$.

cyclohexane + 1,1-diethoxyethane

Mariana Teodorescu, Michael Wilken, Roland Wittig, Jürgen Gmehling, Azeotropic and solid–liquid equilibria data for several binaryorganic systems containing one acetal compound, Fluid Phase Equilibria 204 (2003) 267–280

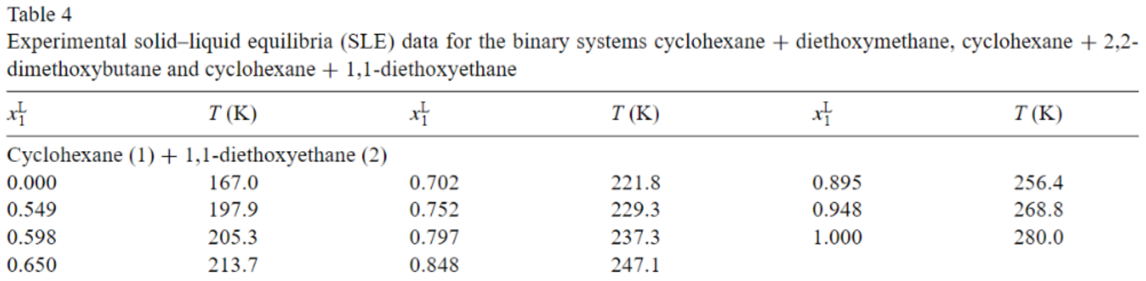


Table 4
Experimental solid–liquid equilibria (SLE) data for the binary systems cyclohexane + diethoxymethane, cyclohexane + 2,2-dimethoxybutane and cyclohexane + 1,1-diethoxyethane

| $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) | $x_1^L$ | $T$ (K) |
|---|---|---|---|---|---|
| Cyclohexane (1) + 1,1-diethoxyethane (2) | | | | | |
| 0.000 | 167.0 | 0.702 | 221.8 | 0.895 | 256.4 |
| 0.549 | 197.9 | 0.752 | 229.3 | 0.948 | 268.8 |
| 0.598 | 205.3 | 0.797 | 237.3 | 1.000 | 280.0 |
| 0.650 | 213.7 | 0.848 | 247.1 | | |

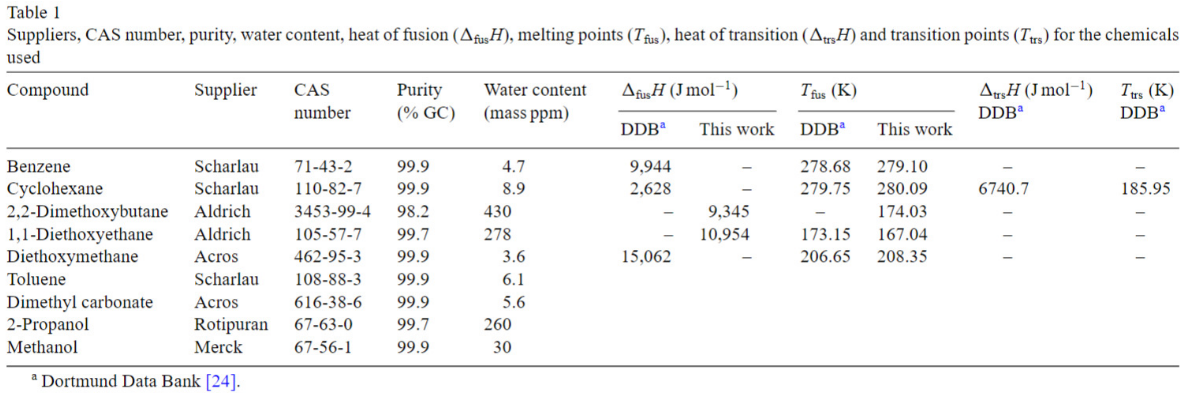


Table 1
Suppliers, CAS number, purity, water content, heat of fusion ($\Delta_{fus}H$), melting points ($T_{fus}$), heat of transition ($\Delta_{trs}H$) and transition points ($T_{trs}$) for the chemicals used

| Compound | Supplier | CAS number | Purity (% GC) | Water content (mass ppm) | $\Delta_{fus}H$ (J mol$^{-1}$) | | $T_{fus}$ (K) | | $\Delta_{trs}H$ (J mol$^{-1}$) DDB[a] | $T_{trs}$ (K) DDB[a] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | DDB[a] | This work | DDB[a] | This work | | |
| Benzene | Scharlau | 71-43-2 | 99.9 | 4.7 | 9,944 | – | 278.68 | 279.10 | – | – |
| Cyclohexane | Scharlau | 110-82-7 | 99.9 | 8.9 | 2,628 | – | 279.75 | 280.09 | 6740.7 | 185.95 |
| 2,2-Dimethoxybutane | Aldrich | 3453-99-4 | 98.2 | 430 | – | 9,345 | – | 174.03 | – | – |
| 1,1-Diethoxyethane | Aldrich | 105-57-7 | 99.7 | 278 | – | 10,954 | 173.15 | 167.04 | – | – |
| Diethoxymethane | Acros | 462-95-3 | 99.9 | 3.6 | 15,062 | – | 206.65 | 208.35 | – | – |
| Toluene | Scharlau | 108-88-3 | 99.9 | 6.1 | | | | | | |
| Dimethyl carbonate | Acros | 616-38-6 | 99.9 | 5.6 | | | | | | |
| 2-Propanol | Rotipuran | 67-63-0 | 99.7 | 260 | | | | | | |
| Methanol | Merck | 67-56-1 | 99.9 | 30 | | | | | | |

[a] Dortmund Data Bank [24].

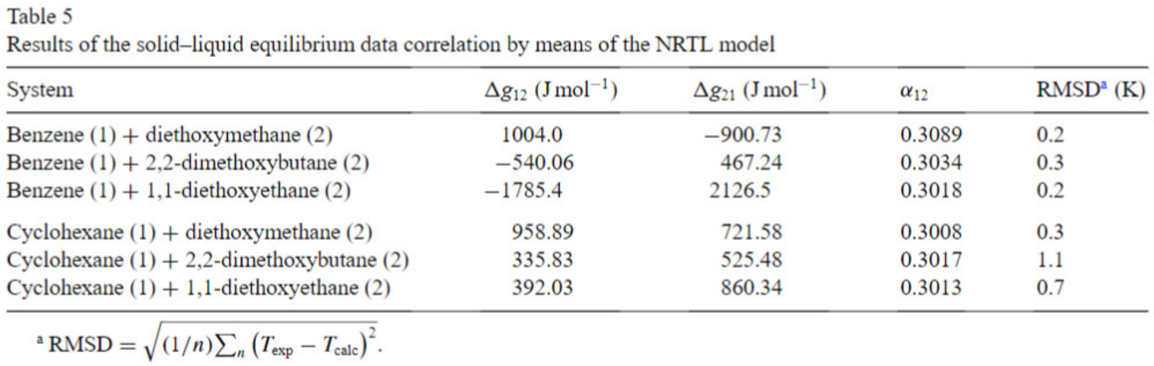


Table 5
Results of the solid–liquid equilibrium data correlation by means of the NRTL model

| System | $\Delta g_{12}$ (J mol$^{-1}$) | $\Delta g_{21}$ (J mol$^{-1}$) | $\alpha_{12}$ | RMSD[a] (K) |
|---|---|---|---|---|
| Benzene (1) + diethoxymethane (2) | 1004.0 | −900.73 | 0.3089 | 0.2 |
| Benzene (1) + 2,2-dimethoxybutane (2) | −540.06 | 467.24 | 0.3034 | 0.3 |
| Benzene (1) + 1,1-diethoxyethane (2) | −1785.4 | 2126.5 | 0.3018 | 0.2 |
| Cyclohexane (1) + diethoxymethane (2) | 958.89 | 721.58 | 0.3008 | 0.3 |
| Cyclohexane (1) + 2,2-dimethoxybutane (2) | 335.83 | 525.48 | 0.3017 | 1.1 |
| Cyclohexane (1) + 1,1-diethoxyethane (2) | 392.03 | 860.34 | 0.3013 | 0.7 |

[a] $\mathrm{RMSD} = \sqrt{(1/n)\sum_n \left(T_{exp} - T_{calc}\right)^2}$.

propanoic acid + acetic acid

P. Abrman, I. Malijevska, Solid–liquid equilibira in the acetic acid–propanoic acid andpropanoic acid–trifluoroacetic acid systems, Fluid Phase Equilibria 166 (1999) 47–52.

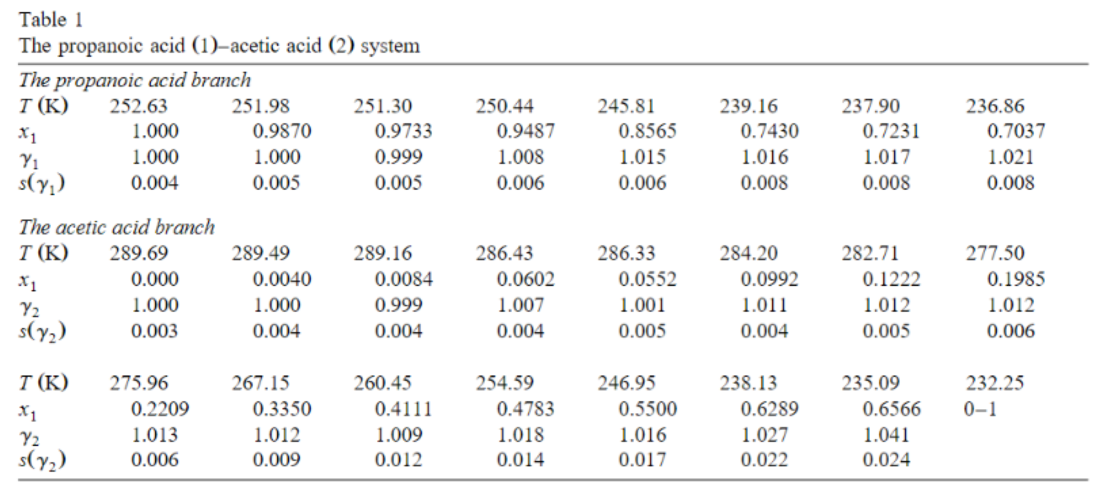


Table 1
The propanoic acid (1)–acetic acid (2) system

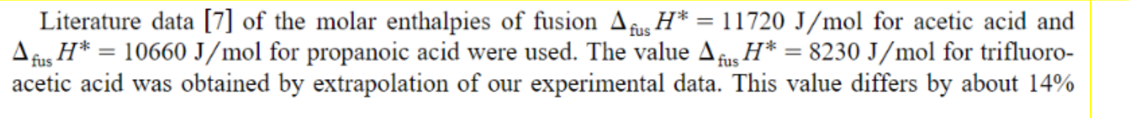
*The propanoic acid branch*

| $T$ (K) | 252.63 | 251.98 | 251.30 | 250.44 | 245.81 | 239.16 | 237.90 | 236.86 |
|---|---|---|---|---|---|---|---|---|
| $x_1$ | 1.000 | 0.9870 | 0.9733 | 0.9487 | 0.8565 | 0.7430 | 0.7231 | 0.7037 |
| $\gamma_1$ | 1.000 | 1.000 | 0.999 | 1.008 | 1.015 | 1.016 | 1.017 | 1.021 |
| $s(\gamma_1)$ | 0.004 | 0.005 | 0.005 | 0.006 | 0.006 | 0.008 | 0.008 | 0.008 |

*The acetic acid branch*

| $T$ (K) | 289.69 | 289.49 | 289.16 | 286.43 | 286.33 | 284.20 | 282.71 | 277.50 |
|---|---|---|---|---|---|---|---|---|
| $x_1$ | 0.000 | 0.0040 | 0.0084 | 0.0602 | 0.0552 | 0.0992 | 0.1222 | 0.1985 |
| $\gamma_2$ | 1.000 | 1.000 | 0.999 | 1.007 | 1.001 | 1.011 | 1.012 | 1.012 |
| $s(\gamma_2)$ | 0.003 | 0.004 | 0.004 | 0.004 | 0.005 | 0.004 | 0.005 | 0.006 |

| $T$ (K) | 275.96 | 267.15 | 260.45 | 254.59 | 246.95 | 238.13 | 235.09 | 232.25 |
|---|---|---|---|---|---|---|---|---|
| $x_1$ | 0.2209 | 0.3350 | 0.4111 | 0.4783 | 0.5500 | 0.6289 | 0.6566 | 0–1 |
| $\gamma_2$ | 1.013 | 1.012 | 1.009 | 1.018 | 1.016 | 1.027 | 1.041 | |
| $s(\gamma_2)$ | 0.006 | 0.009 | 0.012 | 0.014 | 0.017 | 0.022 | 0.024 | |



Literature data [7] of the molar enthalpies of fusion $\Delta_{\mathrm{fus}}H^* = 11720$ J/mol for acetic acid and $\Delta_{\mathrm{fus}}H^* = 10660$ J/mol for propanoic acid were used. The value $\Delta_{\mathrm{fus}}H^* = 8230$ J/mol for trifluoroacetic acid was obtained by extrapolation of our experimental data. This value differs by about 14%

propanoic acid + trifluoroacetic acid

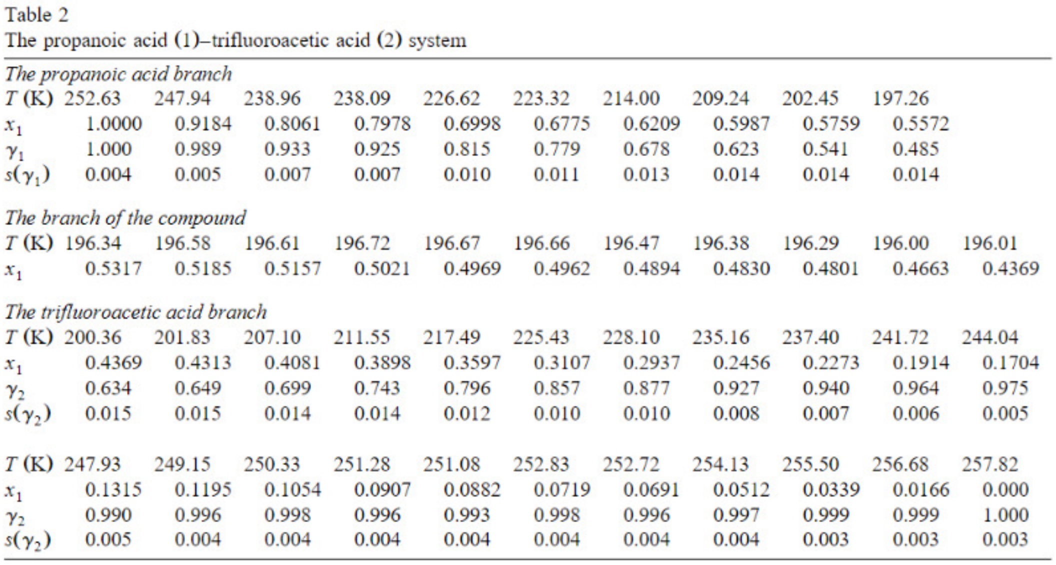
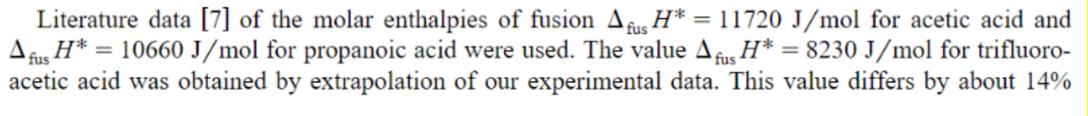


Table 2
The propanoic acid (1)–trifluoroacetic acid (2) system

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *The propanoic acid branch* | | | | | | | | | | | |
| $T$ (K) | 252.63 | 247.94 | 238.96 | 238.09 | 226.62 | 223.32 | 214.00 | 209.24 | 202.45 | 197.26 | |
| $x_1$ | 1.0000 | 0.9184 | 0.8061 | 0.7978 | 0.6998 | 0.6775 | 0.6209 | 0.5987 | 0.5759 | 0.5572 | |
| $\gamma_1$ | 1.000 | 0.989 | 0.933 | 0.925 | 0.815 | 0.779 | 0.678 | 0.623 | 0.541 | 0.485 | |
| $s(\gamma_1)$ | 0.004 | 0.005 | 0.007 | 0.007 | 0.010 | 0.011 | 0.013 | 0.014 | 0.014 | 0.014 | |
| *The branch of the compound* | | | | | | | | | | | |
| $T$ (K) | 196.34 | 196.58 | 196.61 | 196.72 | 196.67 | 196.66 | 196.47 | 196.38 | 196.29 | 196.00 | 196.01 |
| $x_1$ | 0.5317 | 0.5185 | 0.5157 | 0.5021 | 0.4969 | 0.4962 | 0.4894 | 0.4830 | 0.4801 | 0.4663 | 0.4369 |
| *The trifluoroacetic acid branch* | | | | | | | | | | | |
| $T$ (K) | 200.36 | 201.83 | 207.10 | 211.55 | 217.49 | 225.43 | 228.10 | 235.16 | 237.40 | 241.72 | 244.04 |
| $x_1$ | 0.4369 | 0.4313 | 0.4081 | 0.3898 | 0.3597 | 0.3107 | 0.2937 | 0.2456 | 0.2273 | 0.1914 | 0.1704 |
| $\gamma_2$ | 0.634 | 0.649 | 0.699 | 0.743 | 0.796 | 0.857 | 0.877 | 0.927 | 0.940 | 0.964 | 0.975 |
| $s(\gamma_2)$ | 0.015 | 0.015 | 0.014 | 0.014 | 0.012 | 0.010 | 0.010 | 0.008 | 0.007 | 0.006 | 0.005 |
| $T$ (K) | 247.93 | 249.15 | 250.33 | 251.28 | 251.08 | 252.83 | 252.72 | 254.13 | 255.50 | 256.68 | 257.82 |
| $x_1$ | 0.1315 | 0.1195 | 0.1054 | 0.0907 | 0.0882 | 0.0719 | 0.0691 | 0.0512 | 0.0339 | 0.0166 | 0.000 |
| $\gamma_2$ | 0.990 | 0.996 | 0.998 | 0.996 | 0.993 | 0.998 | 0.996 | 0.997 | 0.999 | 0.999 | 1.000 |
| $s(\gamma_2)$ | 0.005 | 0.004 | 0.004 | 0.004 | 0.004 | 0.004 | 0.004 | 0.004 | 0.003 | 0.003 | 0.003 |



Literature data [7] of the molar enthalpies of fusion $\Delta_{\text{fus}}H^* = 11720$ J/mol for acetic acid and $\Delta_{\text{fus}}H^* = 10660$ J/mol for propanoic acid were used. The value $\Delta_{\text{fus}}H^* = 8230$ J/mol for trifluoroacetic acid was obtained by extrapolation of our experimental data. This value differs by about 14%

N-methyl-2-pyrrolidinone + phenol

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria and solid-compound formation in (*N*-methyl-2-pyrrolidinone + phenol, or 3,5-dimethylphenol), Fluid Phase Equilibria 232 (2005) 214–218

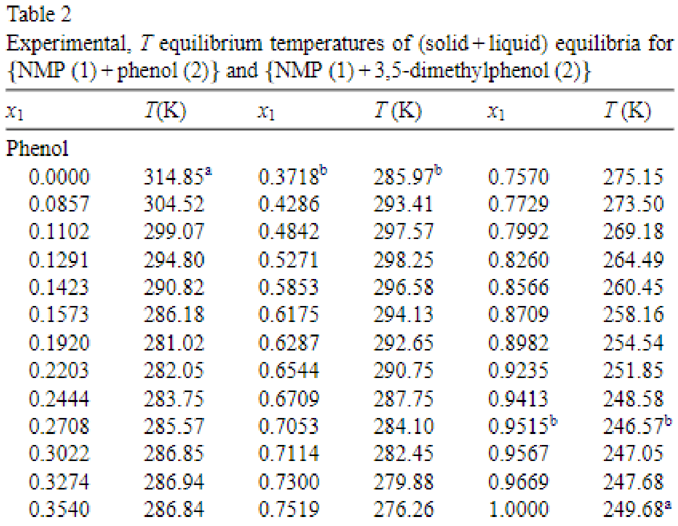


Table 2

Experimental, $T$ equilibrium temperatures of (solid + liquid) equilibria for {NMP (1) + phenol (2)} and {NMP (1) + 3,5-dimethylphenol (2)}

| $x_1$ | $T$(K) | $x_1$ | $T$ (K) | $x_1$ | $T$ (K) |
|---|---|---|---|---|---|
| Phenol | | | | | |
| 0.0000 | $314.85^{a}$ | $0.3718^{b}$ | $285.97^{b}$ | 0.7570 | 275.15 |
| 0.0857 | 304.52 | 0.4286 | 293.41 | 0.7729 | 273.50 |
| 0.1102 | 299.07 | 0.4842 | 297.57 | 0.7992 | 269.18 |
| 0.1291 | 294.80 | 0.5271 | 298.25 | 0.8260 | 264.49 |
| 0.1423 | 290.82 | 0.5853 | 296.58 | 0.8566 | 260.45 |
| 0.1573 | 286.18 | 0.6175 | 294.13 | 0.8709 | 258.16 |
| 0.1920 | 281.02 | 0.6287 | 292.65 | 0.8982 | 254.54 |
| 0.2203 | 282.05 | 0.6544 | 290.75 | 0.9235 | 251.85 |
| 0.2444 | 283.75 | 0.6709 | 287.75 | 0.9413 | 248.58 |
| 0.2708 | 285.57 | 0.7053 | 284.10 | $0.9515^{b}$ | $246.57^{b}$ |
| 0.3022 | 286.85 | 0.7114 | 282.45 | 0.9567 | 247.05 |
| 0.3274 | 286.94 | 0.7300 | 279.88 | 0.9669 | 247.68 |
| 0.3540 | 286.84 | 0.7519 | 276.26 | 1.0000 | $249.68^{a}$ |

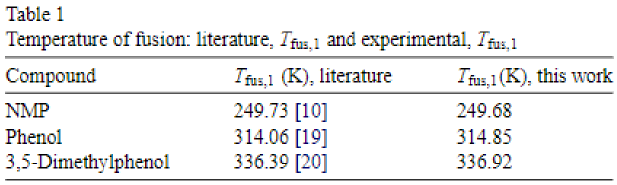


Table 1

Temperature of fusion: literature, $T_{\text{fus},1}$ and experimental, $T_{\text{fus},1}$

| Compound | $T_{\text{fus},1}$ (K), literature | $T_{\text{fus},1}$(K), this work |
|---|---|---|
| NMP | 249.73 [10] | 249.68 |
| Phenol | 314.06 [19] | 314.85 |
| 3,5-Dimethylphenol | 336.39 [20] | 336.92 |

# N-methyl-2-pyrrolidinone + 3,5-dimethylphenol

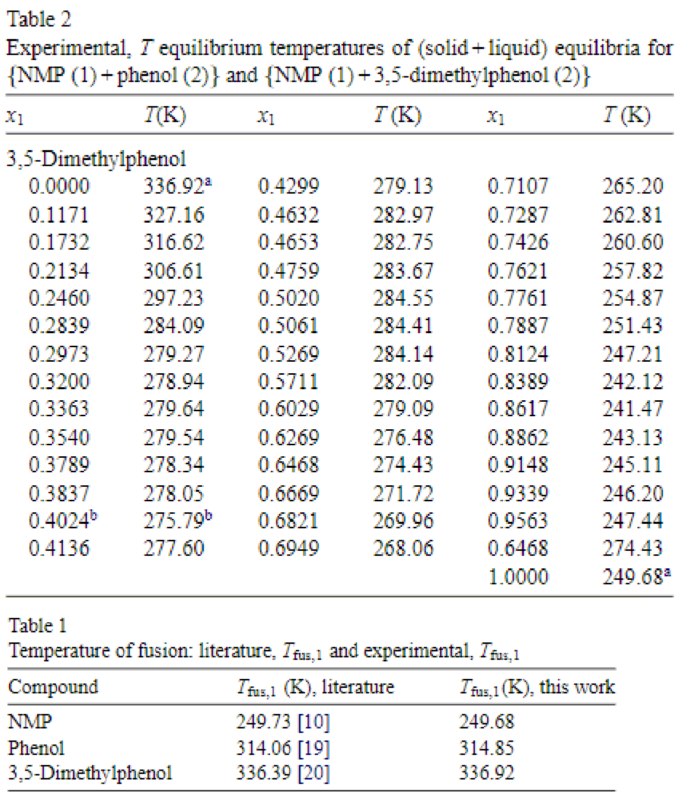


Table 2
Experimental, $T$ equilibrium temperatures of (solid + liquid) equilibria for {NMP (1) + phenol (2)} and {NMP (1) + 3,5-dimethylphenol (2)}

| $x_1$ | $T$(K) | $x_1$ | $T$ (K) | $x_1$ | $T$ (K) |
|---|---|---|---|---|---|
| 3,5-Dimethylphenol | | | | | |
| 0.0000 | 336.92[a] | 0.4299 | 279.13 | 0.7107 | 265.20 |
| 0.1171 | 327.16 | 0.4632 | 282.97 | 0.7287 | 262.81 |
| 0.1732 | 316.62 | 0.4653 | 282.75 | 0.7426 | 260.60 |
| 0.2134 | 306.61 | 0.4759 | 283.67 | 0.7621 | 257.82 |
| 0.2460 | 297.23 | 0.5020 | 284.55 | 0.7761 | 254.87 |
| 0.2839 | 284.09 | 0.5061 | 284.41 | 0.7887 | 251.43 |
| 0.2973 | 279.27 | 0.5269 | 284.14 | 0.8124 | 247.21 |
| 0.3200 | 278.94 | 0.5711 | 282.09 | 0.8389 | 242.12 |
| 0.3363 | 279.64 | 0.6029 | 279.09 | 0.8617 | 241.47 |
| 0.3540 | 279.54 | 0.6269 | 276.48 | 0.8862 | 243.13 |
| 0.3789 | 278.34 | 0.6468 | 274.43 | 0.9148 | 245.11 |
| 0.3837 | 278.05 | 0.6669 | 271.72 | 0.9339 | 246.20 |
| 0.4024[b] | 275.79[b] | 0.6821 | 269.96 | 0.9563 | 247.44 |
| 0.4136 | 277.60 | 0.6949 | 268.06 | 0.6468 | 274.43 |
| | | | | 1.0000 | 249.68[a] |

Table 1
Temperature of fusion: literature, $T_{fus,1}$ and experimental, $T_{fus,1}$

| Compound | $T_{fus,1}$ (K), literature | $T_{fus,1}$ (K), this work |
|---|---|---|
| NMP | 249.73 [10] | 249.68 |
| Phenol | 314.06 [19] | 314.85 |
| 3,5-Dimethylphenol | 336.39 [20] | 336.92 |

*N*-methyl-2-pyrrolidinone + dipropyl ether

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria of binary mixtures containingN-methyl-2-pyrrolidinone and ethers at atmospheric pressure, Fluid Phase Equilibria 227 (2005) 135–143

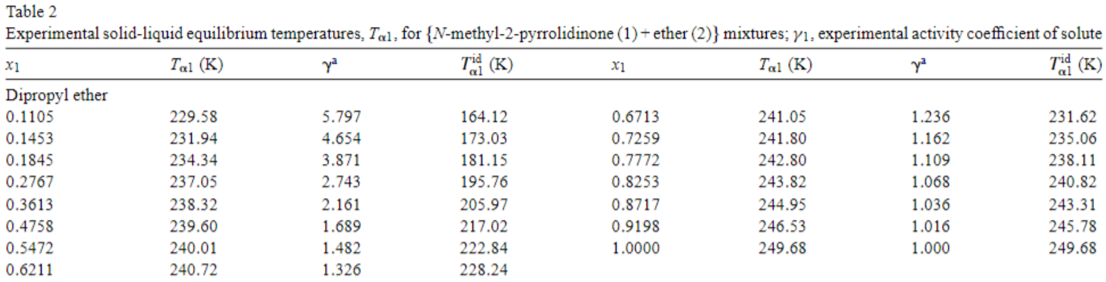


Table 2

Experimental solid-liquid equilibrium temperatures, $T_{\alpha 1}$, for {*N*-methyl-2-pyrrolidinone (1) + ether (2)} mixtures; $\gamma_1$, experimental activity coefficient of solute

| $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) | $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) |
|---|---|---|---|---|---|---|---|
| Dipropyl ether | | | | | | | |
| 0.1105 | 229.58 | 5.797 | 164.12 | 0.6713 | 241.05 | 1.236 | 231.62 |
| 0.1453 | 231.94 | 4.654 | 173.03 | 0.7259 | 241.80 | 1.162 | 235.06 |
| 0.1845 | 234.34 | 3.871 | 181.15 | 0.7772 | 242.80 | 1.109 | 238.11 |
| 0.2767 | 237.05 | 2.743 | 195.76 | 0.8253 | 243.82 | 1.068 | 240.82 |
| 0.3613 | 238.32 | 2.161 | 205.97 | 0.8717 | 244.95 | 1.036 | 243.31 |
| 0.4758 | 239.60 | 1.689 | 217.02 | 0.9198 | 246.53 | 1.016 | 245.78 |
| 0.5472 | 240.01 | 1.482 | 222.84 | 1.0000 | 249.68 | 1.000 | 249.68 |
| 0.6211 | 240.72 | 1.326 | 228.24 | | | | |

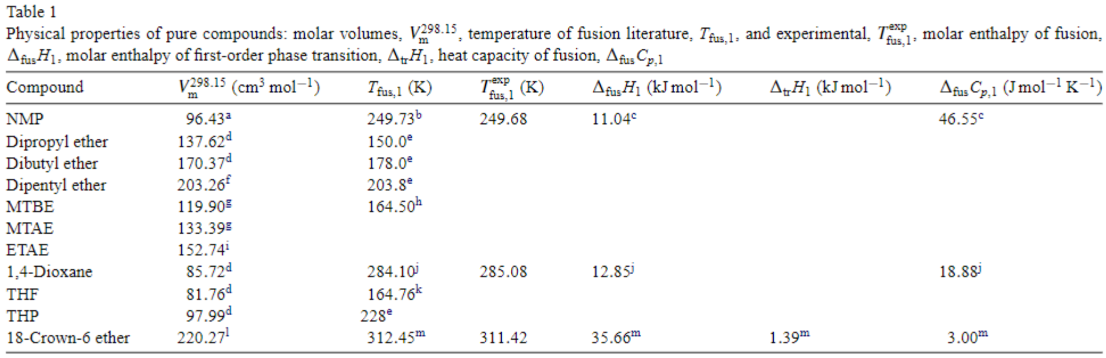


Table 1

Physical properties of pure compounds: molar volumes, $V_m^{298.15}$, temperature of fusion literature, $T_{fus,1}$, and experimental, $T_{fus,1}^{exp}$, molar enthalpy of fusion, $\Delta_{fus}H_1$, molar enthalpy of first-order phase transition, $\Delta_{tr}H_1$, heat capacity of fusion, $\Delta_{fus}C_{p,1}$

| Compound | $V_m^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{exp}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{tr}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| NMP | 96.43[a] | 249.73[b] | 249.68 | 11.04[c] | | 46.55[c] |
| Dipropyl ether | 137.62[d] | 150.0[e] | | | | |
| Dibutyl ether | 170.37[d] | 178.0[e] | | | | |
| Dipentyl ether | 203.26[f] | 203.8[e] | | | | |
| MTBE | 119.90[g] | 164.50[h] | | | | |
| MTAE | 133.39[g] | | | | | |
| ETAE | 152.74[i] | | | | | |
| 1,4-Dioxane | 85.72[d] | 284.10[j] | 285.08 | 12.85[j] | | 18.88[j] |
| THF | 81.76[d] | 164.76[k] | | | | |
| THP | 97.99[d] | 228[e] | | | | |
| 18-Crown-6 ether | 220.27[l] | 312.45[m] | 311.42 | 35.66[m] | 1.39[m] | 3.00[m] |

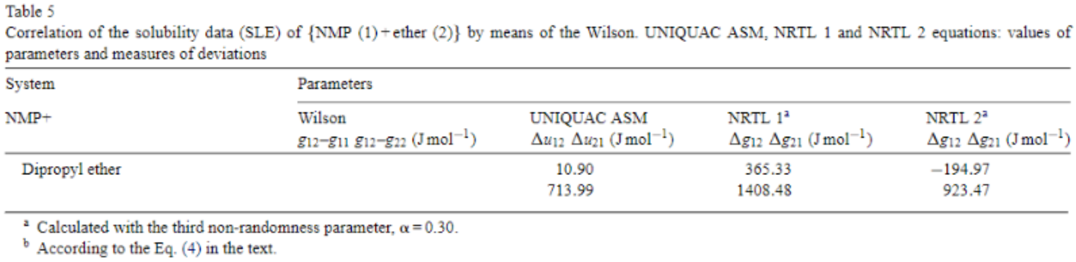


Table 5

Correlation of the solubility data (SLE) of {NMP (1) + ether (2)} by means of the Wilson. UNIQUAC ASM, NRTL 1 and NRTL 2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| NMP+ | Wilson<br>$g_{12}-g_{11}$ $g_{12}-g_{22}$ (J mol$^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$ $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) | NRTL 2[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) |
| Dipropyl ether | | 10.90<br>713.99 | 365.33<br>1408.48 | −194.97<br>923.47 |

[a] Calculated with the third non-randomness parameter, $\alpha = 0.30$.

[b] According to the Eq. (4) in the text.

ODABRATI JEDAN MODEL

*N*-methyl-2-pyrrolidinone + dibutyl ether

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria of binary mixtures containingN-methyl-2-pyrrolidinone and ethers at atmospheric pressure, Fluid Phase Equilibria 227 (2005) 135–143

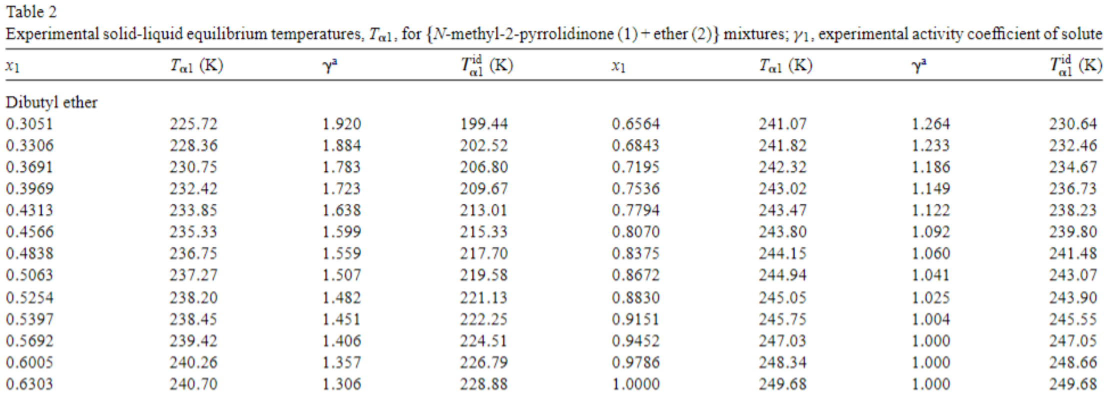


Table 2

Experimental solid-liquid equilibrium temperatures, $T_{\alpha 1}$, for {*N*-methyl-2-pyrrolidinone (1) + ether (2)} mixtures; $\gamma_1$, experimental activity coefficient of solute

| $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) | $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) |
|---|---|---|---|---|---|---|---|
| Dibutyl ether | | | | | | | |
| 0.3051 | 225.72 | 1.920 | 199.44 | 0.6564 | 241.07 | 1.264 | 230.64 |
| 0.3306 | 228.36 | 1.884 | 202.52 | 0.6843 | 241.82 | 1.233 | 232.46 |
| 0.3691 | 230.75 | 1.783 | 206.80 | 0.7195 | 242.32 | 1.186 | 234.67 |
| 0.3969 | 232.42 | 1.723 | 209.67 | 0.7536 | 243.02 | 1.149 | 236.73 |
| 0.4313 | 233.85 | 1.638 | 213.01 | 0.7794 | 243.47 | 1.122 | 238.23 |
| 0.4566 | 235.33 | 1.599 | 215.33 | 0.8070 | 243.80 | 1.092 | 239.80 |
| 0.4838 | 236.75 | 1.559 | 217.70 | 0.8375 | 244.15 | 1.060 | 241.48 |
| 0.5063 | 237.27 | 1.507 | 219.58 | 0.8672 | 244.94 | 1.041 | 243.07 |
| 0.5254 | 238.20 | 1.482 | 221.13 | 0.8830 | 245.05 | 1.025 | 243.90 |
| 0.5397 | 238.45 | 1.451 | 222.25 | 0.9151 | 245.75 | 1.004 | 245.55 |
| 0.5692 | 239.42 | 1.406 | 224.51 | 0.9452 | 247.03 | 1.000 | 247.05 |
| 0.6005 | 240.26 | 1.357 | 226.79 | 0.9786 | 248.34 | 1.000 | 248.66 |
| 0.6303 | 240.70 | 1.306 | 228.88 | 1.0000 | 249.68 | 1.000 | 249.68 |

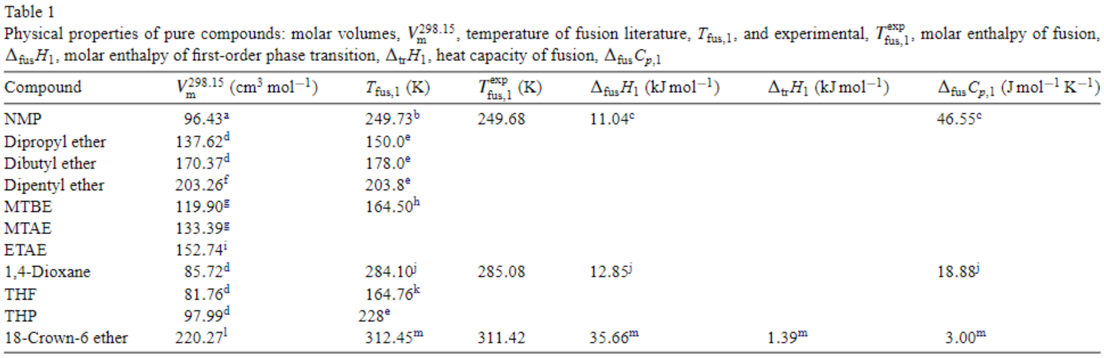


Table 1

Physical properties of pure compounds: molar volumes, $V_m^{298.15}$, temperature of fusion literature, $T_{fus,1}$, and experimental, $T_{fus,1}^{exp}$, molar enthalpy of fusion, $\Delta_{fus}H_1$, molar enthalpy of first-order phase transition, $\Delta_{tr}H_1$, heat capacity of fusion, $\Delta_{fus}C_{p,1}$

| Compound | $V_m^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{exp}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{tr}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| NMP | 96.43$^a$ | 249.73$^b$ | 249.68 | 11.04$^c$ | | 46.55$^c$ |
| Dipropyl ether | 137.62$^d$ | 150.0$^e$ | | | | |
| Dibutyl ether | 170.37$^d$ | 178.0$^e$ | | | | |
| Dipentyl ether | 203.26$^f$ | 203.8$^e$ | | | | |
| MTBE | 119.90$^g$ | 164.50$^h$ | | | | |
| MTAE | 133.39$^g$ | | | | | |
| ETAE | 152.74$^i$ | | | | | |
| 1,4-Dioxane | 85.72$^d$ | 284.10$^j$ | 285.08 | 12.85$^j$ | | 18.88$^j$ |
| THF | 81.76$^d$ | 164.76$^k$ | | | | |
| THP | 97.99$^d$ | 228$^e$ | | | | |
| 18-Crown-6 ether | 220.27$^l$ | 312.45$^m$ | 311.42 | 35.66$^m$ | 1.39$^m$ | 3.00$^m$ |

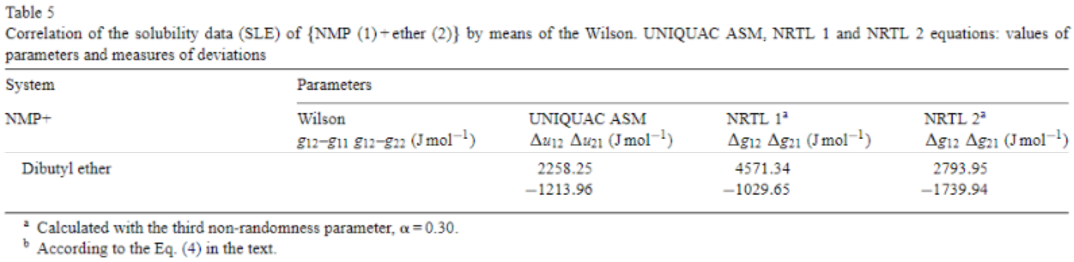


Table 5

Correlation of the solubility data (SLE) of {NMP (1) + ether (2)} by means of the Wilson. UNIQUAC ASM, NRTL 1 and NRTL 2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| NMP+ | Wilson<br>$g_{12}-g_{11}$ $g_{12}-g_{22}$ (J mol$^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$ $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1$^a$<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) | NRTL 2$^a$<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) |
| Dibutyl ether | | 2258.25<br>−1213.96 | 4571.34<br>−1029.65 | 2793.95<br>−1739.94 |

[a] Calculated with the third non-randomness parameter, $\alpha = 0.30$.

[b] According to the Eq. (4) in the text.

ODABRATI JEDAN MODEL

*N*-methyl-2-pyrrolidinone + dipentyl ether

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria of binary mixtures containingN-methyl-2-pyrrolidinone and ethers at atmospheric pressure, Fluid Phase Equilibria 227 (2005) 135–143

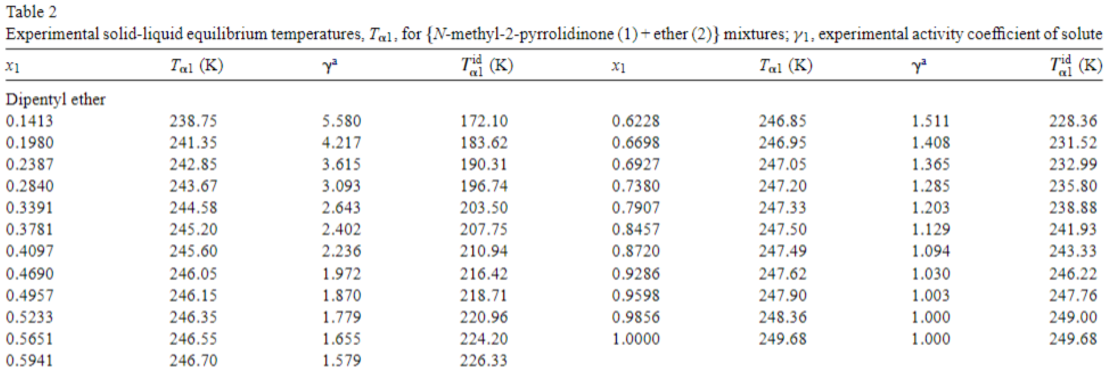


Table 2

Experimental solid-liquid equilibrium temperatures, $T_{\alpha 1}$, for {*N*-methyl-2-pyrrolidinone (1) + ether (2)} mixtures; $\gamma_1$, experimental activity coefficient of solute

| $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) | $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) |
|---|---|---|---|---|---|---|---|
| Dipentyl ether | | | | | | | |
| 0.1413 | 238.75 | 5.580 | 172.10 | 0.6228 | 246.85 | 1.511 | 228.36 |
| 0.1980 | 241.35 | 4.217 | 183.62 | 0.6698 | 246.95 | 1.408 | 231.52 |
| 0.2387 | 242.85 | 3.615 | 190.31 | 0.6927 | 247.05 | 1.365 | 232.99 |
| 0.2840 | 243.67 | 3.093 | 196.74 | 0.7380 | 247.20 | 1.285 | 235.80 |
| 0.3391 | 244.58 | 2.643 | 203.50 | 0.7907 | 247.33 | 1.203 | 238.88 |
| 0.3781 | 245.20 | 2.402 | 207.75 | 0.8457 | 247.50 | 1.129 | 241.93 |
| 0.4097 | 245.60 | 2.236 | 210.94 | 0.8720 | 247.49 | 1.094 | 243.33 |
| 0.4690 | 246.05 | 1.972 | 216.42 | 0.9286 | 247.62 | 1.030 | 246.22 |
| 0.4957 | 246.15 | 1.870 | 218.71 | 0.9598 | 247.90 | 1.003 | 247.76 |
| 0.5233 | 246.35 | 1.779 | 220.96 | 0.9856 | 248.36 | 1.000 | 249.00 |
| 0.5651 | 246.55 | 1.655 | 224.20 | 1.0000 | 249.68 | 1.000 | 249.68 |
| 0.5941 | 246.70 | 1.579 | 226.33 | | | | |

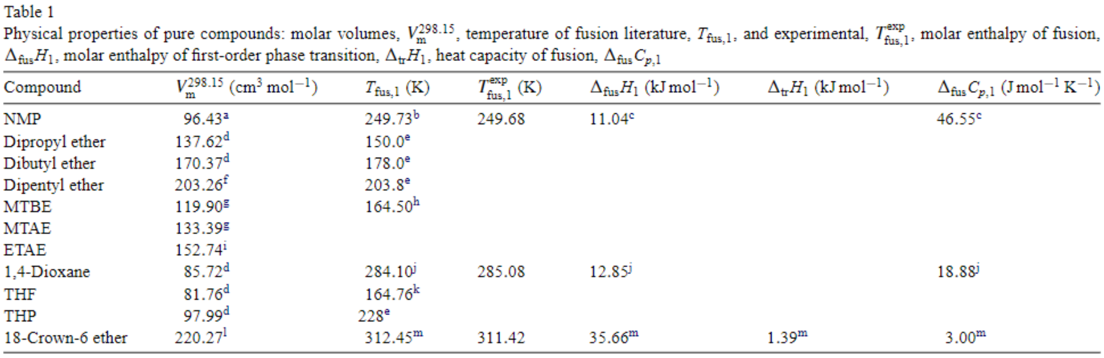


Table 1

Physical properties of pure compounds: molar volumes, $V_m^{298.15}$, temperature of fusion literature, $T_{fus,1}$, and experimental, $T_{fus,1}^{exp}$, molar enthalpy of fusion, $\Delta_{fus}H_1$, molar enthalpy of first-order phase transition, $\Delta_{tr}H_1$, heat capacity of fusion, $\Delta_{fus}C_{p,1}$

| Compound | $V_m^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{exp}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{tr}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| NMP | 96.43[a] | 249.73[b] | 249.68 | 11.04[c] | | 46.55[c] |
| Dipropyl ether | 137.62[d] | 150.0[e] | | | | |
| Dibutyl ether | 170.37[d] | 178.0[e] | | | | |
| Dipentyl ether | 203.26[f] | 203.8[e] | | | | |
| MTBE | 119.90[g] | 164.50[h] | | | | |
| MTAE | 133.39[g] | | | | | |
| ETAE | 152.74[i] | | | | | |
| 1,4-Dioxane | 85.72[d] | 284.10[j] | 285.08 | 12.85[j] | | 18.88[j] |
| THF | 81.76[d] | 164.76[k] | | | | |
| THP | 97.99[d] | 228[e] | | | | |
| 18-Crown-6 ether | 220.27[l] | 312.45[m] | 311.42 | 35.66[m] | 1.39[m] | 3.00[m] |

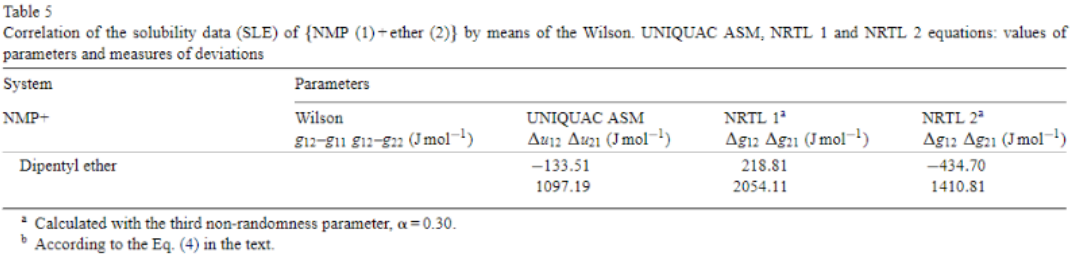


Table 5

Correlation of the solubility data (SLE) of {NMP (1) + ether (2)} by means of the Wilson. UNIQUAC ASM, NRTL 1 and NRTL 2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| NMP+ | Wilson<br>$g_{12}-g_{11}$ $g_{12}-g_{22}$ (J mol$^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$ $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) | NRTL 2[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) |
| Dipentyl ether | | −133.51<br>1097.19 | 218.81<br>2054.11 | −434.70<br>1410.81 |

[a] Calculated with the third non-randomness parameter, $\alpha = 0.30$.

[b] According to the Eq. (4) in the text.

ODABRATI JEDAN MODEL

*N*-methyl-2-pyrrolidinone + methyl 1,1-dimethylethyl ether

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria of binary mixtures containingN-methyl-2-pyrrolidinone and ethers at atmospheric pressure, Fluid Phase Equilibria 227 (2005) 135–143

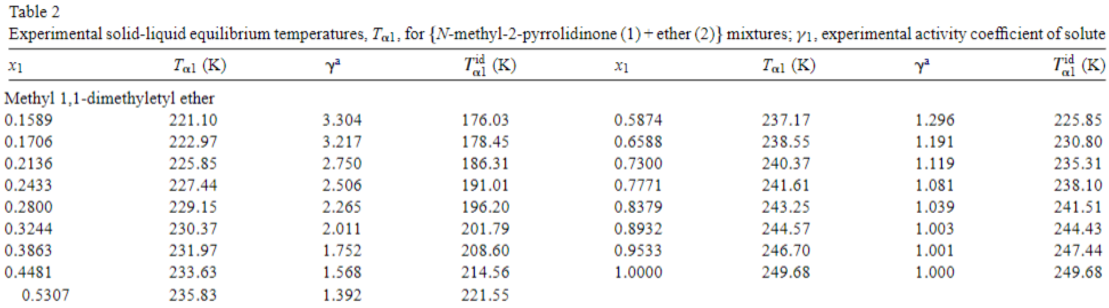


Table 2

Experimental solid-liquid equilibrium temperatures, $T_{\alpha 1}$, for {*N*-methyl-2-pyrrolidinone (1) + ether (2)} mixtures; $\gamma_1$, experimental activity coefficient of solute

| $x_1$ | $T_{\alpha 1}$ (K) | $\gamma$[a] | $T_{\alpha 1}^{id}$ (K) | $x_1$ | $T_{\alpha 1}$ (K) | $\gamma$[a] | $T_{\alpha 1}^{id}$ (K) |
|---|---|---|---|---|---|---|---|
| Methyl 1,1-dimethyletyl ether | | | | | | | |
| 0.1589 | 221.10 | 3.304 | 176.03 | 0.5874 | 237.17 | 1.296 | 225.85 |
| 0.1706 | 222.97 | 3.217 | 178.45 | 0.6588 | 238.55 | 1.191 | 230.80 |
| 0.2136 | 225.85 | 2.750 | 186.31 | 0.7300 | 240.37 | 1.119 | 235.31 |
| 0.2433 | 227.44 | 2.506 | 191.01 | 0.7771 | 241.61 | 1.081 | 238.10 |
| 0.2800 | 229.15 | 2.265 | 196.20 | 0.8379 | 243.25 | 1.039 | 241.51 |
| 0.3244 | 230.37 | 2.011 | 201.79 | 0.8932 | 244.57 | 1.003 | 244.43 |
| 0.3863 | 231.97 | 1.752 | 208.60 | 0.9533 | 246.70 | 1.001 | 247.44 |
| 0.4481 | 233.63 | 1.568 | 214.56 | 1.0000 | 249.68 | 1.000 | 249.68 |
| 0.5307 | 235.83 | 1.392 | 221.55 | | | | |

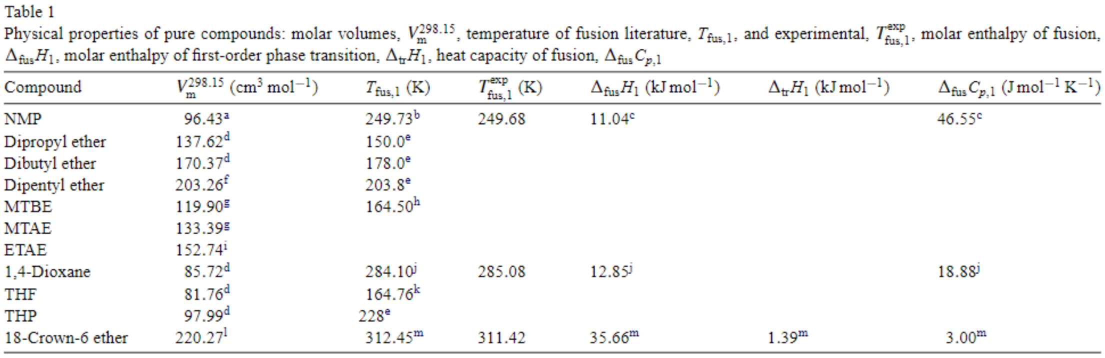


Table 1

Physical properties of pure compounds: molar volumes, $V_m^{298.15}$, temperature of fusion literature, $T_{fus,1}$, and experimental, $T_{fus,1}^{exp}$, molar enthalpy of fusion, $\Delta_{fus}H_1$, molar enthalpy of first-order phase transition, $\Delta_{tr}H_1$, heat capacity of fusion, $\Delta_{fus}C_{p,1}$

| Compound | $V_m^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{exp}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{tr}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| NMP | 96.43[a] | 249.73[b] | 249.68 | 11.04[c] | | 46.55[c] |
| Dipropyl ether | 137.62[d] | 150.0[e] | | | | |
| Dibutyl ether | 170.37[d] | 178.0[e] | | | | |
| Dipentyl ether | 203.26[f] | 203.8[e] | | | | |
| MTBE | 119.90[g] | 164.50[h] | | | | |
| MTAE | 133.39[g] | | | | | |
| ETAE | 152.74[i] | | | | | |
| 1,4-Dioxane | 85.72[d] | 284.10[j] | 285.08 | 12.85[j] | | 18.88[j] |
| THF | 81.76[d] | 164.76[k] | | | | |
| THP | 97.99[d] | 228[e] | | | | |
| 18-Crown-6 ether | 220.27[l] | 312.45[m] | 311.42 | 35.66[m] | 1.39[m] | 3.00[m] |

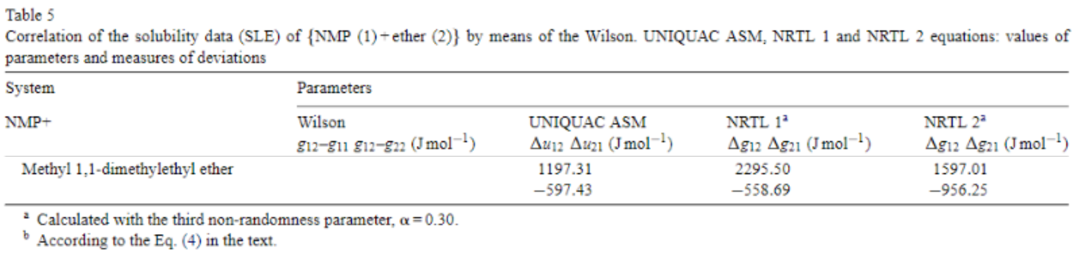


Table 5

Correlation of the solubility data (SLE) of {NMP (1) + ether (2)} by means of the Wilson. UNIQUAC ASM, NRTL 1 and NRTL 2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| NMP+ | Wilson<br>$g_{12}-g_{11}$ $g_{12}-g_{22}$ (J mol$^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$ $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) | NRTL 2[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) |
| Methyl 1,1-dimethylethyl ether | | 1197.31<br>−597.43 | 2295.50<br>−558.69 | 1597.01<br>−956.25 |

[a] Calculated with the third non-randomness parameter, $\alpha = 0.30$.

[b] According to the Eq. (4) in the text.

ODABRATI JEDAN MODEL

*N*-methyl-2-pyrrolidinone + methyl 1,1-dimethylpropylether

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria of binary mixtures containingN-methyl-2-pyrrolidinone and ethers at atmospheric pressure, Fluid Phase Equilibria 227 (2005) 135–143

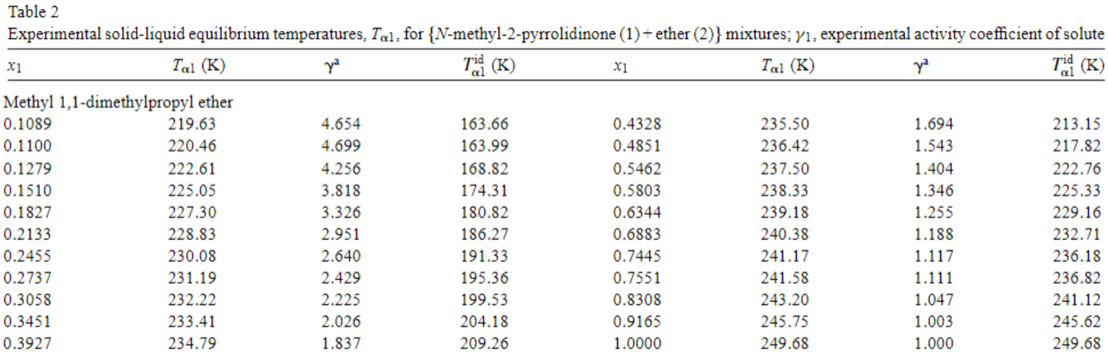


Table 2

Experimental solid-liquid equilibrium temperatures, $T_{\alpha 1}$, for {*N*-methyl-2-pyrrolidinone (1) + ether (2)} mixtures; $\gamma_1$, experimental activity coefficient of solute

| $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T^{id}_{\alpha 1}$ (K) | $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T^{id}_{\alpha 1}$ (K) |
|---|---|---|---|---|---|---|---|
| Methyl 1,1-dimethylpropyl ether | | | | | | | |
| 0.1089 | 219.63 | 4.654 | 163.66 | 0.4328 | 235.50 | 1.694 | 213.15 |
| 0.1100 | 220.46 | 4.699 | 163.99 | 0.4851 | 236.42 | 1.543 | 217.82 |
| 0.1279 | 222.61 | 4.256 | 168.82 | 0.5462 | 237.50 | 1.404 | 222.76 |
| 0.1510 | 225.05 | 3.818 | 174.31 | 0.5803 | 238.33 | 1.346 | 225.33 |
| 0.1827 | 227.30 | 3.326 | 180.82 | 0.6344 | 239.18 | 1.255 | 229.16 |
| 0.2133 | 228.83 | 2.951 | 186.27 | 0.6883 | 240.38 | 1.188 | 232.71 |
| 0.2455 | 230.08 | 2.640 | 191.33 | 0.7445 | 241.17 | 1.117 | 236.18 |
| 0.2737 | 231.19 | 2.429 | 195.36 | 0.7551 | 241.58 | 1.111 | 236.82 |
| 0.3058 | 232.22 | 2.225 | 199.53 | 0.8308 | 243.20 | 1.047 | 241.12 |
| 0.3451 | 233.41 | 2.026 | 204.18 | 0.9165 | 245.75 | 1.003 | 245.62 |
| 0.3927 | 234.79 | 1.837 | 209.26 | 1.0000 | 249.68 | 1.000 | 249.68 |

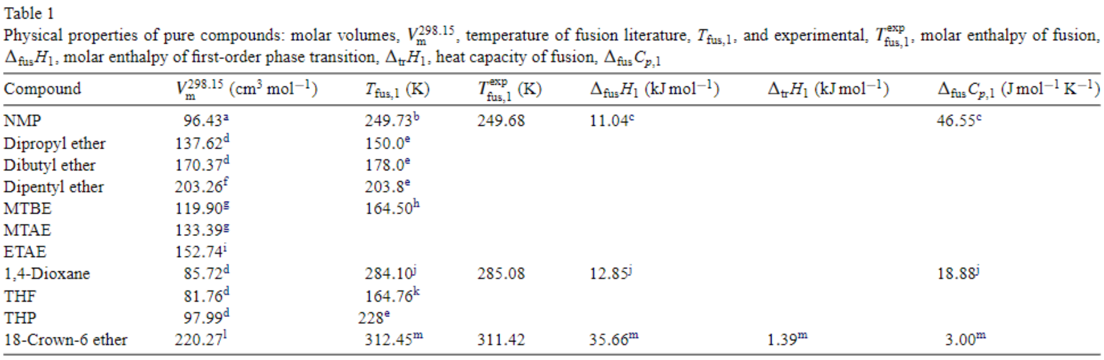


Table 1

Physical properties of pure compounds: molar volumes, $V_m^{298.15}$, temperature of fusion literature, $T_{fus,1}$, and experimental, $T^{exp}_{fus,1}$, molar enthalpy of fusion, $\Delta_{fus}H_1$, molar enthalpy of first-order phase transition, $\Delta_{tr}H_1$, heat capacity of fusion, $\Delta_{fus}C_{p,1}$

| Compound | $V_m^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T^{exp}_{fus,1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{tr}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| NMP | 96.43[a] | 249.73[b] | 249.68 | 11.04[c] | | 46.55[c] |
| Dipropyl ether | 137.62[d] | 150.0[e] | | | | |
| Dibutyl ether | 170.37[d] | 178.0[e] | | | | |
| Dipentyl ether | 203.26[f] | 203.8[e] | | | | |
| MTBE | 119.90[g] | 164.50[h] | | | | |
| MTAE | 133.39[g] | | | | | |
| ETAE | 152.74[i] | | | | | |
| 1,4-Dioxane | 85.72[d] | 284.10[j] | 285.08 | 12.85[j] | | 18.88[j] |
| THF | 81.76[d] | 164.76[k] | | | | |
| THP | 97.99[d] | 228[e] | | | | |
| 18-Crown-6 ether | 220.27[l] | 312.45[m] | 311.42 | 35.66[m] | 1.39[m] | 3.00[m] |

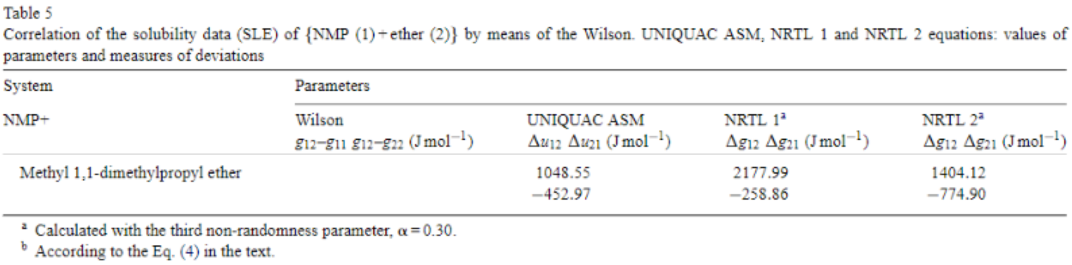


Table 5

Correlation of the solubility data (SLE) of {NMP (1) + ether (2)} by means of the Wilson. UNIQUAC ASM, NRTL 1 and NRTL 2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| NMP+ | Wilson<br>$g_{12}-g_{11}$ $g_{12}-g_{22}$ (J mol$^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$ $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) | NRTL 2[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) |
| Methyl 1,1-dimethylpropyl ether | | 1048.55<br>−452.97 | 2177.99<br>−258.86 | 1404.12<br>−774.90 |

[a] Calculated with the third non-randomness parameter, α = 0.30.

[b] According to the Eq. (4) in the text.

ODABRATI JEDAN MODEL

*N*-methyl-2-pyrrolidinone + ethyl 1,1-dimethylpropyl ether

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria of binary mixtures containingN-methyl-2-pyrrolidinone and ethers at atmospheric pressure, Fluid Phase Equilibria 227 (2005) 135–143

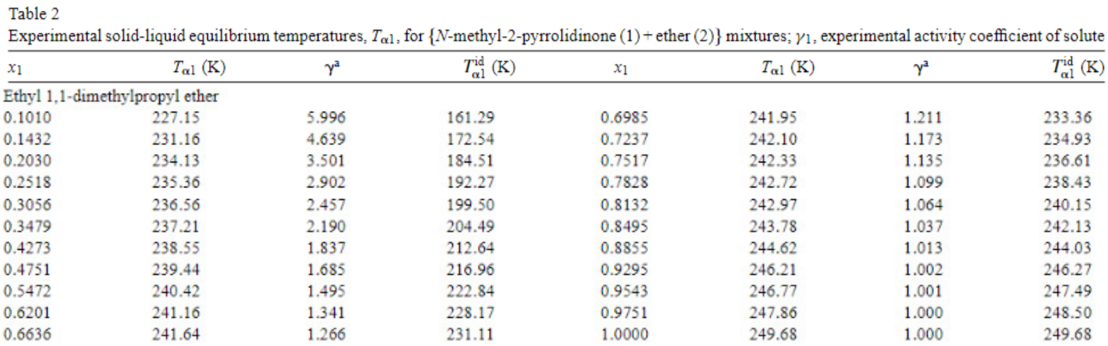


Table 2

Experimental solid-liquid equilibrium temperatures, $T_{\alpha 1}$, for {*N*-methyl-2-pyrrolidinone (1) + ether (2)} mixtures; $\gamma_1$, experimental activity coefficient of solute

| $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) | $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) |
|---|---|---|---|---|---|---|---|
| Ethyl 1,1-dimethylpropyl ether | | | | | | | |
| 0.1010 | 227.15 | 5.996 | 161.29 | 0.6985 | 241.95 | 1.211 | 233.36 |
| 0.1432 | 231.16 | 4.639 | 172.54 | 0.7237 | 242.10 | 1.173 | 234.93 |
| 0.2030 | 234.13 | 3.501 | 184.51 | 0.7517 | 242.33 | 1.135 | 236.61 |
| 0.2518 | 235.36 | 2.902 | 192.27 | 0.7828 | 242.72 | 1.099 | 238.43 |
| 0.3056 | 236.56 | 2.457 | 199.50 | 0.8132 | 242.97 | 1.064 | 240.15 |
| 0.3479 | 237.21 | 2.190 | 204.49 | 0.8495 | 243.78 | 1.037 | 242.13 |
| 0.4273 | 238.55 | 1.837 | 212.64 | 0.8855 | 244.62 | 1.013 | 244.03 |
| 0.4751 | 239.44 | 1.685 | 216.96 | 0.9295 | 246.21 | 1.002 | 246.27 |
| 0.5472 | 240.42 | 1.495 | 222.84 | 0.9543 | 246.77 | 1.001 | 247.49 |
| 0.6201 | 241.16 | 1.341 | 228.17 | 0.9751 | 247.86 | 1.000 | 248.50 |
| 0.6636 | 241.64 | 1.266 | 231.11 | 1.0000 | 249.68 | 1.000 | 249.68 |

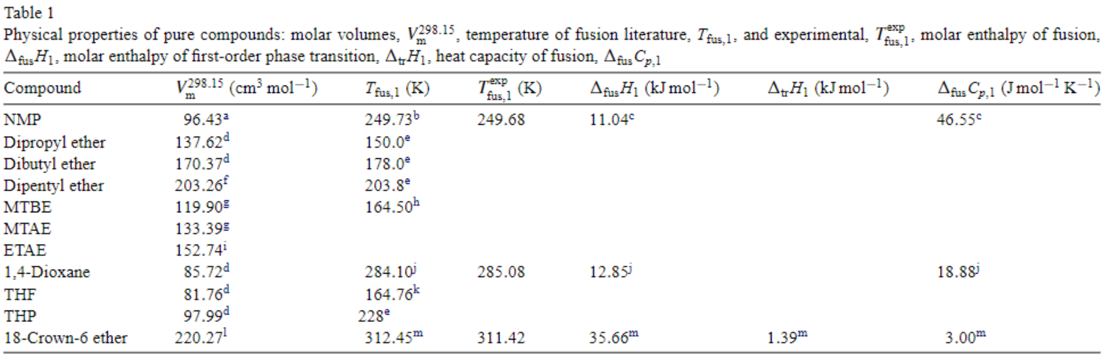


Table 1

Physical properties of pure compounds: molar volumes, $V_m^{298.15}$, temperature of fusion literature, $T_{fus,1}$, and experimental, $T_{fus,1}^{exp}$, molar enthalpy of fusion, $\Delta_{fus}H_1$, molar enthalpy of first-order phase transition, $\Delta_{tr}H_1$, heat capacity of fusion, $\Delta_{fus}C_{p,1}$

| Compound | $V_m^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{exp}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{tr}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| NMP | 96.43[a] | 249.73[b] | 249.68 | 11.04[c] | | 46.55[c] |
| Dipropyl ether | 137.62[d] | 150.0[e] | | | | |
| Dibutyl ether | 170.37[d] | 178.0[e] | | | | |
| Dipentyl ether | 203.26[f] | 203.8[e] | | | | |
| MTBE | 119.90[g] | 164.50[h] | | | | |
| MTAE | 133.39[g] | | | | | |
| ETAE | 152.74[i] | | | | | |
| 1,4-Dioxane | 85.72[d] | 284.10[j] | 285.08 | 12.85[j] | | 18.88[j] |
| THF | 81.76[d] | 164.76[k] | | | | |
| THP | 97.99[d] | 228[e] | | | | |
| 18-Crown-6 ether | 220.27[l] | 312.45[m] | 311.42 | 35.66[m] | 1.39[m] | 3.00[m] |

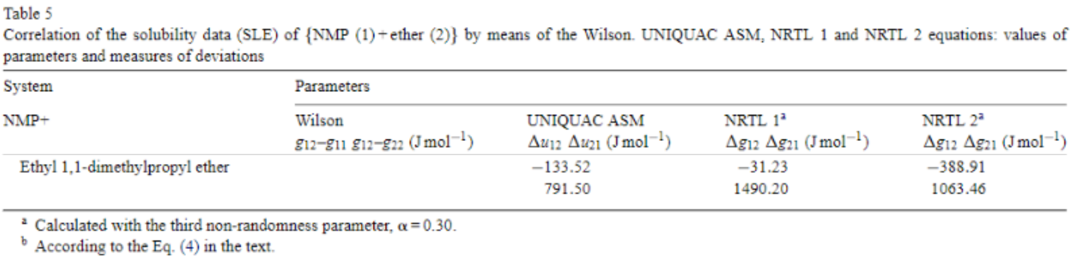


Table 5

Correlation of the solubility data (SLE) of {NMP (1) + ether (2)} by means of the Wilson. UNIQUAC ASM, NRTL 1 and NRTL 2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| NMP+ | Wilson<br>$g_{12}-g_{11}$ $g_{12}-g_{22}$ (J mol$^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$ $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) | NRTL 2[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) |
| Ethyl 1,1-dimethylpropyl ether | | −133.52<br>791.50 | −31.23<br>1490.20 | −388.91<br>1063.46 |

[a] Calculated with the third non-randomness parameter, $\alpha = 0.30$.

[b] According to the Eq. (4) in the text.

ODABRATI JEDAN MODEL

*N*-methyl-2-pyrrolidinone + tetrahydrofuran

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria of binary mixtures containingN-methyl-2-pyrrolidinone and ethers at atmospheric pressure, Fluid Phase Equilibria 227 (2005) 135–143

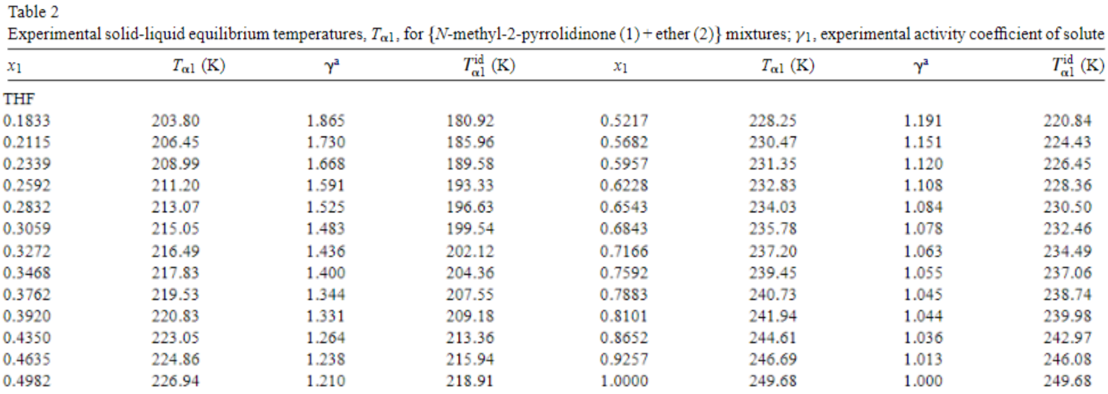


Table 2

Experimental solid-liquid equilibrium temperatures, $T_{\alpha 1}$, for {*N*-methyl-2-pyrrolidinone (1) + ether (2)} mixtures; $\gamma_1$, experimental activity coefficient of solute

| $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) | $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) |
|---|---|---|---|---|---|---|---|
| THF | | | | | | | |
| 0.1833 | 203.80 | 1.865 | 180.92 | 0.5217 | 228.25 | 1.191 | 220.84 |
| 0.2115 | 206.45 | 1.730 | 185.96 | 0.5682 | 230.47 | 1.151 | 224.43 |
| 0.2339 | 208.99 | 1.668 | 189.58 | 0.5957 | 231.35 | 1.120 | 226.45 |
| 0.2592 | 211.20 | 1.591 | 193.33 | 0.6228 | 232.83 | 1.108 | 228.36 |
| 0.2832 | 213.07 | 1.525 | 196.63 | 0.6543 | 234.03 | 1.084 | 230.50 |
| 0.3059 | 215.05 | 1.483 | 199.54 | 0.6843 | 235.78 | 1.078 | 232.46 |
| 0.3272 | 216.49 | 1.436 | 202.12 | 0.7166 | 237.20 | 1.063 | 234.49 |
| 0.3468 | 217.83 | 1.400 | 204.36 | 0.7592 | 239.45 | 1.055 | 237.06 |
| 0.3762 | 219.53 | 1.344 | 207.55 | 0.7883 | 240.73 | 1.045 | 238.74 |
| 0.3920 | 220.83 | 1.331 | 209.18 | 0.8101 | 241.94 | 1.044 | 239.98 |
| 0.4350 | 223.05 | 1.264 | 213.36 | 0.8652 | 244.61 | 1.036 | 242.97 |
| 0.4635 | 224.86 | 1.238 | 215.94 | 0.9257 | 246.69 | 1.013 | 246.08 |
| 0.4982 | 226.94 | 1.210 | 218.91 | 1.0000 | 249.68 | 1.000 | 249.68 |

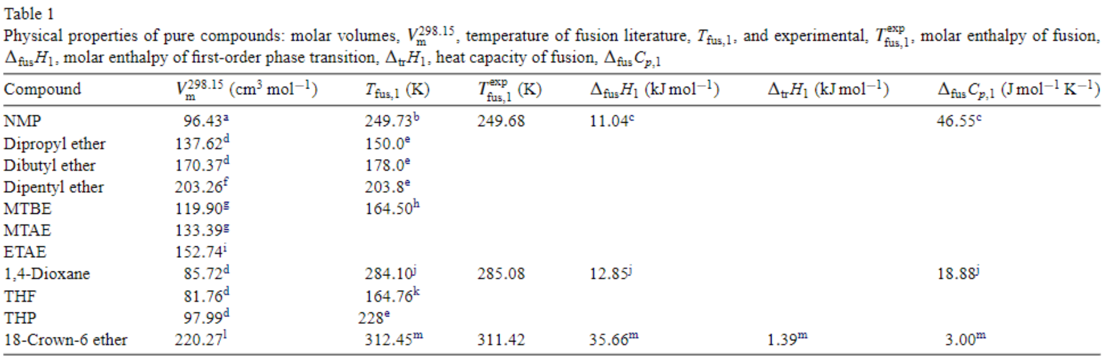


Table 1

Physical properties of pure compounds: molar volumes, $V_m^{298.15}$, temperature of fusion literature, $T_{fus,1}$, and experimental, $T_{fus,1}^{exp}$, molar enthalpy of fusion, $\Delta_{fus}H_1$, molar enthalpy of first-order phase transition, $\Delta_{tr}H_1$, heat capacity of fusion, $\Delta_{fus}C_{p,1}$

| Compound | $V_m^{298.15}$ ($cm^3\ mol^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{exp}$ (K) | $\Delta_{fus}H_1$ ($kJ\ mol^{-1}$) | $\Delta_{tr}H_1$ ($kJ\ mol^{-1}$) | $\Delta_{fus}C_{p,1}$ ($J\ mol^{-1}\ K^{-1}$) |
|---|---|---|---|---|---|---|
| NMP | 96.43[a] | 249.73[b] | 249.68 | 11.04[c] | | 46.55[c] |
| Dipropyl ether | 137.62[d] | 150.0[e] | | | | |
| Dibutyl ether | 170.37[d] | 178.0[e] | | | | |
| Dipentyl ether | 203.26[f] | 203.8[e] | | | | |
| MTBE | 119.90[g] | 164.50[h] | | | | |
| MTAE | 133.39[g] | | | | | |
| ETAE | 152.74[i] | | | | | |
| 1,4-Dioxane | 85.72[d] | 284.10[j] | 285.08 | 12.85[j] | | 18.88[j] |
| THF | 81.76[d] | 164.76[k] | | | | |
| THP | 97.99[d] | 228[e] | | | | |
| 18-Crown-6 ether | 220.27[l] | 312.45[m] | 311.42 | 35.66[m] | 1.39[m] | 3.00[m] |

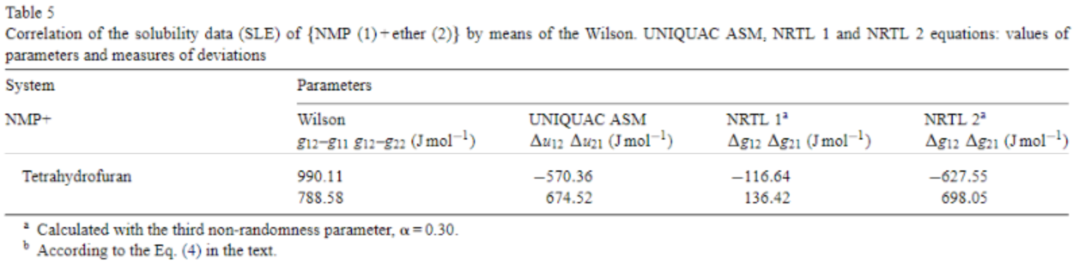


Table 5

Correlation of the solubility data (SLE) of {NMP (1) + ether (2)} by means of the Wilson. UNIQUAC ASM, NRTL 1 and NRTL 2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| NMP+ | Wilson<br>$g_{12}-g_{11}$ $g_{12}-g_{22}$ ($J\ mol^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$ $\Delta u_{21}$ ($J\ mol^{-1}$) | NRTL 1[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ ($J\ mol^{-1}$) | NRTL 2[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ ($J\ mol^{-1}$) |
| Tetrahydrofuran | 990.11 | −570.36 | −116.64 | −627.55 |
| | 788.58 | 674.52 | 136.42 | 698.05 |

[a] Calculated with the third non-randomness parameter, $\alpha = 0.30$.

[b] According to the Eq. (4) in the text.

ODABRATI JEDAN MODEL

*N*-methyl-2-pyrrolidinone + tetrahydropyran

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria of binary mixtures containingN-methyl-2-pyrrolidinone and ethers at atmospheric pressure, Fluid Phase Equilibria 227 (2005) 135–143

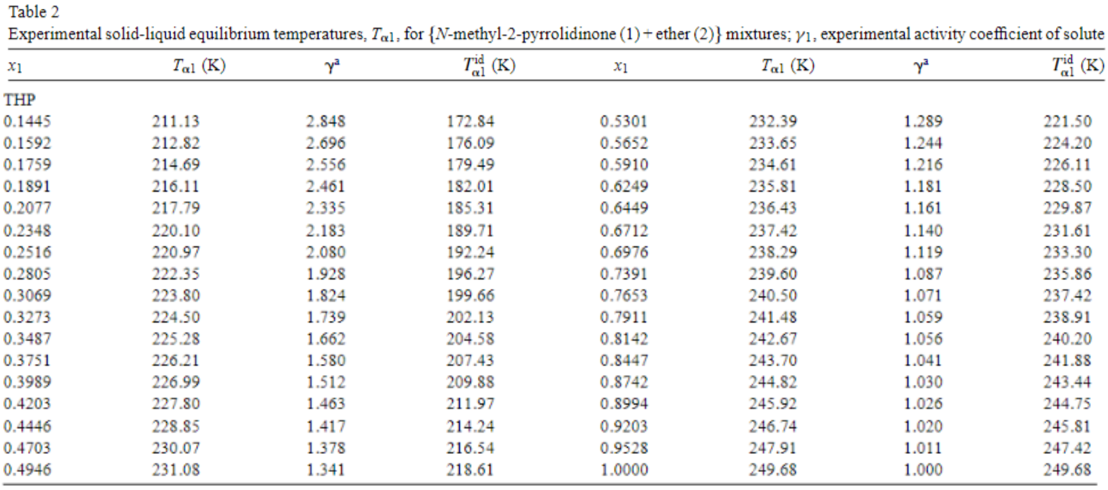


Table 2

Experimental solid-liquid equilibrium temperatures, $T_{\alpha 1}$, for {*N*-methyl-2-pyrrolidinone (1) + ether (2)} mixtures; $\gamma_1$, experimental activity coefficient of solute

| $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) | $x_1$ | $T_{\alpha 1}$ (K) | $\gamma^a$ | $T_{\alpha 1}^{id}$ (K) |
|---|---|---|---|---|---|---|---|
| THP | | | | | | | |
| 0.1445 | 211.13 | 2.848 | 172.84 | 0.5301 | 232.39 | 1.289 | 221.50 |
| 0.1592 | 212.82 | 2.696 | 176.09 | 0.5652 | 233.65 | 1.244 | 224.20 |
| 0.1759 | 214.69 | 2.556 | 179.49 | 0.5910 | 234.61 | 1.216 | 226.11 |
| 0.1891 | 216.11 | 2.461 | 182.01 | 0.6249 | 235.81 | 1.181 | 228.50 |
| 0.2077 | 217.79 | 2.335 | 185.31 | 0.6449 | 236.43 | 1.161 | 229.87 |
| 0.2348 | 220.10 | 2.183 | 189.71 | 0.6712 | 237.42 | 1.140 | 231.61 |
| 0.2516 | 220.97 | 2.080 | 192.24 | 0.6976 | 238.29 | 1.119 | 233.30 |
| 0.2805 | 222.35 | 1.928 | 196.27 | 0.7391 | 239.60 | 1.087 | 235.86 |
| 0.3069 | 223.80 | 1.824 | 199.66 | 0.7653 | 240.50 | 1.071 | 237.42 |
| 0.3273 | 224.50 | 1.739 | 202.13 | 0.7911 | 241.48 | 1.059 | 238.91 |
| 0.3487 | 225.28 | 1.662 | 204.58 | 0.8142 | 242.67 | 1.056 | 240.20 |
| 0.3751 | 226.21 | 1.580 | 207.43 | 0.8447 | 243.70 | 1.041 | 241.88 |
| 0.3989 | 226.99 | 1.512 | 209.88 | 0.8742 | 244.82 | 1.030 | 243.44 |
| 0.4203 | 227.80 | 1.463 | 211.97 | 0.8994 | 245.92 | 1.026 | 244.75 |
| 0.4446 | 228.85 | 1.417 | 214.24 | 0.9203 | 246.74 | 1.020 | 245.81 |
| 0.4703 | 230.07 | 1.378 | 216.54 | 0.9528 | 247.91 | 1.011 | 247.42 |
| 0.4946 | 231.08 | 1.341 | 218.61 | 1.0000 | 249.68 | 1.000 | 249.68 |

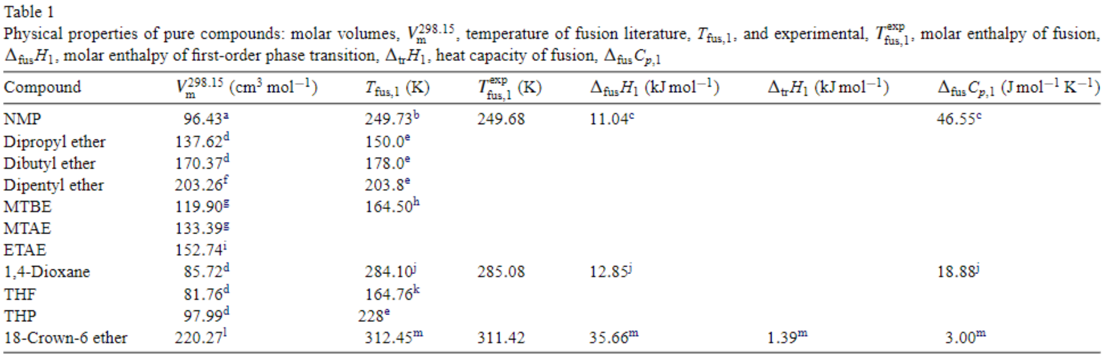


Table 1

Physical properties of pure compounds: molar volumes, $V_m^{298.15}$, temperature of fusion literature, $T_{fus,1}$, and experimental, $T_{fus,1}^{exp}$, molar enthalpy of fusion, $\Delta_{fus}H_1$, molar enthalpy of first-order phase transition, $\Delta_{tr}H_1$, heat capacity of fusion, $\Delta_{fus}C_{p,1}$

| Compound | $V_m^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{exp}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{tr}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| NMP | 96.43[a] | 249.73[b] | 249.68 | 11.04[c] | | 46.55[c] |
| Dipropyl ether | 137.62[d] | 150.0[e] | | | | |
| Dibutyl ether | 170.37[d] | 178.0[e] | | | | |
| Dipentyl ether | 203.26[f] | 203.8[e] | | | | |
| MTBE | 119.90[g] | 164.50[h] | | | | |
| MTAE | 133.39[g] | | | | | |
| ETAE | 152.74[i] | | | | | |
| 1,4-Dioxane | 85.72[d] | 284.10[j] | 285.08 | 12.85[j] | | 18.88[j] |
| THF | 81.76[d] | 164.76[k] | | | | |
| THP | 97.99[d] | 228[e] | | | | |
| 18-Crown-6 ether | 220.27[l] | 312.45[m] | 311.42 | 35.66[m] | 1.39[m] | 3.00[m] |

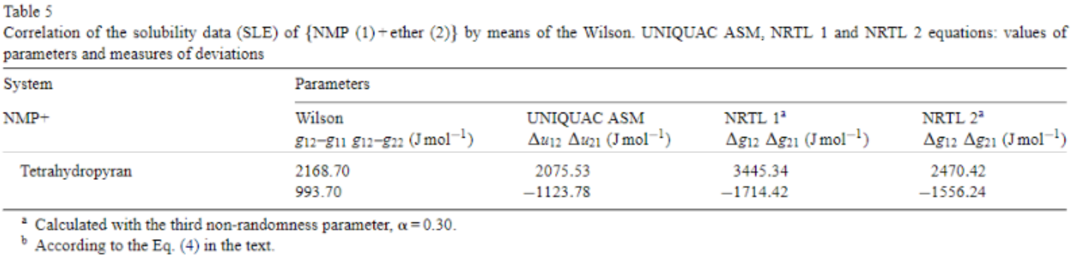


Table 5

Correlation of the solubility data (SLE) of {NMP (1) + ether (2)} by means of the Wilson. UNIQUAC ASM, NRTL 1 and NRTL 2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| NMP+ | Wilson<br>$g_{12}-g_{11}$ $g_{12}-g_{22}$ (J mol$^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$ $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) | NRTL 2[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) |
| Tetrahydropyran | 2168.70<br>993.70 | 2075.53<br>−1123.78 | 3445.34<br>−1714.42 | 2470.42<br>−1556.24 |

[a] Calculated with the third non-randomness parameter, $\alpha = 0.30$.

[b] According to the Eq. (4) in the text.

ODABRATI JEDAN MODEL

*N*-methyl-2-pyrrolidinone + 1,4-dioxane

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria of binary mixtures containingN-methyl-2-pyrrolidinone and ethers at atmospheric pressure, Fluid Phase Equilibria 227 (2005) 135–143

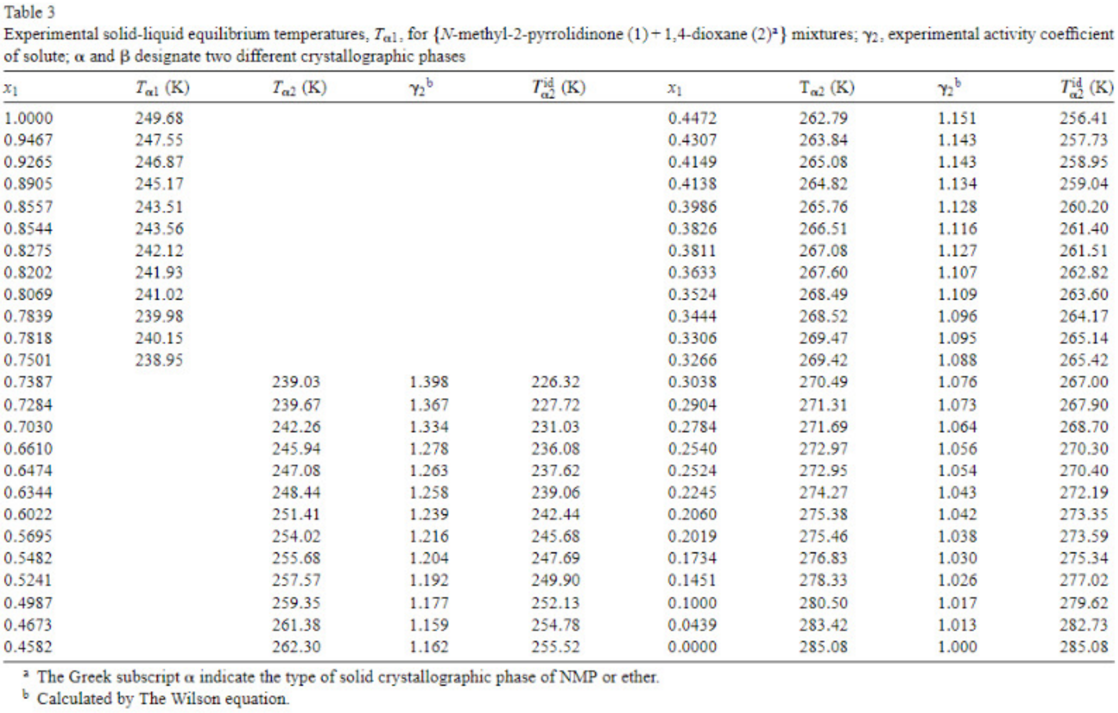


Table 3
Experimental solid-liquid equilibrium temperatures, $T_{\alpha 1}$, for {*N*-methyl-2-pyrrolidinone (1) + 1,4-dioxane (2)[a]} mixtures; $\gamma_2$, experimental activity coefficient of solute; α and β designate two different crystallographic phases

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{\alpha 2}$ (K) | $\gamma_2$[b] | $T^{id}_{\alpha 2}$ (K) | $x_1$ | $T_{\alpha 2}$ (K) | $\gamma_2$[b] | $T^{id}_{\alpha 2}$ (K) |
|---|---|---|---|---|---|---|---|---|
| 1.0000 | 249.68 | | | | 0.4472 | 262.79 | 1.151 | 256.41 |
| 0.9467 | 247.55 | | | | 0.4307 | 263.84 | 1.143 | 257.73 |
| 0.9265 | 246.87 | | | | 0.4149 | 265.08 | 1.143 | 258.95 |
| 0.8905 | 245.17 | | | | 0.4138 | 264.82 | 1.134 | 259.04 |
| 0.8557 | 243.51 | | | | 0.3986 | 265.76 | 1.128 | 260.20 |
| 0.8544 | 243.56 | | | | 0.3826 | 266.51 | 1.116 | 261.40 |
| 0.8275 | 242.12 | | | | 0.3811 | 267.08 | 1.127 | 261.51 |
| 0.8202 | 241.93 | | | | 0.3633 | 267.60 | 1.107 | 262.82 |
| 0.8069 | 241.02 | | | | 0.3524 | 268.49 | 1.109 | 263.60 |
| 0.7839 | 239.98 | | | | 0.3444 | 268.52 | 1.096 | 264.17 |
| 0.7818 | 240.15 | | | | 0.3306 | 269.47 | 1.095 | 265.14 |
| 0.7501 | 238.95 | | | | 0.3266 | 269.42 | 1.088 | 265.42 |
| 0.7387 | | 239.03 | 1.398 | 226.32 | 0.3038 | 270.49 | 1.076 | 267.00 |
| 0.7284 | | 239.67 | 1.367 | 227.72 | 0.2904 | 271.31 | 1.073 | 267.90 |
| 0.7030 | | 242.26 | 1.334 | 231.03 | 0.2784 | 271.69 | 1.064 | 268.70 |
| 0.6610 | | 245.94 | 1.278 | 236.08 | 0.2540 | 272.97 | 1.056 | 270.30 |
| 0.6474 | | 247.08 | 1.263 | 237.62 | 0.2524 | 272.95 | 1.054 | 270.40 |
| 0.6344 | | 248.44 | 1.258 | 239.06 | 0.2245 | 274.27 | 1.043 | 272.19 |
| 0.6022 | | 251.41 | 1.239 | 242.44 | 0.2060 | 275.38 | 1.042 | 273.35 |
| 0.5695 | | 254.02 | 1.216 | 245.68 | 0.2019 | 275.46 | 1.038 | 273.59 |
| 0.5482 | | 255.68 | 1.204 | 247.69 | 0.1734 | 276.83 | 1.030 | 275.34 |
| 0.5241 | | 257.57 | 1.192 | 249.90 | 0.1451 | 278.33 | 1.026 | 277.02 |
| 0.4987 | | 259.35 | 1.177 | 252.13 | 0.1000 | 280.50 | 1.017 | 279.62 |
| 0.4673 | | 261.38 | 1.159 | 254.78 | 0.0439 | 283.42 | 1.013 | 282.73 |
| 0.4582 | | 262.30 | 1.162 | 255.52 | 0.0000 | 285.08 | 1.000 | 285.08 |

[a] The Greek subscript α indicate the type of solid crystallographic phase of NMP or ether.
[b] Calculated by The Wilson equation.

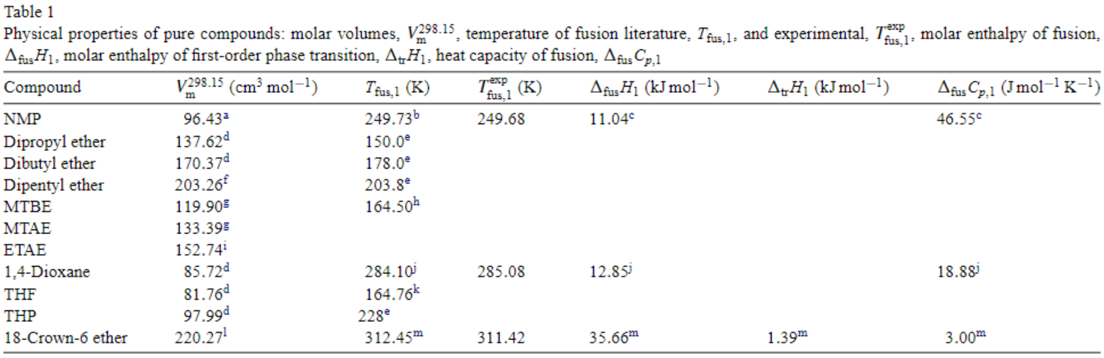


Table 1
Physical properties of pure compounds: molar volumes, $V_m^{298.15}$, temperature of fusion literature, $T_{fus,1}$, and experimental, $T_{fus,1}^{exp}$, molar enthalpy of fusion, $\Delta_{fus}H_1$, molar enthalpy of first-order phase transition, $\Delta_{tr}H_1$, heat capacity of fusion, $\Delta_{fus}C_{p,1}$

| Compound | $V_m^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{exp}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{tr}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| NMP | 96.43[a] | 249.73[b] | 249.68 | 11.04[c] | | 46.55[c] |
| Dipropyl ether | 137.62[d] | 150.0[e] | | | | |
| Dibutyl ether | 170.37[d] | 178.0[e] | | | | |
| Dipentyl ether | 203.26[f] | 203.8[e] | | | | |
| MTBE | 119.90[g] | 164.50[h] | | | | |
| MTAE | 133.39[g] | | | | | |
| ETAE | 152.74[i] | | | | | |
| 1,4-Dioxane | 85.72[d] | 284.10[j] | 285.08 | 12.85[j] | | 18.88[j] |
| THF | 81.76[d] | 164.76[k] | | | | |
| THP | 97.99[d] | 228[e] | | | | |
| 18-Crown-6 ether | 220.27[l] | 312.45[m] | 311.42 | 35.66[m] | 1.39[m] | 3.00[m] |

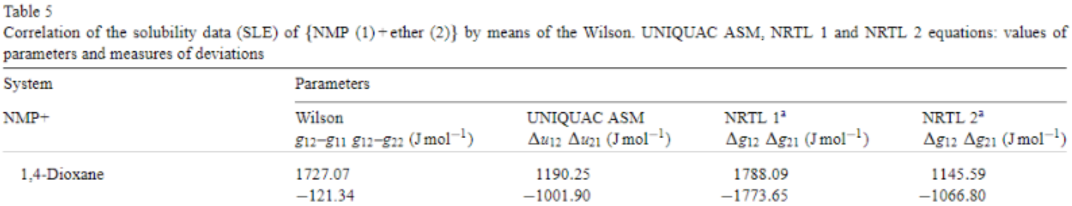


Table 5
Correlation of the solubility data (SLE) of {NMP (1) + ether (2)} by means of the Wilson. UNIQUAC ASM, NRTL 1 and NRTL 2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| NMP+ | Wilson<br>$g_{12}-g_{11}$ $g_{12}-g_{22}$ (J mol$^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$ $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) | NRTL 2[a]<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) |
| 1,4-Dioxane | 1727.07<br>−121.34 | 1190.25<br>−1001.90 | 1788.09<br>−1773.65 | 1145.59<br>−1066.80 |

ODABRATI JEDAN MODEL

*N*-methyl-2-pyrrolidinone + tetrahydropyran, 18-crown-6

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria of binary mixtures containingN-methyl-2-pyrrolidinone and ethers at atmospheric pressure, Fluid Phase Equilibria 227 (2005) 135–143

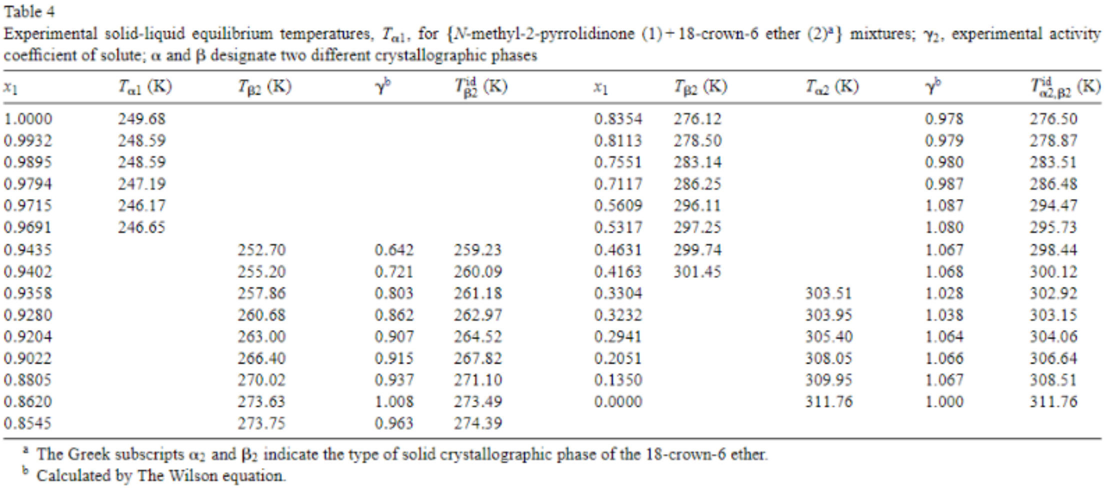


Table 4

Experimental solid-liquid equilibrium temperatures, $T_{\alpha 1}$, for {*N*-methyl-2-pyrrolidinone (1) + 18-crown-6 ether (2)[a]} mixtures; $\gamma_2$, experimental activity coefficient of solute; α and β designate two different crystallographic phases

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{\beta 2}$ (K) | $\gamma^b$ | $T^{id}_{\beta 2}$ (K) | $x_1$ | $T_{\beta 2}$ (K) | $T_{\alpha 2}$ (K) | $\gamma^b$ | $T^{id}_{\alpha 2,\beta 2}$ (K) |
|---|---|---|---|---|---|---|---|---|---|
| 1.0000 | 249.68 | | | | 0.8354 | 276.12 | | 0.978 | 276.50 |
| 0.9932 | 248.59 | | | | 0.8113 | 278.50 | | 0.979 | 278.87 |
| 0.9895 | 248.59 | | | | 0.7551 | 283.14 | | 0.980 | 283.51 |
| 0.9794 | 247.19 | | | | 0.7117 | 286.25 | | 0.987 | 286.48 |
| 0.9715 | 246.17 | | | | 0.5609 | 296.11 | | 1.087 | 294.47 |
| 0.9691 | 246.65 | | | | 0.5317 | 297.25 | | 1.080 | 295.73 |
| 0.9435 | | 252.70 | 0.642 | 259.23 | 0.4631 | 299.74 | | 1.067 | 298.44 |
| 0.9402 | | 255.20 | 0.721 | 260.09 | 0.4163 | 301.45 | | 1.068 | 300.12 |
| 0.9358 | | 257.86 | 0.803 | 261.18 | 0.3304 | | 303.51 | 1.028 | 302.92 |
| 0.9280 | | 260.68 | 0.862 | 262.97 | 0.3232 | | 303.95 | 1.038 | 303.15 |
| 0.9204 | | 263.00 | 0.907 | 264.52 | 0.2941 | | 305.40 | 1.064 | 304.06 |
| 0.9022 | | 266.40 | 0.915 | 267.82 | 0.2051 | | 308.05 | 1.066 | 306.64 |
| 0.8805 | | 270.02 | 0.937 | 271.10 | 0.1350 | | 309.95 | 1.067 | 308.51 |
| 0.8620 | | 273.63 | 1.008 | 273.49 | 0.0000 | | 311.76 | 1.000 | 311.76 |
| 0.8545 | | 273.75 | 0.963 | 274.39 | | | | | |

[a] The Greek subscripts $\alpha_2$ and $\beta_2$ indicate the type of solid crystallographic phase of the 18-crown-6 ether.

[b] Calculated by The Wilson equation.

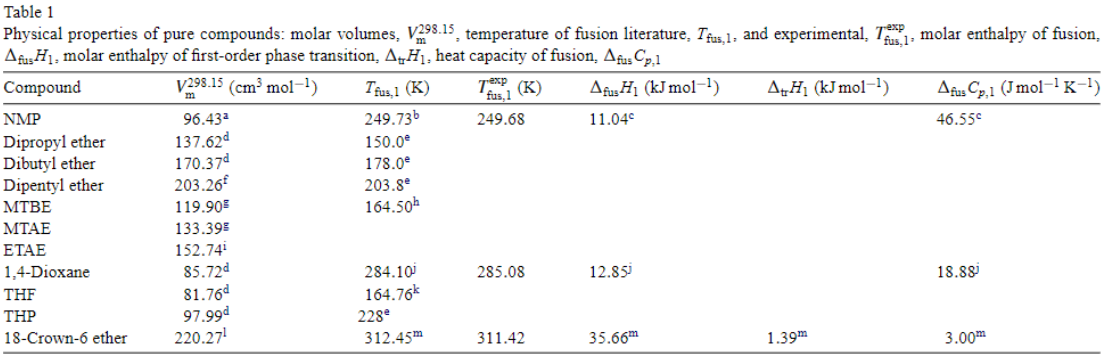


Table 1

Physical properties of pure compounds: molar volumes, $V_m^{298.15}$, temperature of fusion literature, $T_{fus,1}$, and experimental, $T_{fus,1}^{exp}$, molar enthalpy of fusion, $\Delta_{fus}H_1$, molar enthalpy of first-order phase transition, $\Delta_{tr}H_1$, heat capacity of fusion, $\Delta_{fus}C_{p,1}$

| Compound | $V_m^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{exp}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{tr}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|---|
| NMP | 96.43$^a$ | 249.73$^b$ | 249.68 | 11.04$^c$ | | 46.55$^c$ |
| Dipropyl ether | 137.62$^d$ | 150.0$^e$ | | | | |
| Dibutyl ether | 170.37$^d$ | 178.0$^e$ | | | | |
| Dipentyl ether | 203.26$^f$ | 203.8$^e$ | | | | |
| MTBE | 119.90$^g$ | 164.50$^h$ | | | | |
| MTAE | 133.39$^g$ | | | | | |
| ETAE | 152.74$^i$ | | | | | |
| 1,4-Dioxane | 85.72$^d$ | 284.10$^j$ | 285.08 | 12.85$^j$ | | 18.88$^j$ |
| THF | 81.76$^d$ | 164.76$^k$ | | | | |
| THP | 97.99$^d$ | 228$^e$ | | | | |
| 18-Crown-6 ether | 220.27$^l$ | 312.45$^m$ | 311.42 | 35.66$^m$ | 1.39$^m$ | 3.00$^m$ |

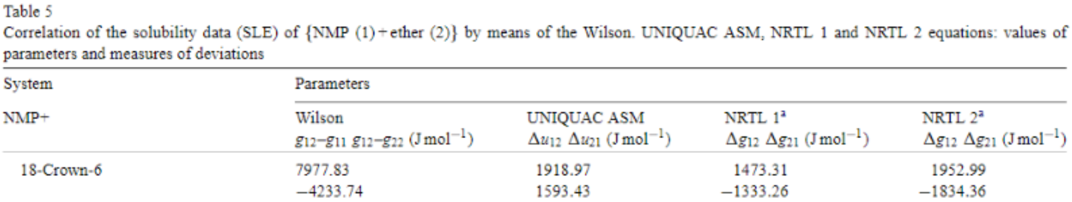


Table 5

Correlation of the solubility data (SLE) of {NMP (1) + ether (2)} by means of the Wilson. UNIQUAC ASM, NRTL 1 and NRTL 2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| NMP+ | Wilson<br>$g_{12}-g_{11}$ $g_{12}-g_{22}$ (J mol$^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$ $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1$^a$<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) | NRTL 2$^a$<br>$\Delta g_{12}$ $\Delta g_{21}$ (J mol$^{-1}$) |
| 18-Crown-6 | 7977.83<br>−4233.74 | 1918.97<br>1593.43 | 1473.31<br>−1333.26 | 1952.99<br>−1834.36 |

ODABRATI JEDAN MODEL

acenaphthene + *o*-dichlorobenzene

Dongwei Wei, Lishuo Wang, Fengchun Yan, Chao Zhang, Solid–liquid equilibria of acenaphthene witho-,m-, or p-dichlorobenzene, Fluid Phase Equilibria 291 (2010) 66–70

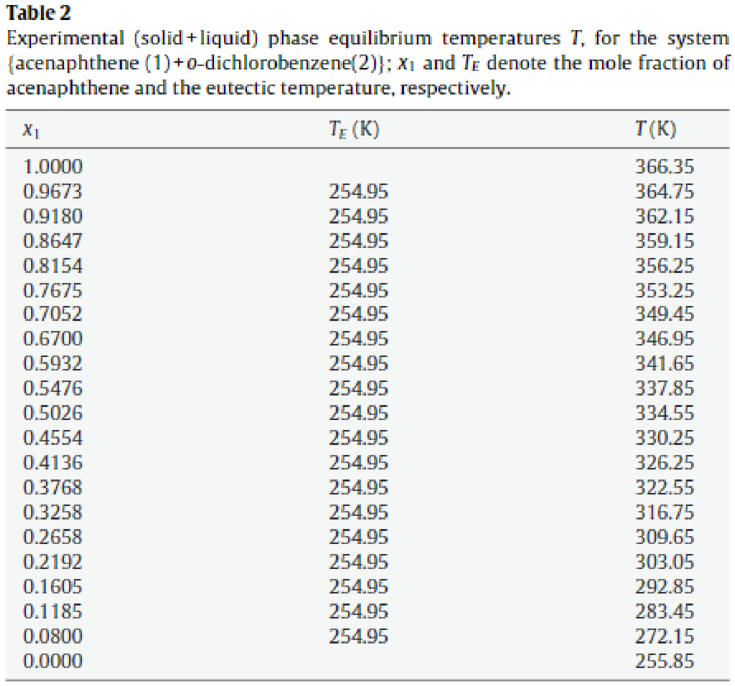


**Table 2**

Experimental (solid + liquid) phase equilibrium temperatures $T$, for the system {acenaphthene (1) + *o*-dichlorobenzene(2)}; $x_1$ and $T_E$ denote the mole fraction of acenaphthene and the eutectic temperature, respectively.

| $x_1$ | $T_E$ (K) | $T$ (K) |
|---|---|---|
| 1.0000 | | 366.35 |
| 0.9673 | 254.95 | 364.75 |
| 0.9180 | 254.95 | 362.15 |
| 0.8647 | 254.95 | 359.15 |
| 0.8154 | 254.95 | 356.25 |
| 0.7675 | 254.95 | 353.25 |
| 0.7052 | 254.95 | 349.45 |
| 0.6700 | 254.95 | 346.95 |
| 0.5932 | 254.95 | 341.65 |
| 0.5476 | 254.95 | 337.85 |
| 0.5026 | 254.95 | 334.55 |
| 0.4554 | 254.95 | 330.25 |
| 0.4136 | 254.95 | 326.25 |
| 0.3768 | 254.95 | 322.55 |
| 0.3258 | 254.95 | 316.75 |
| 0.2658 | 254.95 | 309.65 |
| 0.2192 | 254.95 | 303.05 |
| 0.1605 | 254.95 | 292.85 |
| 0.1185 | 254.95 | 283.45 |
| 0.0800 | 254.95 | 272.15 |
| 0.0000 | | 255.85 |

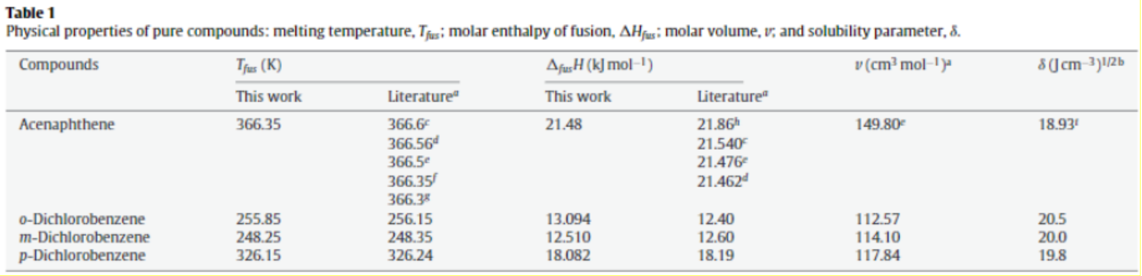


**Table 1**

Physical properties of pure compounds: melting temperature, $T_{fus}$; molar enthalpy of fusion, $\Delta H_{fus}$; molar volume, $v$; and solubility parameter, $\delta$.

| Compounds | $T_{fus}$ (K) | | $\Delta_{fus}H$ (kJ mol$^{-1}$) | | $v$ (cm$^3$ mol$^{-1}$)$^a$ | $\delta$ (J cm$^{-3}$)$^{1/2b}$ |
|---|---|---|---|---|---|---|
| | This work | Literature$^a$ | This work | Literature$^a$ | | |
| Acenaphthene | 366.35 | 366.6$^c$<br>366.56$^d$<br>366.5$^e$<br>366.35$^f$<br>366.3$^g$ | 21.48 | 21.86$^h$<br>21.540$^c$<br>21.476$^e$<br>21.462$^d$ | 149.80$^e$ | 18.93$^i$ |
| *o*-Dichlorobenzene | 255.85 | 256.15 | 13.094 | 12.40 | 112.57 | 20.5 |
| *m*-Dichlorobenzene | 248.25 | 248.35 | 12.510 | 12.60 | 114.10 | 20.0 |
| *p*-Dichlorobenzene | 326.15 | 326.24 | 18.082 | 18.19 | 117.84 | 19.8 |

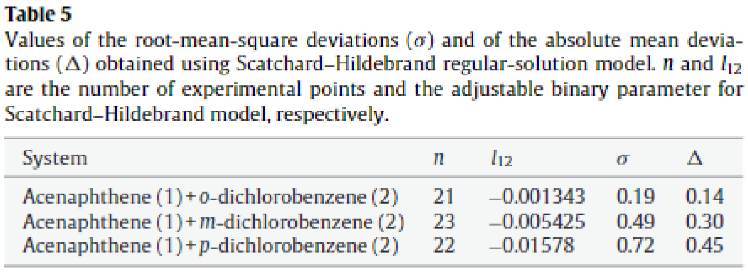


**Table 5**

Values of the root-mean-square deviations ($\sigma$) and of the absolute mean deviations ($\Delta$) obtained using Scatchard–Hildebrand regular-solution model. $n$ and $l_{12}$ are the number of experimental points and the adjustable binary parameter for Scatchard–Hildebrand model, respectively.

| System | $n$ | $l_{12}$ | $\sigma$ | $\Delta$ |
|---|---|---|---|---|
| Acenaphthene (1) + *o*-dichlorobenzene (2) | 21 | –0.001343 | 0.19 | 0.14 |
| Acenaphthene (1) + *m*-dichlorobenzene (2) | 23 | –0.005425 | 0.49 | 0.30 |
| Acenaphthene (1) + *p*-dichlorobenzene (2) | 22 | –0.01578 | 0.72 | 0.45 |

acenaphthene + *m*-dichlorobenzene
Dongwei Wei, Lishuo Wang, Fengchun Yan, Chao Zhang, Solid–liquid equilibria of acenaphthene witho-,m-, or p-dichlorobenzene, Fluid Phase Equilibria 291 (2010) 66–70

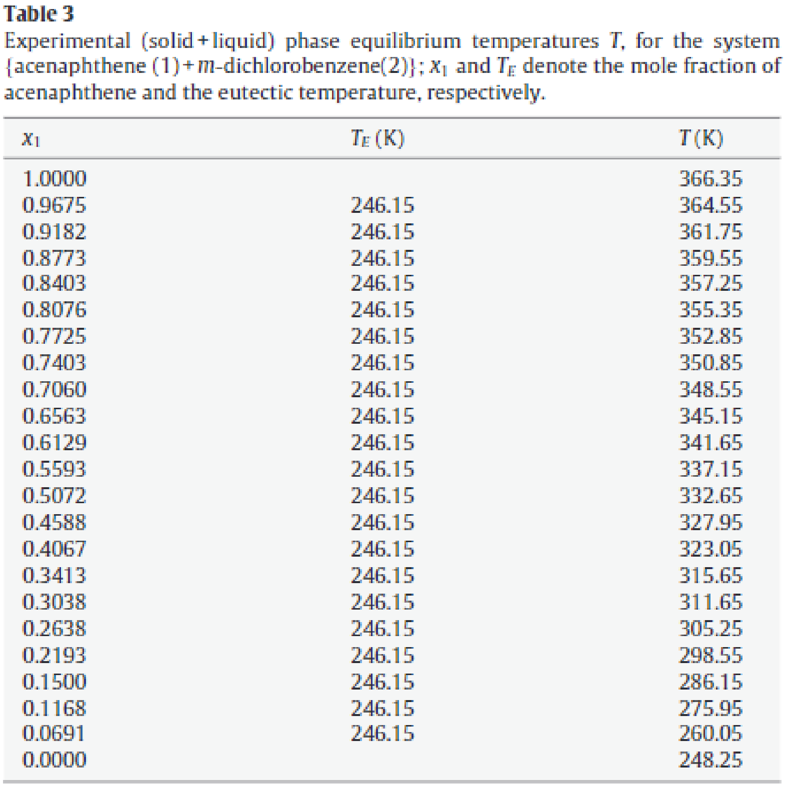


**Table 3**
Experimental (solid + liquid) phase equilibrium temperatures $T$, for the system {acenaphthene (1) + *m*-dichlorobenzene(2)}; $x_1$ and $T_E$ denote the mole fraction of acenaphthene and the eutectic temperature, respectively.

| $x_1$ | $T_E$ (K) | $T$ (K) |
|---|---|---|
| 1.0000 | | 366.35 |
| 0.9675 | 246.15 | 364.55 |
| 0.9182 | 246.15 | 361.75 |
| 0.8773 | 246.15 | 359.55 |
| 0.8403 | 246.15 | 357.25 |
| 0.8076 | 246.15 | 355.35 |
| 0.7725 | 246.15 | 352.85 |
| 0.7403 | 246.15 | 350.85 |
| 0.7060 | 246.15 | 348.55 |
| 0.6563 | 246.15 | 345.15 |
| 0.6129 | 246.15 | 341.65 |
| 0.5593 | 246.15 | 337.15 |
| 0.5072 | 246.15 | 332.65 |
| 0.4588 | 246.15 | 327.95 |
| 0.4067 | 246.15 | 323.05 |
| 0.3413 | 246.15 | 315.65 |
| 0.3038 | 246.15 | 311.65 |
| 0.2638 | 246.15 | 305.25 |
| 0.2193 | 246.15 | 298.55 |
| 0.1500 | 246.15 | 286.15 |
| 0.1168 | 246.15 | 275.95 |
| 0.0691 | 246.15 | 260.05 |
| 0.0000 | | 248.25 |

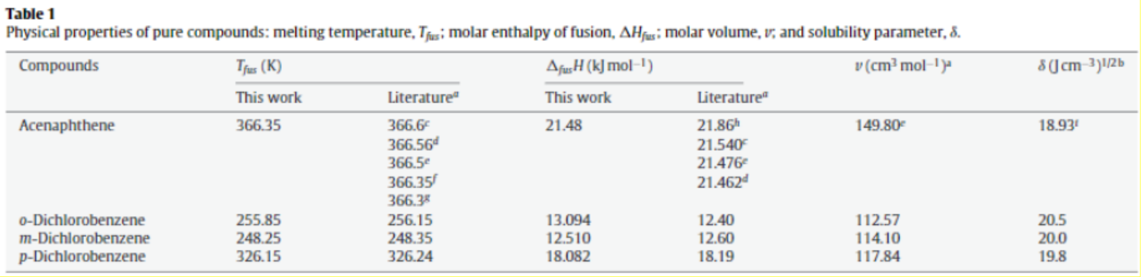


**Table 1**
Physical properties of pure compounds: melting temperature, $T_{fus}$; molar enthalpy of fusion, $\Delta H_{fus}$; molar volume, $v$; and solubility parameter, $\delta$.

| Compounds | $T_{fus}$ (K) | | $\Delta_{fus}H$ (kJ mol$^{-1}$) | | $v$ (cm$^3$ mol$^{-1}$)$^a$ | $\delta$ (J cm$^{-3}$)$^{1/2b}$ |
|---|---|---|---|---|---|---|
| | This work | Literature$^a$ | This work | Literature$^a$ | | |
| Acenaphthene | 366.35 | 366.6$^c$<br>366.56$^d$<br>366.5$^e$<br>366.35$^f$<br>366.3$^g$ | 21.48 | 21.86$^h$<br>21.540$^c$<br>21.476$^e$<br>21.462$^d$ | 149.80$^e$ | 18.93$^i$ |
| *o*-Dichlorobenzene | 255.85 | 256.15 | 13.094 | 12.40 | 112.57 | 20.5 |
| *m*-Dichlorobenzene | 248.25 | 248.35 | 12.510 | 12.60 | 114.10 | 20.0 |
| *p*-Dichlorobenzene | 326.15 | 326.24 | 18.082 | 18.19 | 117.84 | 19.8 |

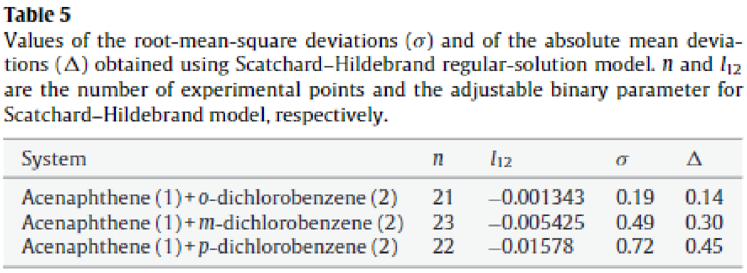


**Table 5**
Values of the root-mean-square deviations ($\sigma$) and of the absolute mean deviations ($\Delta$) obtained using Scatchard–Hildebrand regular-solution model. $n$ and $l_{12}$ are the number of experimental points and the adjustable binary parameter for Scatchard–Hildebrand model, respectively.

| System | $n$ | $l_{12}$ | $\sigma$ | $\Delta$ |
|---|---|---|---|---|
| Acenaphthene (1) + *o*-dichlorobenzene (2) | 21 | –0.001343 | 0.19 | 0.14 |
| Acenaphthene (1) + *m*-dichlorobenzene (2) | 23 | –0.005425 | 0.49 | 0.30 |
| Acenaphthene (1) + *p*-dichlorobenzene (2) | 22 | –0.01578 | 0.72 | 0.45 |

acenaphthene + *p*-dichlorobenzene

Dongwei Wei, Lishuo Wang, Fengchun Yan, Chao Zhang, Solid–liquid equilibria of acenaphthene witho-,m-, or p-dichlorobenzene, Fluid Phase Equilibria 291 (2010) 66–70

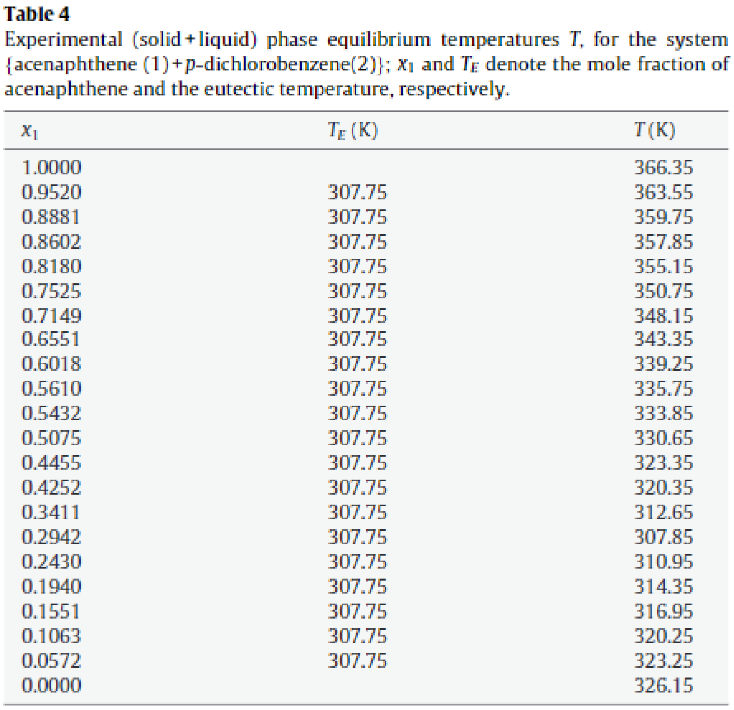


**Table 4**

Experimental (solid + liquid) phase equilibrium temperatures $T$, for the system {acenaphthene (1) + *p*-dichlorobenzene(2)}; $x_1$ and $T_E$ denote the mole fraction of acenaphthene and the eutectic temperature, respectively.

| $x_1$ | $T_E$ (K) | $T$ (K) |
|---|---|---|
| 1.0000 | | 366.35 |
| 0.9520 | 307.75 | 363.55 |
| 0.8881 | 307.75 | 359.75 |
| 0.8602 | 307.75 | 357.85 |
| 0.8180 | 307.75 | 355.15 |
| 0.7525 | 307.75 | 350.75 |
| 0.7149 | 307.75 | 348.15 |
| 0.6551 | 307.75 | 343.35 |
| 0.6018 | 307.75 | 339.25 |
| 0.5610 | 307.75 | 335.75 |
| 0.5432 | 307.75 | 333.85 |
| 0.5075 | 307.75 | 330.65 |
| 0.4455 | 307.75 | 323.35 |
| 0.4252 | 307.75 | 320.35 |
| 0.3411 | 307.75 | 312.65 |
| 0.2942 | 307.75 | 307.85 |
| 0.2430 | 307.75 | 310.95 |
| 0.1940 | 307.75 | 314.35 |
| 0.1551 | 307.75 | 316.95 |
| 0.1063 | 307.75 | 320.25 |
| 0.0572 | 307.75 | 323.25 |
| 0.0000 | | 326.15 |

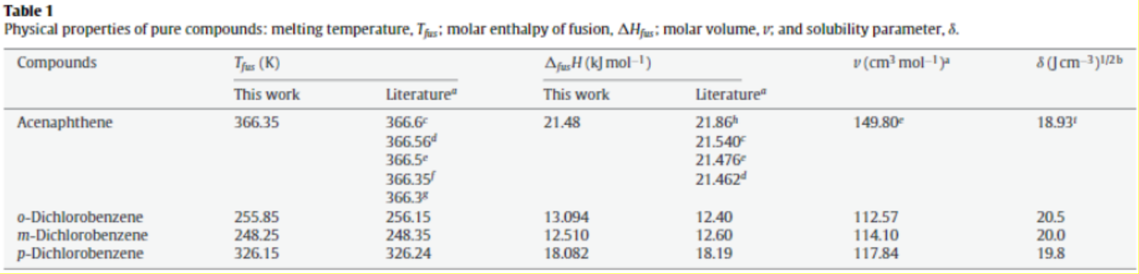


**Table 1**

Physical properties of pure compounds: melting temperature, $T_{fus}$; molar enthalpy of fusion, $\Delta H_{fus}$; molar volume, $v$; and solubility parameter, $\delta$.

| Compounds | $T_{fus}$ (K) | | $\Delta_{fus}H$ (kJ mol$^{-1}$) | | $v$ (cm$^3$ mol$^{-1}$)$^a$ | $\delta$ (J cm$^{-3}$)$^{1/2b}$ |
|---|---|---|---|---|---|---|
| | This work | Literature$^a$ | This work | Literature$^a$ | | |
| Acenaphthene | 366.35 | 366.6$^c$<br>366.56$^d$<br>366.5$^e$<br>366.35$^f$<br>366.3$^g$ | 21.48 | 21.86$^h$<br>21.540$^c$<br>21.476$^e$<br>21.462$^d$ | 149.80$^e$ | 18.93$^f$ |
| *o*-Dichlorobenzene | 255.85 | 256.15 | 13.094 | 12.40 | 112.57 | 20.5 |
| *m*-Dichlorobenzene | 248.25 | 248.35 | 12.510 | 12.60 | 114.10 | 20.0 |
| *p*-Dichlorobenzene | 326.15 | 326.24 | 18.082 | 18.19 | 117.84 | 19.8 |

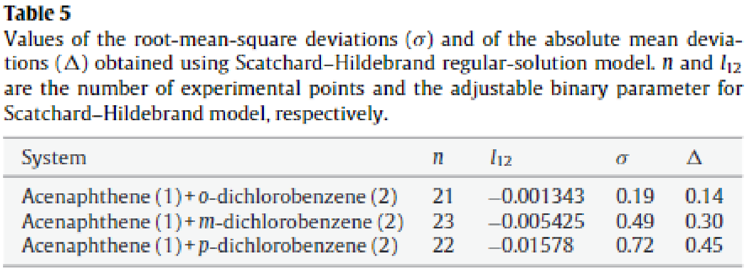


**Table 5**

Values of the root-mean-square deviations ($\sigma$) and of the absolute mean deviations ($\Delta$) obtained using Scatchard–Hildebrand regular-solution model. $n$ and $l_{12}$ are the number of experimental points and the adjustable binary parameter for Scatchard–Hildebrand model, respectively.

| System | $n$ | $l_{12}$ | $\sigma$ | $\Delta$ |
|---|---|---|---|---|
| Acenaphthene (1) + *o*-dichlorobenzene (2) | 21 | −0.001343 | 0.19 | 0.14 |
| Acenaphthene (1) + *m*-dichlorobenzene (2) | 23 | −0.005425 | 0.49 | 0.30 |
| Acenaphthene (1) + *p*-dichlorobenzene (2) | 22 | −0.01578 | 0.72 | 0.45 |

*n*-hexanol + *N*-methyl-2-pyrrolidinone

U. Domanska, J. Łachwa, (Solid+liquid) phase equilibria of binary mixtures containing *N*-methyl-2-pyrrolidinone and long-chain *n*-alkanols at atmospheric pressure, Fluid Phase Equilibria 198 (2002) 1–14

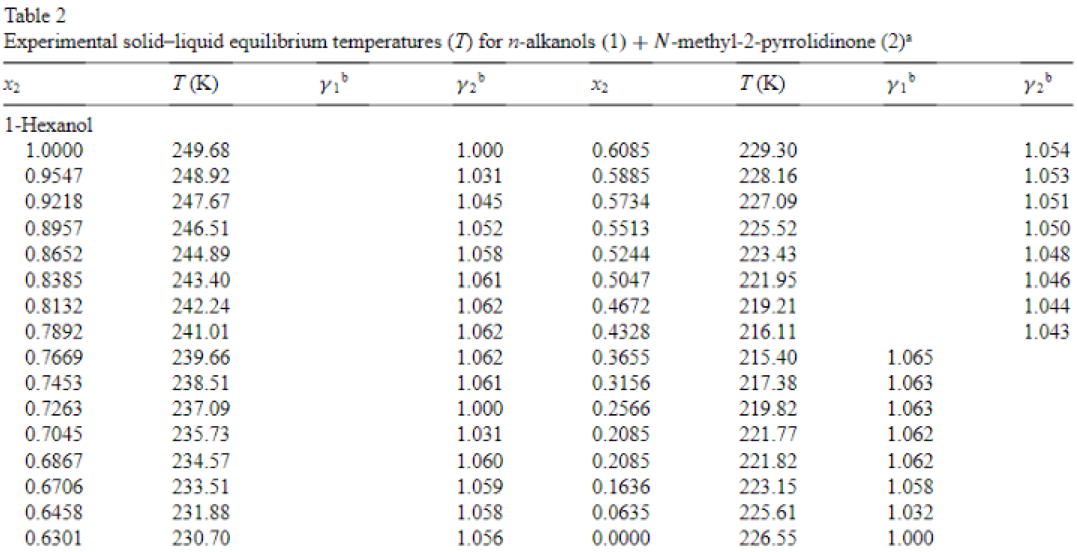


Table 2

Experimental solid–liquid equilibrium temperatures ($T$) for $n$-alkanols (1) + $N$-methyl-2-pyrrolidinone (2)[a]

| $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] | $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] |
|---|---|---|---|---|---|---|---|
| 1-Hexanol | | | | | | | |
| 1.0000 | 249.68 | | 1.000 | 0.6085 | 229.30 | | 1.054 |
| 0.9547 | 248.92 | | 1.031 | 0.5885 | 228.16 | | 1.053 |
| 0.9218 | 247.67 | | 1.045 | 0.5734 | 227.09 | | 1.051 |
| 0.8957 | 246.51 | | 1.052 | 0.5513 | 225.52 | | 1.050 |
| 0.8652 | 244.89 | | 1.058 | 0.5244 | 223.43 | | 1.048 |
| 0.8385 | 243.40 | | 1.061 | 0.5047 | 221.95 | | 1.046 |
| 0.8132 | 242.24 | | 1.062 | 0.4672 | 219.21 | | 1.044 |
| 0.7892 | 241.01 | | 1.062 | 0.4328 | 216.11 | | 1.043 |
| 0.7669 | 239.66 | | 1.062 | 0.3655 | 215.40 | 1.065 | |
| 0.7453 | 238.51 | | 1.061 | 0.3156 | 217.38 | 1.063 | |
| 0.7263 | 237.09 | | 1.000 | 0.2566 | 219.82 | 1.063 | |
| 0.7045 | 235.73 | | 1.031 | 0.2085 | 221.77 | 1.062 | |
| 0.6867 | 234.57 | | 1.060 | 0.2085 | 221.82 | 1.062 | |
| 0.6706 | 233.51 | | 1.059 | 0.1636 | 223.15 | 1.058 | |
| 0.6458 | 231.88 | | 1.058 | 0.0635 | 225.61 | 1.032 | |
| 0.6301 | 230.70 | | 1.056 | 0.0000 | 226.55 | 1.000 | |

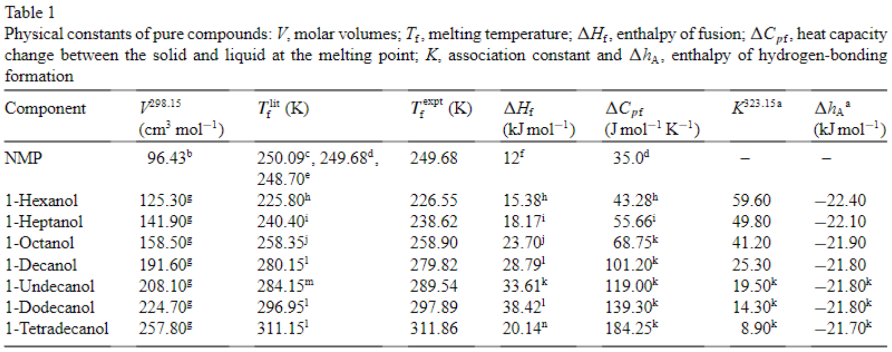


Table 1

Physical constants of pure compounds: $V$, molar volumes; $T_f$, melting temperature; $\Delta H_f$, enthalpy of fusion; $\Delta C_{pf}$, heat capacity change between the solid and liquid at the melting point; $K$, association constant and $\Delta h_A$, enthalpy of hydrogen-bonding formation

| Component | $V^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_f^{\text{lit}}$ (K) | $T_f^{\text{expt}}$ (K) | $\Delta H_f$ (kJ mol$^{-1}$) | $\Delta C_{pf}$ (J mol$^{-1}$ K$^{-1}$) | $K^{323.15\text{a}}$ | $\Delta h_A$[a] (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|---|
| NMP | 96.43[b] | 250.09[c], 249.68[d], 248.70[e] | 249.68 | 12[f] | 35.0[d] | – | – |
| 1-Hexanol | 125.30[g] | 225.80[h] | 226.55 | 15.38[h] | 43.28[h] | 59.60 | –22.40 |
| 1-Heptanol | 141.90[g] | 240.40[i] | 238.62 | 18.17[i] | 55.66[i] | 49.80 | –22.10 |
| 1-Octanol | 158.50[g] | 258.35[j] | 258.90 | 23.70[j] | 68.75[k] | 41.20 | –21.90 |
| 1-Decanol | 191.60[g] | 280.15[l] | 279.82 | 28.79[l] | 101.20[k] | 25.30 | –21.80 |
| 1-Undecanol | 208.10[g] | 284.15[m] | 289.54 | 33.61[k] | 119.00[k] | 19.50[k] | –21.80[k] |
| 1-Dodecanol | 224.70[g] | 296.95[l] | 297.89 | 38.42[l] | 139.30[k] | 14.30[k] | –21.80[k] |
| 1-Tetradecanol | 257.80[g] | 311.15[l] | 311.86 | 20.14[n] | 184.25[k] | 8.90[k] | –21.70[k] |

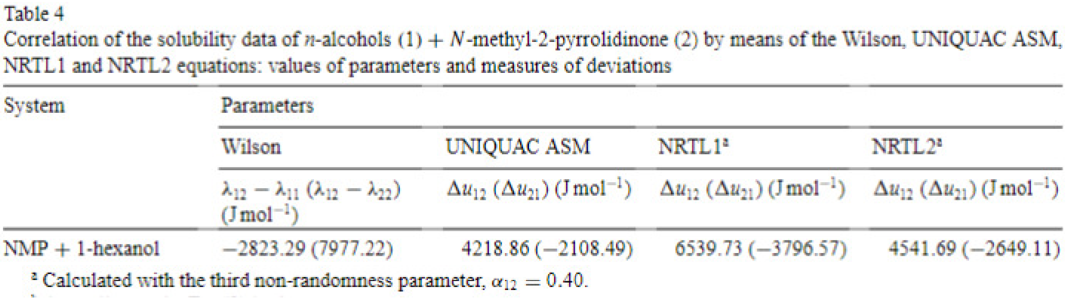


Table 4

Correlation of the solubility data of $n$-alcohols (1) + $N$-methyl-2-pyrrolidinone (2) by means of the Wilson, UNIQUAC ASM, NRTL1 and NRTL2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| | Wilson | UNIQUAC ASM | NRTL1[a] | NRTL2[a] |
| | $\lambda_{12}-\lambda_{11}$ ($\lambda_{12}-\lambda_{22}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) |
| NMP + 1-hexanol | −2823.29 (7977.22) | 4218.86 (−2108.49) | 6539.73 (−3796.57) | 4541.69 (−2649.11) |

[a] Calculated with the third non-randomness parameter, $\alpha_{12} = 0.40$.

ODABRATI JEDAN MODEL

*n*-heptanol + *N*-methyl-2-pyrrolidinone

U. Domanska, J. Łachwa, (Solid+liquid) phase equilibria of binary mixtures containing *N*-methyl-2-pyrrolidinone and long-chain *n*-alkanols at atmospheric pressure, Fluid Phase Equilibria 198 (2002) 1–14

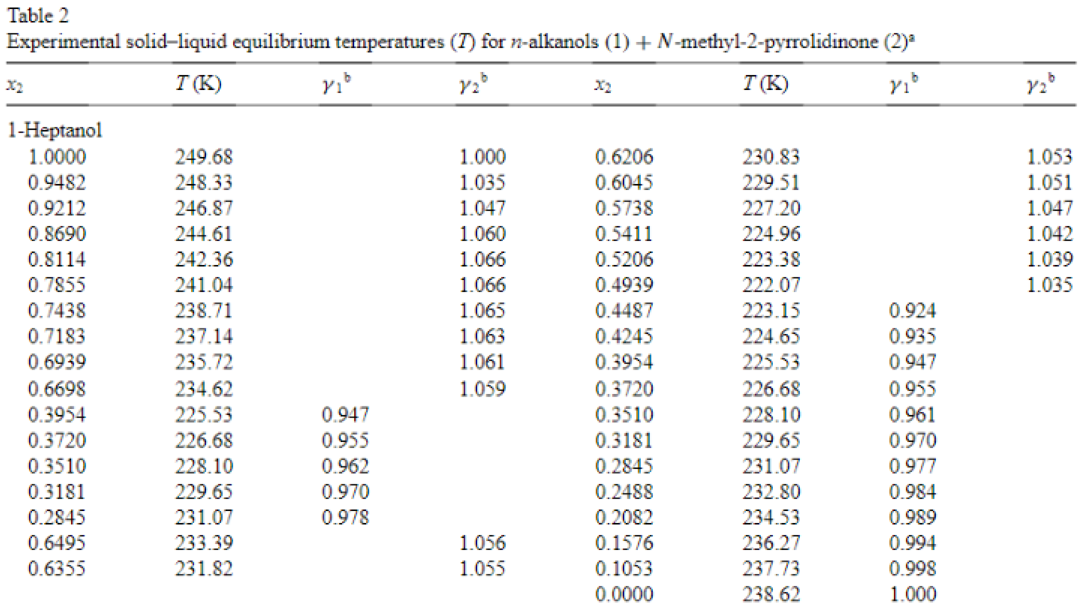


Table 2

Experimental solid–liquid equilibrium temperatures ($T$) for $n$-alkanols (1) + $N$-methyl-2-pyrrolidinone (2)[a]

| $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] | $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] |
|---|---|---|---|---|---|---|---|
| 1-Heptanol | | | | | | | |
| 1.0000 | 249.68 | | 1.000 | 0.6206 | 230.83 | | 1.053 |
| 0.9482 | 248.33 | | 1.035 | 0.6045 | 229.51 | | 1.051 |
| 0.9212 | 246.87 | | 1.047 | 0.5738 | 227.20 | | 1.047 |
| 0.8690 | 244.61 | | 1.060 | 0.5411 | 224.96 | | 1.042 |
| 0.8114 | 242.36 | | 1.066 | 0.5206 | 223.38 | | 1.039 |
| 0.7855 | 241.04 | | 1.066 | 0.4939 | 222.07 | | 1.035 |
| 0.7438 | 238.71 | | 1.065 | 0.4487 | 223.15 | 0.924 | |
| 0.7183 | 237.14 | | 1.063 | 0.4245 | 224.65 | 0.935 | |
| 0.6939 | 235.72 | | 1.061 | 0.3954 | 225.53 | 0.947 | |
| 0.6698 | 234.62 | | 1.059 | 0.3720 | 226.68 | 0.955 | |
| 0.3954 | 225.53 | 0.947 | | 0.3510 | 228.10 | 0.961 | |
| 0.3720 | 226.68 | 0.955 | | 0.3181 | 229.65 | 0.970 | |
| 0.3510 | 228.10 | 0.962 | | 0.2845 | 231.07 | 0.977 | |
| 0.3181 | 229.65 | 0.970 | | 0.2488 | 232.80 | 0.984 | |
| 0.2845 | 231.07 | 0.978 | | 0.2082 | 234.53 | 0.989 | |
| 0.6495 | 233.39 | | 1.056 | 0.1576 | 236.27 | 0.994 | |
| 0.6355 | 231.82 | | 1.055 | 0.1053 | 237.73 | 0.998 | |
| | | | | 0.0000 | 238.62 | 1.000 | |

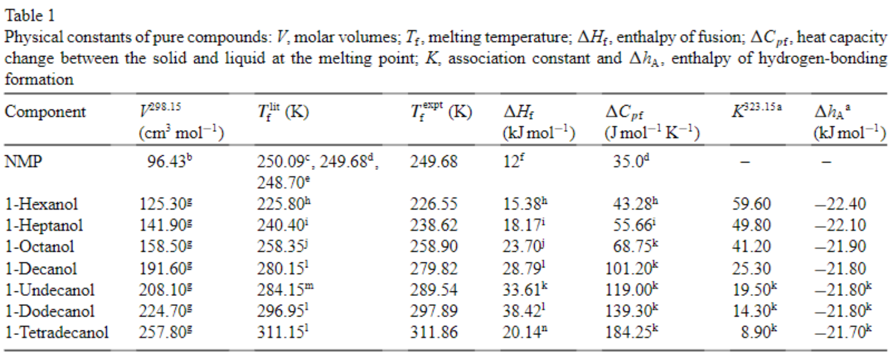


Table 1

Physical constants of pure compounds: $V$, molar volumes; $T_f$, melting temperature; $\Delta H_f$, enthalpy of fusion; $\Delta C_{pf}$, heat capacity change between the solid and liquid at the melting point; $K$, association constant and $\Delta h_A$, enthalpy of hydrogen-bonding formation

| Component | $V^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_f^{\text{lit}}$ (K) | $T_f^{\text{expt}}$ (K) | $\Delta H_f$ (kJ mol$^{-1}$) | $\Delta C_{pf}$ (J mol$^{-1}$ K$^{-1}$) | $K^{323.15\text{a}}$ | $\Delta h_A$[a] (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|---|
| NMP | 96.43[b] | 250.09[c], 249.68[d], 248.70[e] | 249.68 | 12[f] | 35.0[d] | – | – |
| 1-Hexanol | 125.30[g] | 225.80[h] | 226.55 | 15.38[h] | 43.28[h] | 59.60 | –22.40 |
| 1-Heptanol | 141.90[g] | 240.40[i] | 238.62 | 18.17[i] | 55.66[i] | 49.80 | –22.10 |
| 1-Octanol | 158.50[g] | 258.35[j] | 258.90 | 23.70[j] | 68.75[k] | 41.20 | –21.90 |
| 1-Decanol | 191.60[g] | 280.15[l] | 279.82 | 28.79[l] | 101.20[k] | 25.30 | –21.80 |
| 1-Undecanol | 208.10[g] | 284.15[m] | 289.54 | 33.61[k] | 119.00[k] | 19.50[k] | –21.80[k] |
| 1-Dodecanol | 224.70[g] | 296.95[l] | 297.89 | 38.42[l] | 139.30[k] | 14.30[k] | –21.80[k] |
| 1-Tetradecanol | 257.80[g] | 311.15[l] | 311.86 | 20.14[n] | 184.25[k] | 8.90[k] | –21.70[k] |

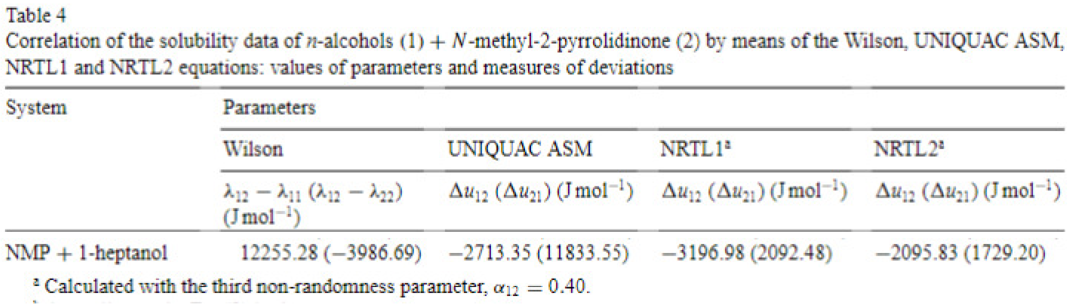


Table 4

Correlation of the solubility data of $n$-alcohols (1) + $N$-methyl-2-pyrrolidinone (2) by means of the Wilson, UNIQUAC ASM, NRTL1 and NRTL2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| | Wilson | UNIQUAC ASM | NRTL1[a] | NRTL2[a] |
| | $\lambda_{12}-\lambda_{11}$ ($\lambda_{12}-\lambda_{22}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) |
| NMP + 1-heptanol | 12255.28 (−3986.69) | −2713.35 (11833.55) | −3196.98 (2092.48) | −2095.83 (1729.20) |

[a] Calculated with the third non-randomness parameter, $\alpha_{12} = 0.40$.

ODABRATI JEDAN MODEL

*n*-octanol + *N*-methyl-2-pyrrolidinone

U. Domanska, J. Łachwa, (Solid+liquid) phase equilibria of binary mixtures containing *N*-methyl-2-pyrrolidinone and long-chain *n*-alkanols at atmospheric pressure, Fluid Phase Equilibria 198 (2002) 1–14

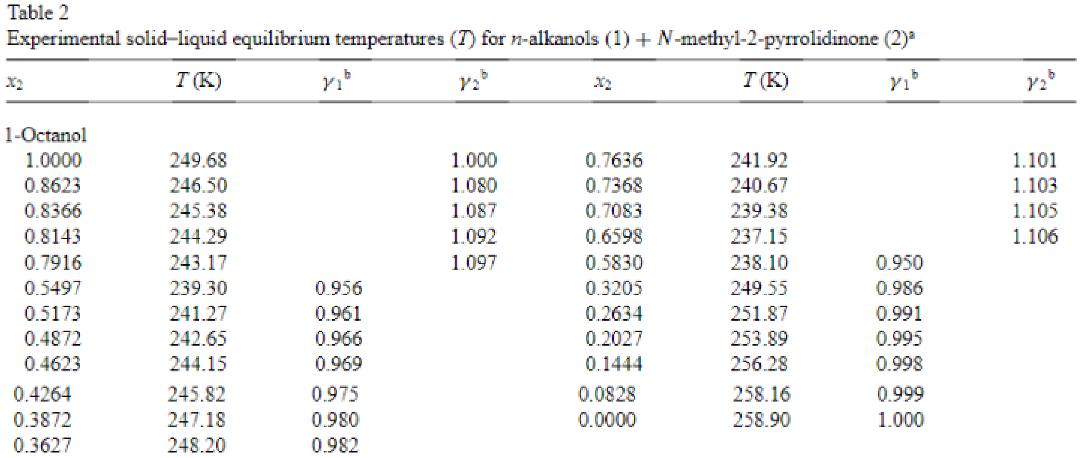


Table 2

Experimental solid–liquid equilibrium temperatures ($T$) for $n$-alkanols (1) + $N$-methyl-2-pyrrolidinone (2)[a]

| $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] | $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] |
|---|---|---|---|---|---|---|---|
| 1-Octanol | | | | | | | |
| 1.0000 | 249.68 | | 1.000 | 0.7636 | 241.92 | | 1.101 |
| 0.8623 | 246.50 | | 1.080 | 0.7368 | 240.67 | | 1.103 |
| 0.8366 | 245.38 | | 1.087 | 0.7083 | 239.38 | | 1.105 |
| 0.8143 | 244.29 | | 1.092 | 0.6598 | 237.15 | | 1.106 |
| 0.7916 | 243.17 | | 1.097 | 0.5830 | 238.10 | 0.950 | |
| 0.5497 | 239.30 | 0.956 | | 0.3205 | 249.55 | 0.986 | |
| 0.5173 | 241.27 | 0.961 | | 0.2634 | 251.87 | 0.991 | |
| 0.4872 | 242.65 | 0.966 | | 0.2027 | 253.89 | 0.995 | |
| 0.4623 | 244.15 | 0.969 | | 0.1444 | 256.28 | 0.998 | |
| 0.4264 | 245.82 | 0.975 | | 0.0828 | 258.16 | 0.999 | |
| 0.3872 | 247.18 | 0.980 | | 0.0000 | 258.90 | 1.000 | |
| 0.3627 | 248.20 | 0.982 | | | | | |

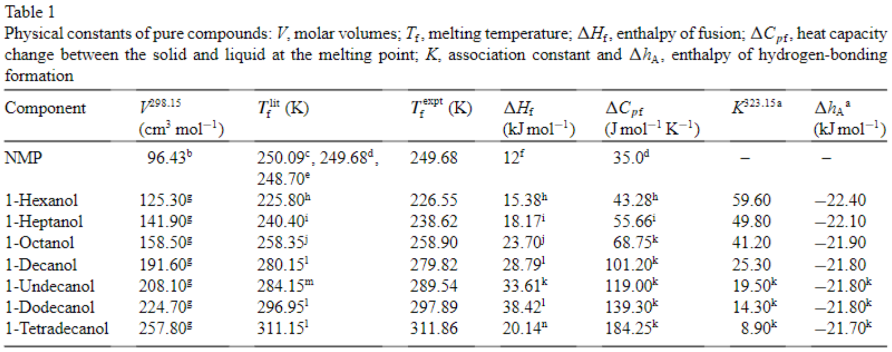


Table 1

Physical constants of pure compounds: $V$, molar volumes; $T_f$, melting temperature; $\Delta H_f$, enthalpy of fusion; $\Delta C_{pf}$, heat capacity change between the solid and liquid at the melting point; $K$, association constant and $\Delta h_A$, enthalpy of hydrogen-bonding formation

| Component | $V^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_f^{lit}$ (K) | $T_f^{expt}$ (K) | $\Delta H_f$ (kJ mol$^{-1}$) | $\Delta C_{pf}$ (J mol$^{-1}$ K$^{-1}$) | $K^{323.15}$[a] | $\Delta h_A$[a] (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|---|
| NMP | 96.43[b] | 250.09[c], 249.68[d], 248.70[e] | 249.68 | 12[f] | 35.0[d] | – | – |
| 1-Hexanol | 125.30[g] | 225.80[h] | 226.55 | 15.38[h] | 43.28[h] | 59.60 | −22.40 |
| 1-Heptanol | 141.90[g] | 240.40[i] | 238.62 | 18.17[i] | 55.66[i] | 49.80 | −22.10 |
| 1-Octanol | 158.50[g] | 258.35[j] | 258.90 | 23.70[j] | 68.75[k] | 41.20 | −21.90 |
| 1-Decanol | 191.60[g] | 280.15[l] | 279.82 | 28.79[l] | 101.20[k] | 25.30 | −21.80 |
| 1-Undecanol | 208.10[g] | 284.15[m] | 289.54 | 33.61[k] | 119.00[k] | 19.50[k] | −21.80[k] |
| 1-Dodecanol | 224.70[g] | 296.95[l] | 297.89 | 38.42[l] | 139.30[k] | 14.30[k] | −21.80[k] |
| 1-Tetradecanol | 257.80[g] | 311.15[l] | 311.86 | 20.14[n] | 184.25[k] | 8.90[k] | −21.70[k] |

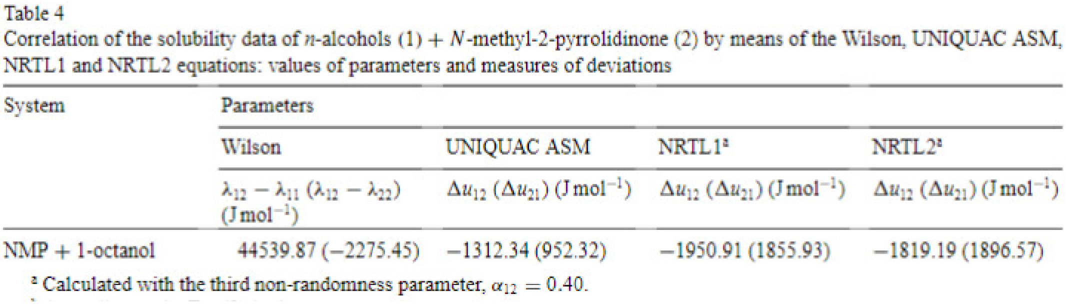


Table 4

Correlation of the solubility data of $n$-alcohols (1) + $N$-methyl-2-pyrrolidinone (2) by means of the Wilson, UNIQUAC ASM, NRTL1 and NRTL2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| | Wilson | UNIQUAC ASM | NRTL1[a] | NRTL2[a] |
| | $\lambda_{12}-\lambda_{11}$ ($\lambda_{12}-\lambda_{22}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) |
| NMP + 1-octanol | 44539.87 (−2275.45) | −1312.34 (952.32) | −1950.91 (1855.93) | −1819.19 (1896.57) |

[a] Calculated with the third non-randomness parameter, $\alpha_{12} = 0.40$.

ODABRATI JEDAN MODEL

*n*-decanol + *N*-methyl-2-pyrrolidinone

U. Domanska, J. Łachwa, (Solid+liquid) phase equilibria of binary mixtures containing *N*-methyl-2-pyrrolidinone and long-chain *n*-alkanols at atmospheric pressure, Fluid Phase Equilibria 198 (2002) 1–14

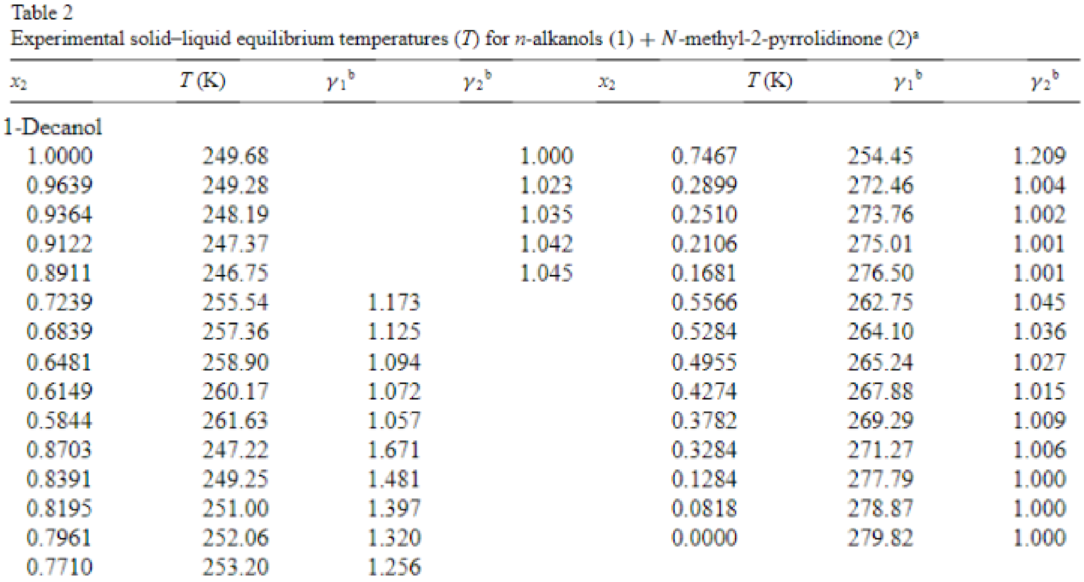


Table 2

Experimental solid–liquid equilibrium temperatures ($T$) for $n$-alkanols (1) + $N$-methyl-2-pyrrolidinone (2)[a]

| $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] | $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] |
|---|---|---|---|---|---|---|---|
| 1-Decanol | | | | | | | |
| 1.0000 | 249.68 | | 1.000 | 0.7467 | 254.45 | 1.209 | |
| 0.9639 | 249.28 | | 1.023 | 0.2899 | 272.46 | 1.004 | |
| 0.9364 | 248.19 | | 1.035 | 0.2510 | 273.76 | 1.002 | |
| 0.9122 | 247.37 | | 1.042 | 0.2106 | 275.01 | 1.001 | |
| 0.8911 | 246.75 | | 1.045 | 0.1681 | 276.50 | 1.001 | |
| 0.7239 | 255.54 | 1.173 | | 0.5566 | 262.75 | 1.045 | |
| 0.6839 | 257.36 | 1.125 | | 0.5284 | 264.10 | 1.036 | |
| 0.6481 | 258.90 | 1.094 | | 0.4955 | 265.24 | 1.027 | |
| 0.6149 | 260.17 | 1.072 | | 0.4274 | 267.88 | 1.015 | |
| 0.5844 | 261.63 | 1.057 | | 0.3782 | 269.29 | 1.009 | |
| 0.8703 | 247.22 | 1.671 | | 0.3284 | 271.27 | 1.006 | |
| 0.8391 | 249.25 | 1.481 | | 0.1284 | 277.79 | 1.000 | |
| 0.8195 | 251.00 | 1.397 | | 0.0818 | 278.87 | 1.000 | |
| 0.7961 | 252.06 | 1.320 | | 0.0000 | 279.82 | 1.000 | |
| 0.7710 | 253.20 | 1.256 | | | | | |

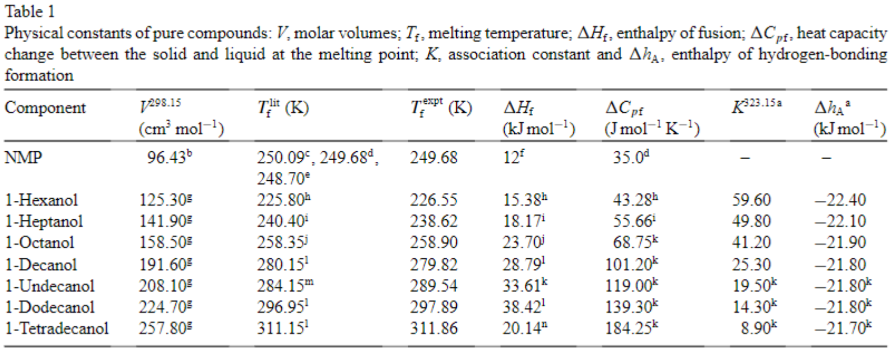


Table 1

Physical constants of pure compounds: $V$, molar volumes; $T_f$, melting temperature; $\Delta H_f$, enthalpy of fusion; $\Delta C_{pf}$, heat capacity change between the solid and liquid at the melting point; $K$, association constant and $\Delta h_A$, enthalpy of hydrogen-bonding formation

| Component | $V^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_f^{lit}$ (K) | $T_f^{expt}$ (K) | $\Delta H_f$ (kJ mol$^{-1}$) | $\Delta C_{pf}$ (J mol$^{-1}$ K$^{-1}$) | $K^{323.15a}$ | $\Delta h_A$[a] (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|---|
| NMP | 96.43[b] | 250.09[c], 249.68[d], 248.70[e] | 249.68 | 12[f] | 35.0[d] | – | – |
| 1-Hexanol | 125.30[g] | 225.80[h] | 226.55 | 15.38[h] | 43.28[h] | 59.60 | −22.40 |
| 1-Heptanol | 141.90[g] | 240.40[i] | 238.62 | 18.17[i] | 55.66[i] | 49.80 | −22.10 |
| 1-Octanol | 158.50[g] | 258.35[j] | 258.90 | 23.70[j] | 68.75[k] | 41.20 | −21.90 |
| 1-Decanol | 191.60[g] | 280.15[l] | 279.82 | 28.79[l] | 101.20[k] | 25.30 | −21.80 |
| 1-Undecanol | 208.10[g] | 284.15[m] | 289.54 | 33.61[k] | 119.00[k] | 19.50[k] | −21.80[k] |
| 1-Dodecanol | 224.70[g] | 296.95[l] | 297.89 | 38.42[l] | 139.30[k] | 14.30[k] | −21.80[k] |
| 1-Tetradecanol | 257.80[g] | 311.15[l] | 311.86 | 20.14[n] | 184.25[k] | 8.90[k] | −21.70[k] |

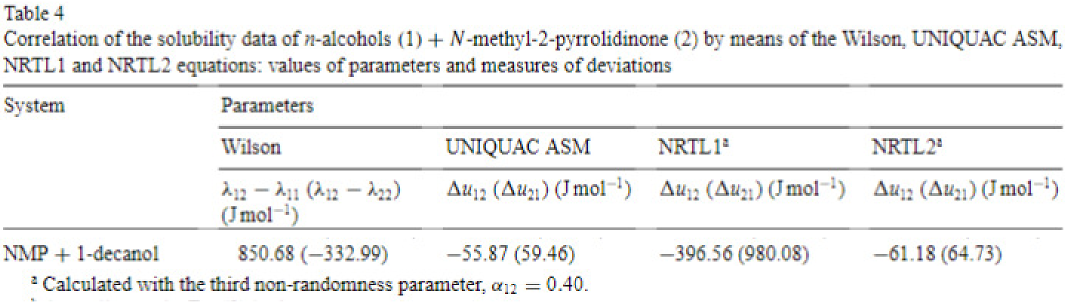


Table 4

Correlation of the solubility data of $n$-alcohols (1) + $N$-methyl-2-pyrrolidinone (2) by means of the Wilson, UNIQUAC ASM, NRTL1 and NRTL2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| | Wilson | UNIQUAC ASM | NRTL1[a] | NRTL2[a] |
| | $\lambda_{12}-\lambda_{11}$ ($\lambda_{12}-\lambda_{22}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) |
| NMP + 1-decanol | 850.68 (−332.99) | −55.87 (59.46) | −396.56 (980.08) | −61.18 (64.73) |

[a] Calculated with the third non-randomness parameter, $\alpha_{12} = 0.40$.

ODABRATI JEDAN MODEL

*n*-undecanol + *N*-methyl-2-pyrrolidinone

U. Domanska, J. Łachwa, (Solid+liquid) phase equilibria of binary mixtures containing *N*-methyl-2-pyrrolidinone and long-chain *n*-alkanols at atmospheric pressure, Fluid Phase Equilibria 198 (2002) 1–14

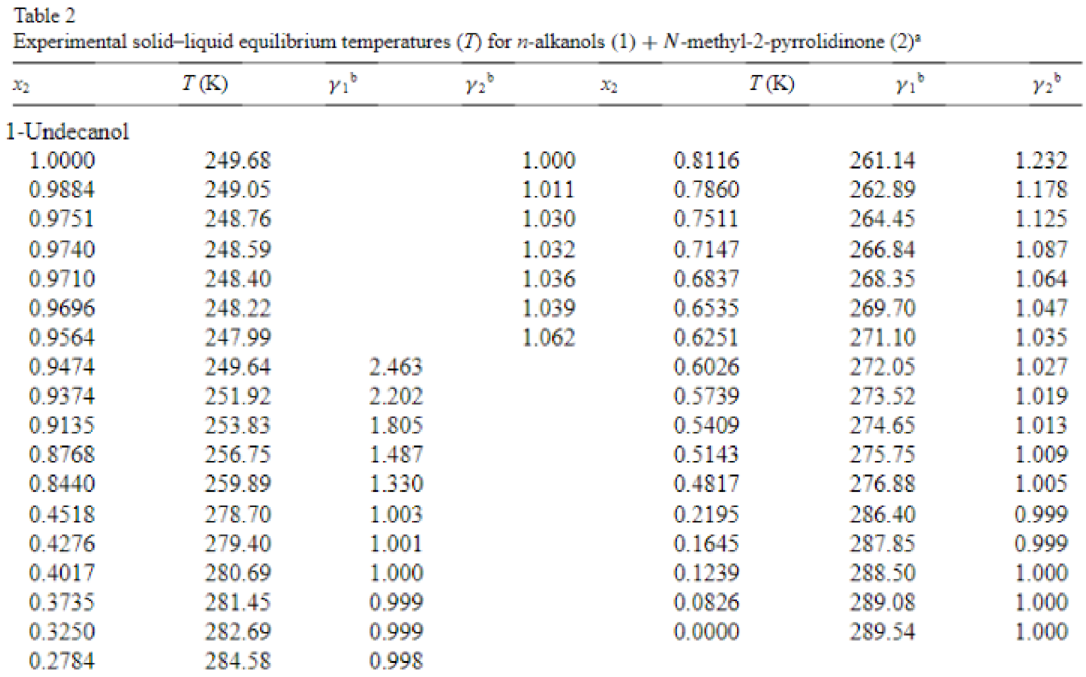


Table 2

Experimental solid–liquid equilibrium temperatures ($T$) for $n$-alkanols (1) + $N$-methyl-2-pyrrolidinone (2)[a]

| $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] | $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] |
|---|---|---|---|---|---|---|---|
| 1-Undecanol | | | | | | | |
| 1.0000 | 249.68 | | 1.000 | 0.8116 | 261.14 | 1.232 | |
| 0.9884 | 249.05 | | 1.011 | 0.7860 | 262.89 | 1.178 | |
| 0.9751 | 248.76 | | 1.030 | 0.7511 | 264.45 | 1.125 | |
| 0.9740 | 248.59 | | 1.032 | 0.7147 | 266.84 | 1.087 | |
| 0.9710 | 248.40 | | 1.036 | 0.6837 | 268.35 | 1.064 | |
| 0.9696 | 248.22 | | 1.039 | 0.6535 | 269.70 | 1.047 | |
| 0.9564 | 247.99 | | 1.062 | 0.6251 | 271.10 | 1.035 | |
| 0.9474 | 249.64 | 2.463 | | 0.6026 | 272.05 | 1.027 | |
| 0.9374 | 251.92 | 2.202 | | 0.5739 | 273.52 | 1.019 | |
| 0.9135 | 253.83 | 1.805 | | 0.5409 | 274.65 | 1.013 | |
| 0.8768 | 256.75 | 1.487 | | 0.5143 | 275.75 | 1.009 | |
| 0.8440 | 259.89 | 1.330 | | 0.4817 | 276.88 | 1.005 | |
| 0.4518 | 278.70 | 1.003 | | 0.2195 | 286.40 | 0.999 | |
| 0.4276 | 279.40 | 1.001 | | 0.1645 | 287.85 | 0.999 | |
| 0.4017 | 280.69 | 1.000 | | 0.1239 | 288.50 | 1.000 | |
| 0.3735 | 281.45 | 0.999 | | 0.0826 | 289.08 | 1.000 | |
| 0.3250 | 282.69 | 0.999 | | 0.0000 | 289.54 | 1.000 | |
| 0.2784 | 284.58 | 0.998 | | | | | |

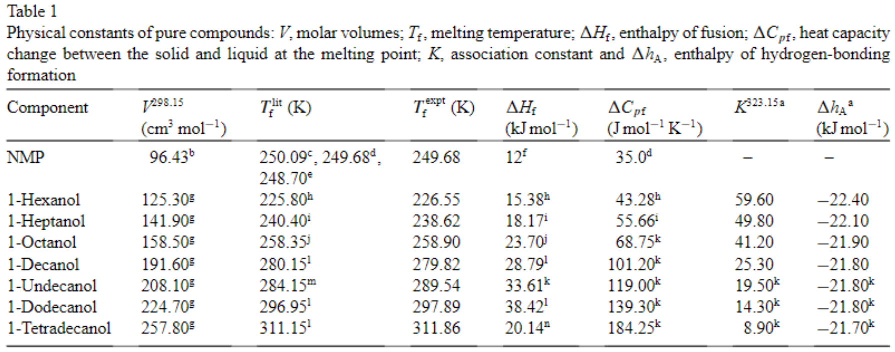


Table 1

Physical constants of pure compounds: $V$, molar volumes; $T_f$, melting temperature; $\Delta H_f$, enthalpy of fusion; $\Delta C_{pf}$, heat capacity change between the solid and liquid at the melting point; $K$, association constant and $\Delta h_A$, enthalpy of hydrogen-bonding formation

| Component | $V^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_f^{lit}$ (K) | $T_f^{expt}$ (K) | $\Delta H_f$ (kJ mol$^{-1}$) | $\Delta C_{pf}$ (J mol$^{-1}$ K$^{-1}$) | $K^{323.15\,a}$ | $\Delta h_A$[a] (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|---|
| NMP | 96.43[b] | 250.09[c], 249.68[d], 248.70[e] | 249.68 | 12[f] | 35.0[d] | – | – |
| 1-Hexanol | 125.30[g] | 225.80[h] | 226.55 | 15.38[h] | 43.28[h] | 59.60 | –22.40 |
| 1-Heptanol | 141.90[g] | 240.40[i] | 238.62 | 18.17[i] | 55.66[i] | 49.80 | –22.10 |
| 1-Octanol | 158.50[g] | 258.35[j] | 258.90 | 23.70[j] | 68.75[k] | 41.20 | –21.90 |
| 1-Decanol | 191.60[g] | 280.15[l] | 279.82 | 28.79[l] | 101.20[k] | 25.30 | –21.80 |
| 1-Undecanol | 208.10[g] | 284.15[m] | 289.54 | 33.61[k] | 119.00[k] | 19.50[k] | –21.80[k] |
| 1-Dodecanol | 224.70[g] | 296.95[l] | 297.89 | 38.42[l] | 139.30[k] | 14.30[k] | –21.80[k] |
| 1-Tetradecanol | 257.80[g] | 311.15[l] | 311.86 | 20.14[n] | 184.25[k] | 8.90[k] | –21.70[k] |

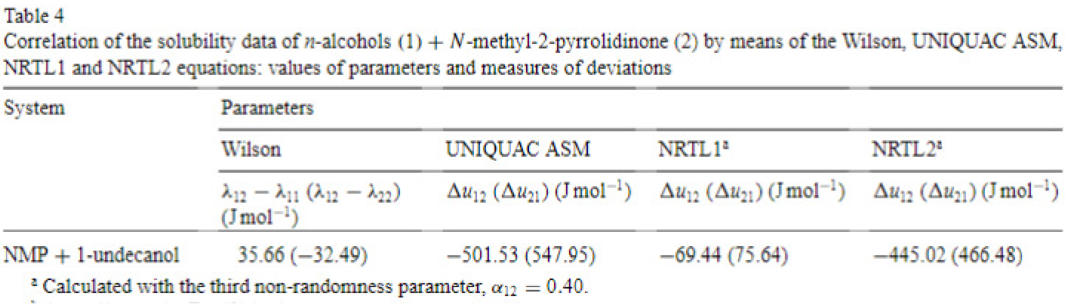


Table 4

Correlation of the solubility data of $n$-alcohols (1) + $N$-methyl-2-pyrrolidinone (2) by means of the Wilson, UNIQUAC ASM, NRTL1 and NRTL2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| | Wilson | UNIQUAC ASM | NRTL1[a] | NRTL2[a] |
| | $\lambda_{12}-\lambda_{11}$ ($\lambda_{12}-\lambda_{22}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) |
| NMP + 1-undecanol | 35.66 (−32.49) | −501.53 (547.95) | −69.44 (75.64) | −445.02 (466.48) |

[a] Calculated with the third non-randomness parameter, $\alpha_{12}$ = 0.40.

ODABRATI JEDAN MODEL

*n*-dodecanol + *N*-methyl-2-pyrrolidinone

U. Domanska, J. Łachwa, (Solid+liquid) phase equilibria of binary mixtures containing *N*-methyl-2-pyrrolidinone and long-chain *n*-alkanols at atmospheric pressure, Fluid Phase Equilibria 198 (2002) 1–14

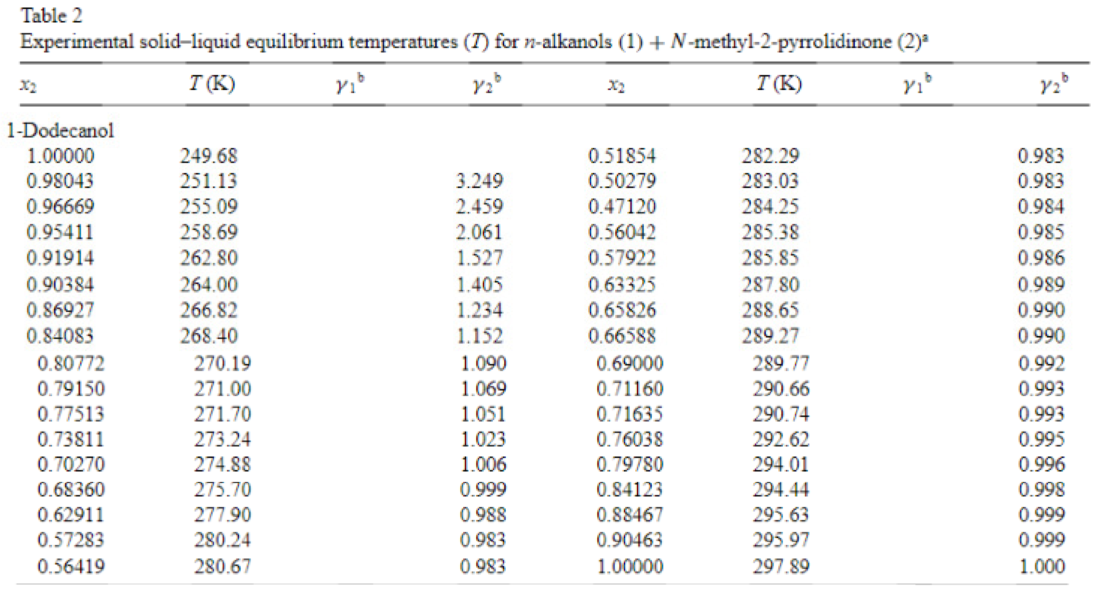


Table 2

Experimental solid–liquid equilibrium temperatures ($T$) for $n$-alkanols (1) + $N$-methyl-2-pyrrolidinone (2)[a]

| $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] | $x_2$ | $T$ (K) | $\gamma_1$[b] | $\gamma_2$[b] |
|---|---|---|---|---|---|---|---|
| 1-Dodecanol | | | | | | | |
| 1.00000 | 249.68 | | | 0.51854 | 282.29 | | 0.983 |
| 0.98043 | 251.13 | | 3.249 | 0.50279 | 283.03 | | 0.983 |
| 0.96669 | 255.09 | | 2.459 | 0.47120 | 284.25 | | 0.984 |
| 0.95411 | 258.69 | | 2.061 | 0.56042 | 285.38 | | 0.985 |
| 0.91914 | 262.80 | | 1.527 | 0.57922 | 285.85 | | 0.986 |
| 0.90384 | 264.00 | | 1.405 | 0.63325 | 287.80 | | 0.989 |
| 0.86927 | 266.82 | | 1.234 | 0.65826 | 288.65 | | 0.990 |
| 0.84083 | 268.40 | | 1.152 | 0.66588 | 289.27 | | 0.990 |
| 0.80772 | 270.19 | | 1.090 | 0.69000 | 289.77 | | 0.992 |
| 0.79150 | 271.00 | | 1.069 | 0.71160 | 290.66 | | 0.993 |
| 0.77513 | 271.70 | | 1.051 | 0.71635 | 290.74 | | 0.993 |
| 0.73811 | 273.24 | | 1.023 | 0.76038 | 292.62 | | 0.995 |
| 0.70270 | 274.88 | | 1.006 | 0.79780 | 294.01 | | 0.996 |
| 0.68360 | 275.70 | | 0.999 | 0.84123 | 294.44 | | 0.998 |
| 0.62911 | 277.90 | | 0.988 | 0.88467 | 295.63 | | 0.999 |
| 0.57283 | 280.24 | | 0.983 | 0.90463 | 295.97 | | 0.999 |
| 0.56419 | 280.67 | | 0.983 | 1.00000 | 297.89 | | 1.000 |

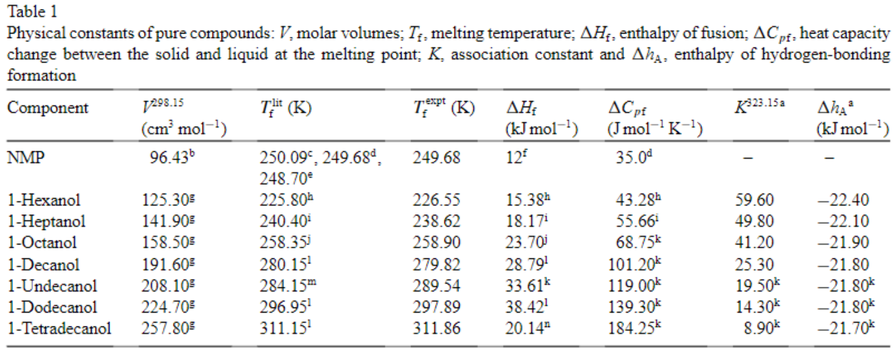


Table 1

Physical constants of pure compounds: $V$, molar volumes; $T_f$, melting temperature; $\Delta H_f$, enthalpy of fusion; $\Delta C_{pf}$, heat capacity change between the solid and liquid at the melting point; $K$, association constant and $\Delta h_A$, enthalpy of hydrogen-bonding formation

| Component | $V^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_f^{\text{lit}}$ (K) | $T_f^{\text{expt}}$ (K) | $\Delta H_f$ (kJ mol$^{-1}$) | $\Delta C_{pf}$ (J mol$^{-1}$ K$^{-1}$) | $K^{323.15\,a}$ | $\Delta h_A$[a] (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|---|
| NMP | 96.43[b] | 250.09[c], 249.68[d], 248.70[e] | 249.68 | 12[f] | 35.0[d] | – | – |
| 1-Hexanol | 125.30[g] | 225.80[h] | 226.55 | 15.38[h] | 43.28[h] | 59.60 | –22.40 |
| 1-Heptanol | 141.90[g] | 240.40[i] | 238.62 | 18.17[i] | 55.66[i] | 49.80 | –22.10 |
| 1-Octanol | 158.50[g] | 258.35[j] | 258.90 | 23.70[j] | 68.75[k] | 41.20 | –21.90 |
| 1-Decanol | 191.60[g] | 280.15[l] | 279.82 | 28.79[l] | 101.20[k] | 25.30 | –21.80 |
| 1-Undecanol | 208.10[g] | 284.15[m] | 289.54 | 33.61[k] | 119.00[k] | 19.50[k] | –21.80[k] |
| 1-Dodecanol | 224.70[g] | 296.95[l] | 297.89 | 38.42[l] | 139.30[k] | 14.30[k] | –21.80[k] |
| 1-Tetradecanol | 257.80[g] | 311.15[l] | 311.86 | 20.14[n] | 184.25[k] | 8.90[k] | –21.70[k] |

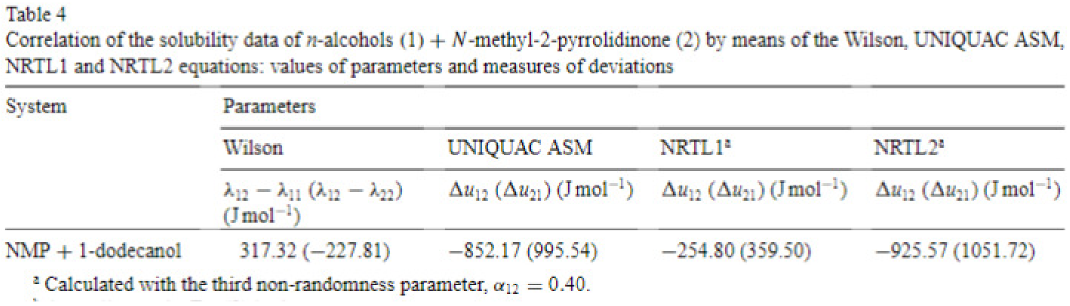


Table 4

Correlation of the solubility data of $n$-alcohols (1) + $N$-methyl-2-pyrrolidinone (2) by means of the Wilson, UNIQUAC ASM, NRTL1 and NRTL2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| | Wilson | UNIQUAC ASM | NRTL1[a] | NRTL2[a] |
| | $\lambda_{12} - \lambda_{11}$ ($\lambda_{12} - \lambda_{22}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) |
| NMP + 1-dodecanol | 317.32 (−227.81) | −852.17 (995.54) | −254.80 (359.50) | −925.57 (1051.72) |

[a] Calculated with the third non-randomness parameter, $\alpha_{12} = 0.40$.

ODABRATI JEDAN MODEL

*n*-tetradecanol + *N*-methyl-2-pyrrolidinone

U. Domanska, J. Łachwa, (Solid+liquid) phase equilibria of binary mixtures containing *N*-methyl-2-pyrrolidinone and long-chain *n*-alkanols at atmospheric pressure, Fluid Phase Equilibria 198 (2002) 1–14

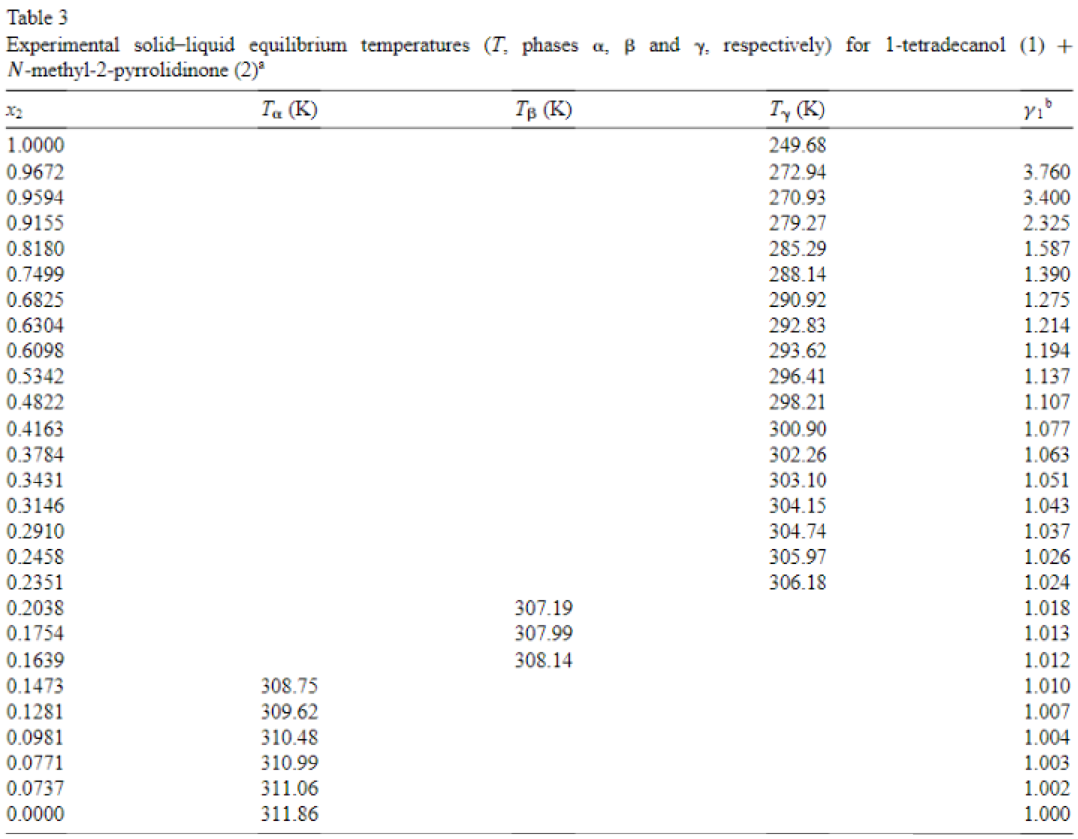


Table 3

Experimental solid–liquid equilibrium temperatures ($T$, phases α, β and γ, respectively) for 1-tetradecanol (1) + $N$-methyl-2-pyrrolidinone (2)[a]

| $x_2$ | $T_\alpha$ (K) | $T_\beta$ (K) | $T_\gamma$ (K) | $\gamma_1$[b] |
|---|---|---|---|---|
| 1.0000 | | | 249.68 | |
| 0.9672 | | | 272.94 | 3.760 |
| 0.9594 | | | 270.93 | 3.400 |
| 0.9155 | | | 279.27 | 2.325 |
| 0.8180 | | | 285.29 | 1.587 |
| 0.7499 | | | 288.14 | 1.390 |
| 0.6825 | | | 290.92 | 1.275 |
| 0.6304 | | | 292.83 | 1.214 |
| 0.6098 | | | 293.62 | 1.194 |
| 0.5342 | | | 296.41 | 1.137 |
| 0.4822 | | | 298.21 | 1.107 |
| 0.4163 | | | 300.90 | 1.077 |
| 0.3784 | | | 302.26 | 1.063 |
| 0.3431 | | | 303.10 | 1.051 |
| 0.3146 | | | 304.15 | 1.043 |
| 0.2910 | | | 304.74 | 1.037 |
| 0.2458 | | | 305.97 | 1.026 |
| 0.2351 | | | 306.18 | 1.024 |
| 0.2038 | | 307.19 | | 1.018 |
| 0.1754 | | 307.99 | | 1.013 |
| 0.1639 | | 308.14 | | 1.012 |
| 0.1473 | 308.75 | | | 1.010 |
| 0.1281 | 309.62 | | | 1.007 |
| 0.0981 | 310.48 | | | 1.004 |
| 0.0771 | 310.99 | | | 1.003 |
| 0.0737 | 311.06 | | | 1.002 |
| 0.0000 | 311.86 | | | 1.000 |

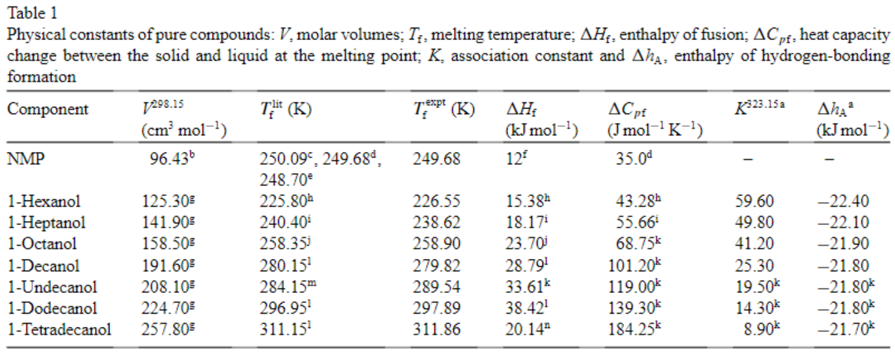


Table 1

Physical constants of pure compounds: $V$, molar volumes; $T_f$, melting temperature; $\Delta H_f$, enthalpy of fusion; $\Delta C_{pf}$, heat capacity change between the solid and liquid at the melting point; $K$, association constant and $\Delta h_A$, enthalpy of hydrogen-bonding formation

| Component | $V^{298.15}$ (cm$^3$ mol$^{-1}$) | $T_f^{lit}$ (K) | $T_f^{expt}$ (K) | $\Delta H_f$ (kJ mol$^{-1}$) | $\Delta C_{pf}$ (J mol$^{-1}$ K$^{-1}$) | $K^{323.15a}$ | $\Delta h_A$[a] (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|---|
| NMP | 96.43[b] | 250.09[c], 249.68[d], 248.70[e] | 249.68 | 12[f] | 35.0[d] | – | – |
| 1-Hexanol | 125.30[g] | 225.80[h] | 226.55 | 15.38[h] | 43.28[h] | 59.60 | −22.40 |
| 1-Heptanol | 141.90[g] | 240.40[i] | 238.62 | 18.17[i] | 55.66[i] | 49.80 | −22.10 |
| 1-Octanol | 158.50[g] | 258.35[j] | 258.90 | 23.70[j] | 68.75[k] | 41.20 | −21.90 |
| 1-Decanol | 191.60[g] | 280.15[l] | 279.82 | 28.79[l] | 101.20[k] | 25.30 | −21.80 |
| 1-Undecanol | 208.10[g] | 284.15[m] | 289.54 | 33.61[k] | 119.00[k] | 19.50[k] | −21.80[k] |
| 1-Dodecanol | 224.70[g] | 296.95[l] | 297.89 | 38.42[l] | 139.30[k] | 14.30[k] | −21.80[k] |
| 1-Tetradecanol | 257.80[g] | 311.15[l] | 311.86 | 20.14[n] | 184.25[k] | 8.90[k] | −21.70[k] |

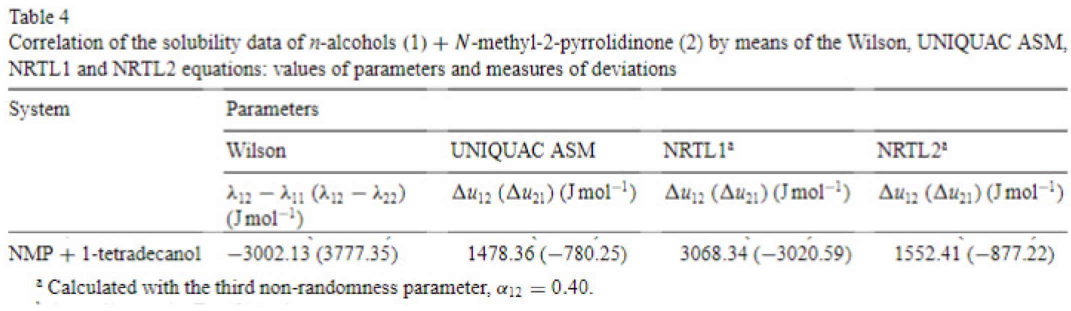


Table 4

Correlation of the solubility data of $n$-alcohols (1) + $N$-methyl-2-pyrrolidinone (2) by means of the Wilson, UNIQUAC ASM, NRTL1 and NRTL2 equations: values of parameters and measures of deviations

| System | Parameters | | | |
|---|---|---|---|---|
| | Wilson | UNIQUAC ASM | NRTL1[a] | NRTL2[a] |
| | $\lambda_{12}-\lambda_{11}$ ($\lambda_{12}-\lambda_{22}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) | $\Delta u_{12}$ ($\Delta u_{21}$) (J mol$^{-1}$) |
| NMP + 1-tetradecanol | −3002.13 (3777.35) | 1478.36 (−780.25) | 3068.34 (−3020.59) | 1552.41 (−877.22) |

[a] Calculated with the third non-randomness parameter, $\alpha_{12}$ = 0.40.

ODABRATI JEDAN MODEL

dimethyl carbonate + diphenyl carbonate
Sang Hong Shin, In-Yong Jeong, Yeong-Seok Jeong, So-Jin Park, Solid–liquid equilibria and the physical properties of binary systems of diphenyl carbonate, dimethyl carbonate, methyl phenyl carbonate, anisole, methanol and phenol, Fluid Phase Equilibria, Volume 376, 25 August 2014, Pages 105-110

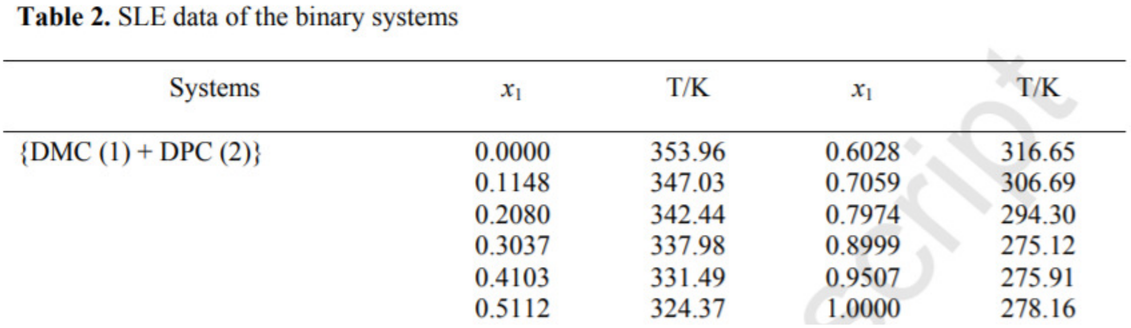


**Table 2.** SLE data of the binary systems

| Systems | $x_1$ | T/K | $x_1$ | T/K |
|---|---|---|---|---|
| {DMC (1) + DPC (2)} | 0.0000 | 353.96 | 0.6028 | 316.65 |
| | 0.1148 | 347.03 | 0.7059 | 306.69 |
| | 0.2080 | 342.44 | 0.7974 | 294.30 |
| | 0.3037 | 337.98 | 0.8999 | 275.12 |
| | 0.4103 | 331.49 | 0.9507 | 275.91 |
| | 0.5112 | 324.37 | 1.0000 | 278.16 |

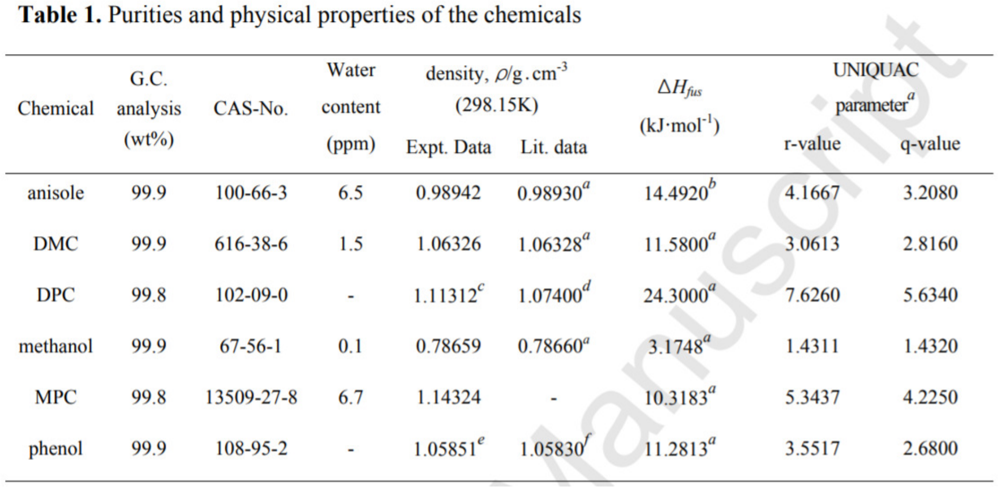


**Table 1.** Purities and physical properties of the chemicals

| Chemical | G.C. analysis (wt%) | CAS-No. | Water content (ppm) | density, $\rho$/g.cm$^{-3}$ (298.15K) | | $\Delta H_{fus}$ (kJ·mol$^{-1}$) | UNIQUAC parameter$^a$ | |
|---|---|---|---|---|---|---|---|---|
| | | | | Expt. Data | Lit. data | | r-value | q-value |
| anisole | 99.9 | 100-66-3 | 6.5 | 0.98942 | 0.98930$^a$ | 14.4920$^b$ | 4.1667 | 3.2080 |
| DMC | 99.9 | 616-38-6 | 1.5 | 1.06326 | 1.06328$^a$ | 11.5800$^a$ | 3.0613 | 2.8160 |
| DPC | 99.8 | 102-09-0 | - | 1.11312$^c$ | 1.07400$^d$ | 24.3000$^a$ | 7.6260 | 5.6340 |
| methanol | 99.9 | 67-56-1 | 0.1 | 0.78659 | 0.78660$^a$ | 3.1748$^a$ | 1.4311 | 1.4320 |
| MPC | 99.8 | 13509-27-8 | 6.7 | 1.14324 | - | 10.3183$^a$ | 5.3437 | 4.2250 |
| phenol | 99.9 | 108-95-2 | - | 1.05851$^e$ | 1.05830$^f$ | 11.2813$^a$ | 3.5517 | 2.6800 |

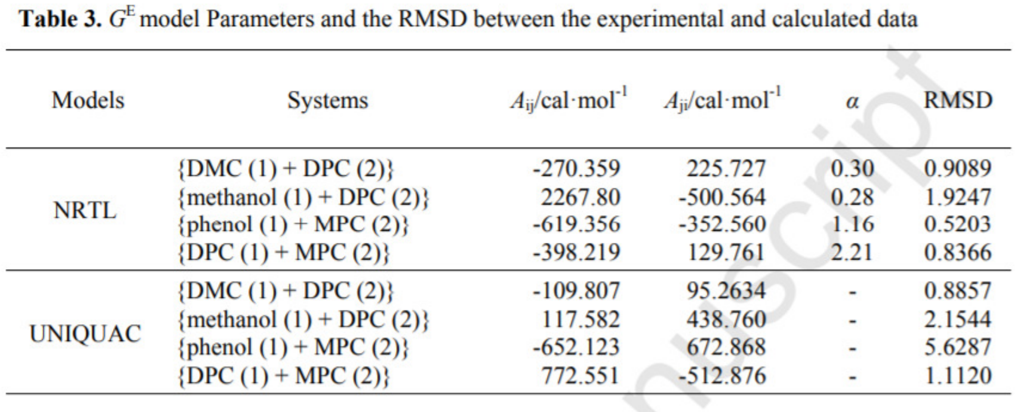


**Table 3.** $G^E$ model Parameters and the RMSD between the experimental and calculated data

| Models | Systems | $A_{ij}$/cal·mol$^{-1}$ | $A_{ji}$/cal·mol$^{-1}$ | $\alpha$ | RMSD |
|---|---|---|---|---|---|
| NRTL | {DMC (1) + DPC (2)} | -270.359 | 225.727 | 0.30 | 0.9089 |
| | {methanol (1) + DPC (2)} | 2267.80 | -500.564 | 0.28 | 1.9247 |
| | {phenol (1) + MPC (2)} | -619.356 | -352.560 | 1.16 | 0.5203 |
| | {DPC (1) + MPC (2)} | -398.219 | 129.761 | 2.21 | 0.8366 |
| UNIQUAC | {DMC (1) + DPC (2)} | -109.807 | 95.2634 | - | 0.8857 |
| | {methanol (1) + DPC (2)} | 117.582 | 438.760 | - | 2.1544 |
| | {phenol (1) + MPC (2)} | -652.123 | 672.868 | - | 5.6287 |
| | {DPC (1) + MPC (2)} | 772.551 | -512.876 | - | 1.1120 |

ODABRATI JEDAN MODEL

methanol + diphenyl carbonate

Sang Hong Shin, In-Yong Jeong, Yeong-Seok Jeong, So-Jin Park, Solid–liquid equilibria and the physical properties of binary systems of diphenyl carbonate, dimethyl carbonate, methyl phenyl carbonate, anisole, methanol and phenol, Fluid Phase Equilibria, Volume 376, 25 August 2014, Pages 105-110

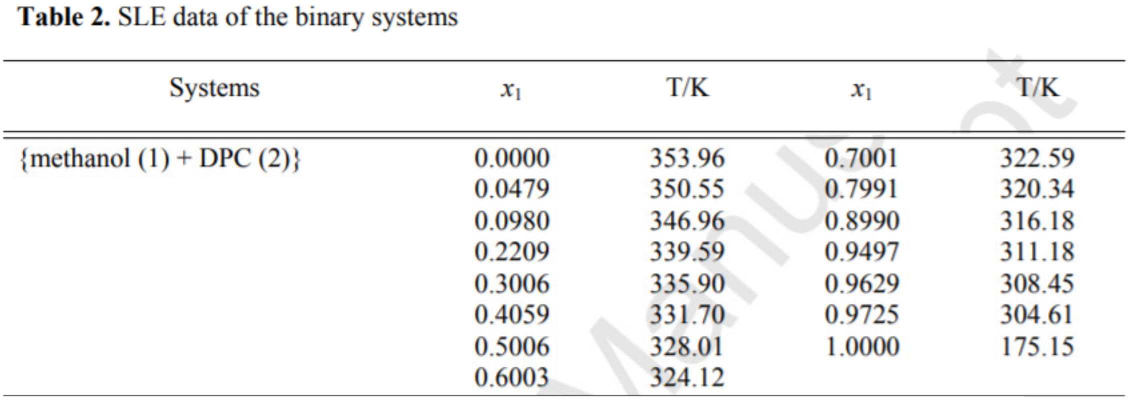


**Table 2.** SLE data of the binary systems

| Systems | $x_1$ | T/K | $x_1$ | T/K |
|---|---|---|---|---|
| {methanol (1) + DPC (2)} | 0.0000 | 353.96 | 0.7001 | 322.59 |
| | 0.0479 | 350.55 | 0.7991 | 320.34 |
| | 0.0980 | 346.96 | 0.8990 | 316.18 |
| | 0.2209 | 339.59 | 0.9497 | 311.18 |
| | 0.3006 | 335.90 | 0.9629 | 308.45 |
| | 0.4059 | 331.70 | 0.9725 | 304.61 |
| | 0.5006 | 328.01 | 1.0000 | 175.15 |
| | 0.6003 | 324.12 | | |

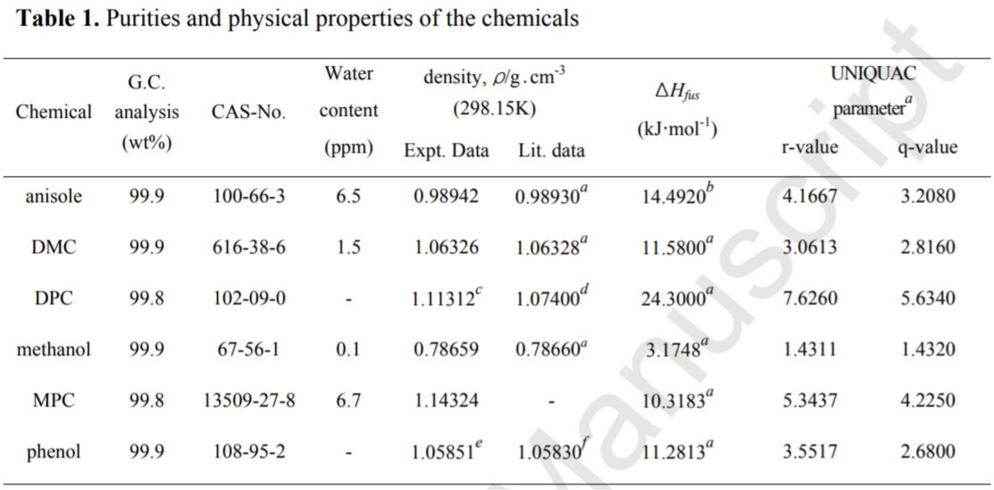


**Table 1.** Purities and physical properties of the chemicals

| Chemical | G.C. analysis (wt%) | CAS-No. | Water content (ppm) | density, $\rho$/g.cm$^{-3}$ (298.15K) | | $\Delta H_{fus}$ (kJ·mol$^{-1}$) | UNIQUAC parameter[a] | |
|---|---|---|---|---|---|---|---|---|
| | | | | Expt. Data | Lit. data | | r-value | q-value |
| anisole | 99.9 | 100-66-3 | 6.5 | 0.98942 | 0.98930[a] | 14.4920[b] | 4.1667 | 3.2080 |
| DMC | 99.9 | 616-38-6 | 1.5 | 1.06326 | 1.06328[a] | 11.5800[a] | 3.0613 | 2.8160 |
| DPC | 99.8 | 102-09-0 | - | 1.11312[c] | 1.07400[d] | 24.3000[a] | 7.6260 | 5.6340 |
| methanol | 99.9 | 67-56-1 | 0.1 | 0.78659 | 0.78660[a] | 3.1748[a] | 1.4311 | 1.4320 |
| MPC | 99.8 | 13509-27-8 | 6.7 | 1.14324 | - | 10.3183[a] | 5.3437 | 4.2250 |
| phenol | 99.9 | 108-95-2 | - | 1.05851[e] | 1.05830[f] | 11.2813[a] | 3.5517 | 2.6800 |

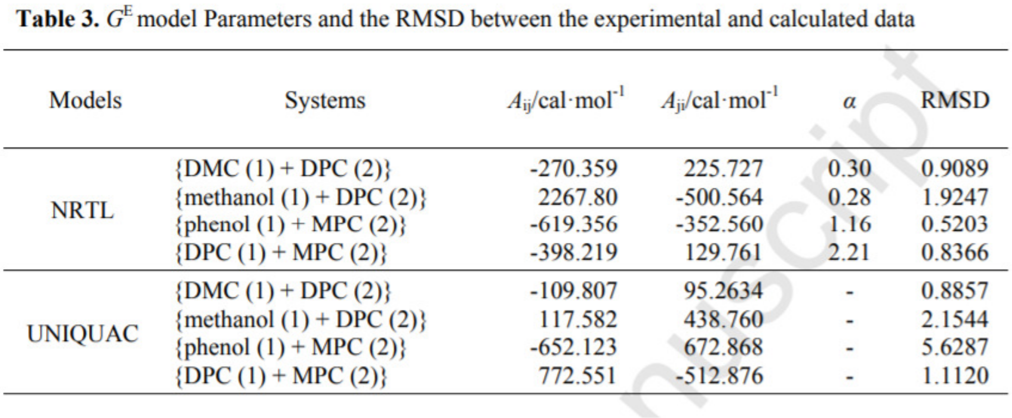


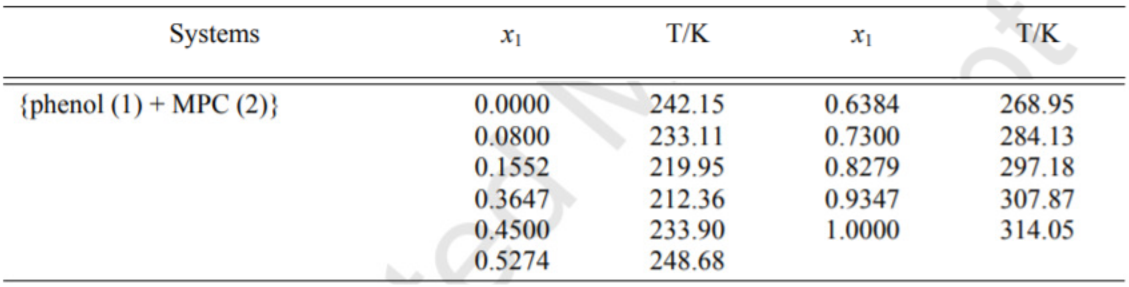
**Table 3.** $G^E$ model Parameters and the RMSD between the experimental and calculated data

| Models | Systems | $A_{ij}$/cal·mol$^{-1}$ | $A_{ji}$/cal·mol$^{-1}$ | $\alpha$ | RMSD |
|---|---|---|---|---|---|
| NRTL | {DMC (1) + DPC (2)} | -270.359 | 225.727 | 0.30 | 0.9089 |
| | {methanol (1) + DPC (2)} | 2267.80 | -500.564 | 0.28 | 1.9247 |
| | {phenol (1) + MPC (2)} | -619.356 | -352.560 | 1.16 | 0.5203 |
| | {DPC (1) + MPC (2)} | -398.219 | 129.761 | 2.21 | 0.8366 |
| UNIQUAC | {DMC (1) + DPC (2)} | -109.807 | 95.2634 | - | 0.8857 |
| | {methanol (1) + DPC (2)} | 117.582 | 438.760 | - | 2.1544 |
| | {phenol (1) + MPC (2)} | -652.123 | 672.868 | - | 5.6287 |
| | {DPC (1) + MPC (2)} | 772.551 | -512.876 | - | 1.1120 |

ODABRATI JEDAN MODEL

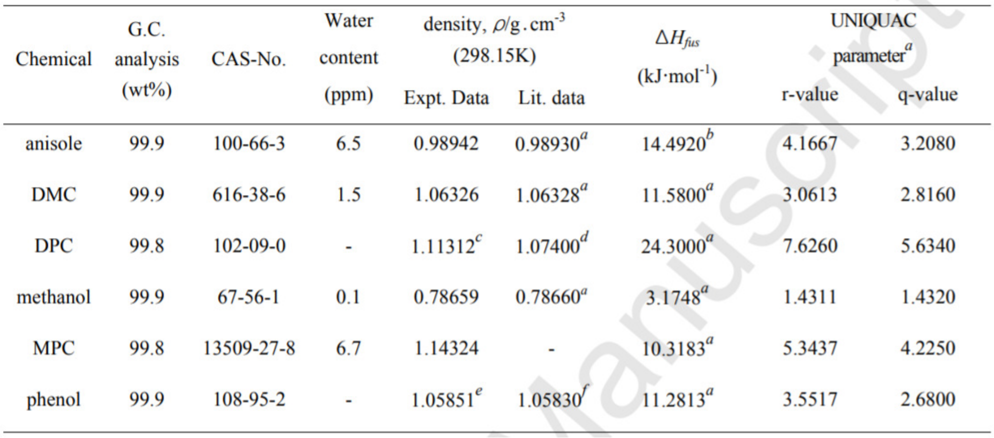
phenol + methyl phenyl carbonate
Sang Hong Shin, In-Yong Jeong, Yeong-Seok Jeong, So-Jin Park, Solid–liquid equilibria and the physical properties of binary systems of diphenyl carbonate, dimethyl carbonate, methyl phenyl carbonate, anisole, methanol and phenol, Fluid Phase Equilibria, Volume 376, 25 August 2014, Pages 105-110

**Table 2.** SLE data of the binary systems



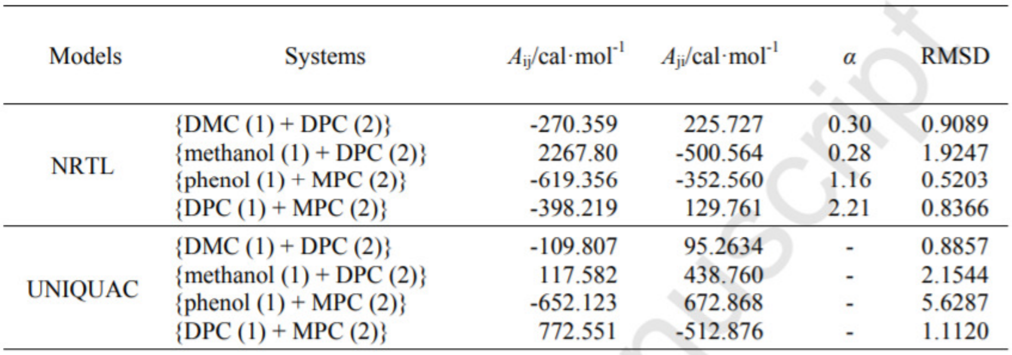
| Systems | $x_1$ | T/K | $x_1$ | T/K |
|---|---|---|---|---|
| {phenol (1) + MPC (2)} | 0.0000 | 242.15 | 0.6384 | 268.95 |
| | 0.0800 | 233.11 | 0.7300 | 284.13 |
| | 0.1552 | 219.95 | 0.8279 | 297.18 |
| | 0.3647 | 212.36 | 0.9347 | 307.87 |
| | 0.4500 | 233.90 | 1.0000 | 314.05 |
| | 0.5274 | 248.68 | | |

**Table 1.** Purities and physical properties of the chemicals



| Chemical | G.C. analysis (wt%) | CAS-No. | Water content (ppm) | density, $\rho$/g.cm$^{-3}$ (298.15K) | | $\Delta H_{fus}$ (kJ·mol$^{-1}$) | UNIQUAC parameter$^a$ | |
|---|---|---|---|---|---|---|---|---|
| | | | | Expt. Data | Lit. data | | r-value | q-value |
| anisole | 99.9 | 100-66-3 | 6.5 | 0.98942 | 0.98930$^a$ | 14.4920$^b$ | 4.1667 | 3.2080 |
| DMC | 99.9 | 616-38-6 | 1.5 | 1.06326 | 1.06328$^a$ | 11.5800$^a$ | 3.0613 | 2.8160 |
| DPC | 99.8 | 102-09-0 | - | 1.11312$^c$ | 1.07400$^d$ | 24.3000$^a$ | 7.6260 | 5.6340 |
| methanol | 99.9 | 67-56-1 | 0.1 | 0.78659 | 0.78660$^a$ | 3.1748$^a$ | 1.4311 | 1.4320 |
| MPC | 99.8 | 13509-27-8 | 6.7 | 1.14324 | - | 10.3183$^a$ | 5.3437 | 4.2250 |
| phenol | 99.9 | 108-95-2 | - | 1.05851$^e$ | 1.05830$^f$ | 11.2813$^a$ | 3.5517 | 2.6800 |

**Table 3.** $G^E$ model Parameters and the RMSD between the experimental and calculated data



| Models | Systems | $A_{ij}$/cal·mol$^{-1}$ | $A_{ji}$/cal·mol$^{-1}$ | $\alpha$ | RMSD |
|---|---|---|---|---|---|
| NRTL | {DMC (1) + DPC (2)} | -270.359 | 225.727 | 0.30 | 0.9089 |
| | {methanol (1) + DPC (2)} | 2267.80 | -500.564 | 0.28 | 1.9247 |
| | {phenol (1) + MPC (2)} | -619.356 | -352.560 | 1.16 | 0.5203 |
| | {DPC (1) + MPC (2)} | -398.219 | 129.761 | 2.21 | 0.8366 |
| UNIQUAC | {DMC (1) + DPC (2)} | -109.807 | 95.2634 | - | 0.8857 |
| | {methanol (1) + DPC (2)} | 117.582 | 438.760 | - | 2.1544 |
| | {phenol (1) + MPC (2)} | -652.123 | 672.868 | - | 5.6287 |
| | {DPC (1) + MPC (2)} | 772.551 | -512.876 | - | 1.1120 |

ODABRATI JEDAN MODEL

diphenyl carbonate + methyl phenyl carbonate

Sang Hong Shin, In-Yong Jeong, Yeong-Seok Jeong, So-Jin Park, Solid–liquid equilibria and the physical properties of binary systems of diphenyl carbonate, dimethyl carbonate, methyl phenyl carbonate, anisole, methanol and phenol, Fluid Phase Equilibria, Volume 376, 25 August 2014, Pages 105-110

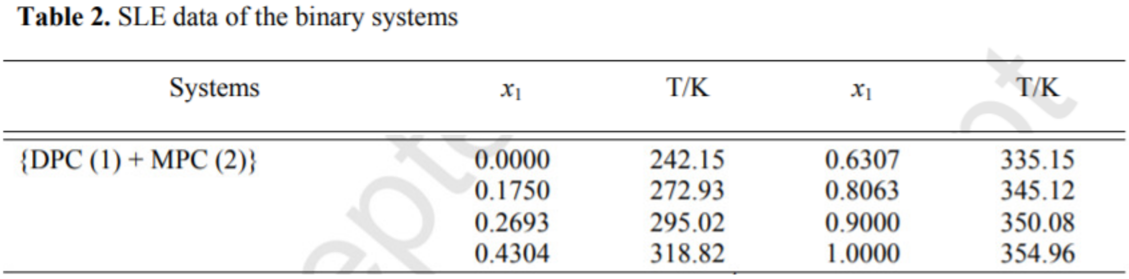


**Table 2.** SLE data of the binary systems

| Systems | $x_1$ | T/K | $x_1$ | T/K |
|---|---|---|---|---|
| {DPC (1) + MPC (2)} | 0.0000 | 242.15 | 0.6307 | 335.15 |
| | 0.1750 | 272.93 | 0.8063 | 345.12 |
| | 0.2693 | 295.02 | 0.9000 | 350.08 |
| | 0.4304 | 318.82 | 1.0000 | 354.96 |

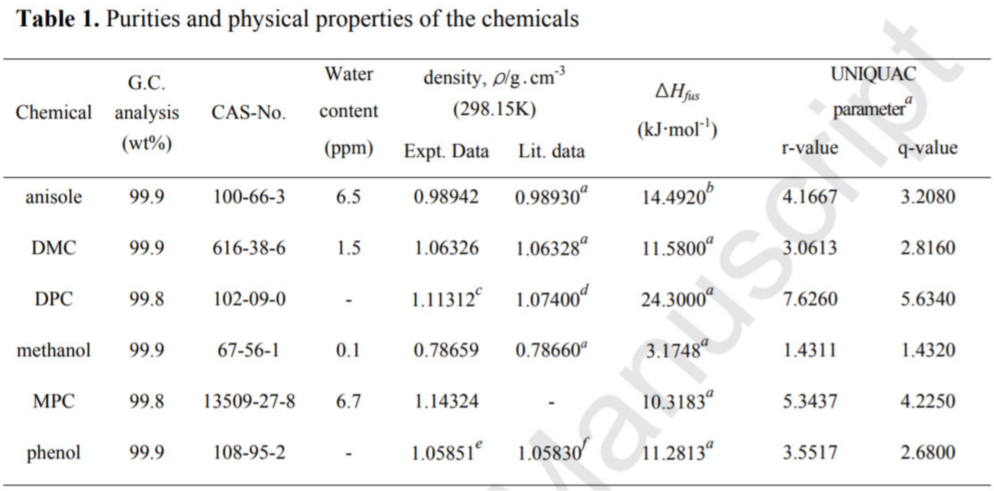


**Table 1.** Purities and physical properties of the chemicals

| Chemical | G.C. analysis (wt%) | CAS-No. | Water content (ppm) | density, $\rho$/g.cm$^{-3}$ (298.15K) | | $\Delta H_{fus}$ (kJ·mol$^{-1}$) | UNIQUAC parameter[a] | |
|---|---|---|---|---|---|---|---|---|
| | | | | Expt. Data | Lit. data | | r-value | q-value |
| anisole | 99.9 | 100-66-3 | 6.5 | 0.98942 | 0.98930[a] | 14.4920[b] | 4.1667 | 3.2080 |
| DMC | 99.9 | 616-38-6 | 1.5 | 1.06326 | 1.06328[a] | 11.5800[a] | 3.0613 | 2.8160 |
| DPC | 99.8 | 102-09-0 | - | 1.11312[c] | 1.07400[d] | 24.3000[a] | 7.6260 | 5.6340 |
| methanol | 99.9 | 67-56-1 | 0.1 | 0.78659 | 0.78660[a] | 3.1748[a] | 1.4311 | 1.4320 |
| MPC | 99.8 | 13509-27-8 | 6.7 | 1.14324 | - | 10.3183[a] | 5.3437 | 4.2250 |
| phenol | 99.9 | 108-95-2 | - | 1.05851[e] | 1.05830[f] | 11.2813[a] | 3.5517 | 2.6800 |

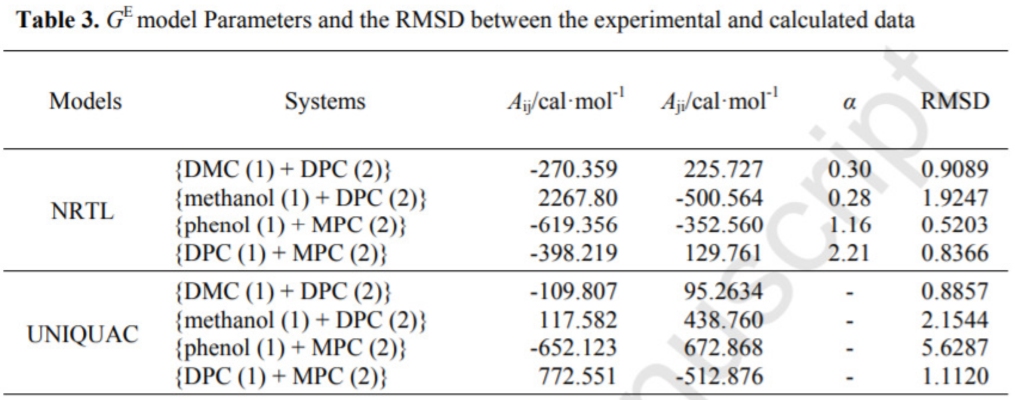


**Table 3.** $G^E$ model Parameters and the RMSD between the experimental and calculated data

| Models | Systems | $A_{ij}$/cal·mol$^{-1}$ | $A_{ji}$/cal·mol$^{-1}$ | $\alpha$ | RMSD |
|---|---|---|---|---|---|
| NRTL | {DMC (1) + DPC (2)} | -270.359 | 225.727 | 0.30 | 0.9089 |
| | {methanol (1) + DPC (2)} | 2267.80 | -500.564 | 0.28 | 1.9247 |
| | {phenol (1) + MPC (2)} | -619.356 | -352.560 | 1.16 | 0.5203 |
| | {DPC (1) + MPC (2)} | -398.219 | 129.761 | 2.21 | 0.8366 |
| UNIQUAC | {DMC (1) + DPC (2)} | -109.807 | 95.2634 | - | 0.8857 |
| | {methanol (1) + DPC (2)} | 117.582 | 438.760 | - | 2.1544 |
| | {phenol (1) + MPC (2)} | -652.123 | 672.868 | - | 5.6287 |
| | {DPC (1) + MPC (2)} | 772.551 | -512.876 | - | 1.1120 |

ODABRATI JEDAN MODEL

cyclohexane + hexadecane
Margreth Tadie, Indra Bahadur, Prashant Reddy, Peterson Thokozani Ngema, Paramespri Naidoo, Nirmala Deenadayalu, Deresh Ramjugernath, Solid–liquid equilibria measurements for binary systems comprising (butyric acid + propionic or pentanoic acid) and (heptanoic acid + propionic or butyric or pentanoic or hexanoic acid), J. Chem. Thermodynamics 57 (2013) 485–492

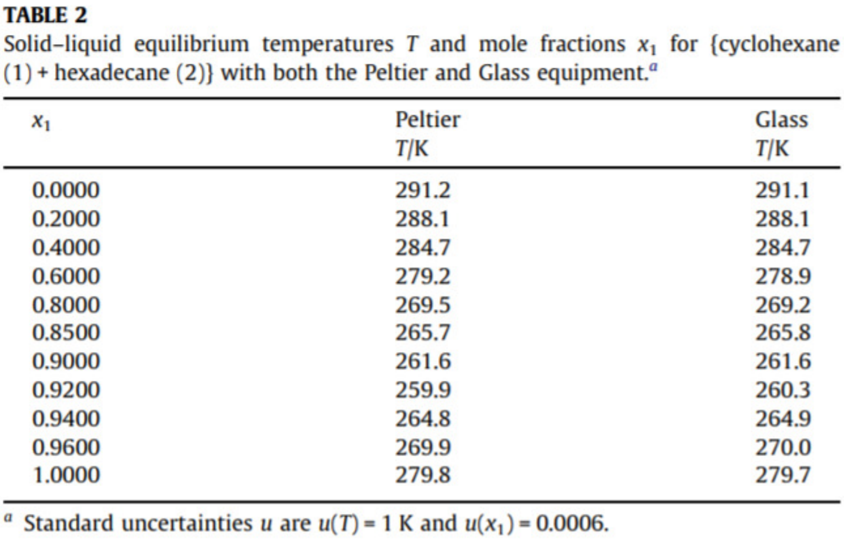


**TABLE 2**

Solid–liquid equilibrium temperatures $T$ and mole fractions $x_1$ for {cyclohexane (1) + hexadecane (2)} with both the Peltier and Glass equipment.[a]

| $x_1$ | Peltier $T$/K | Glass $T$/K |
|---|---|---|
| 0.0000 | 291.2 | 291.1 |
| 0.2000 | 288.1 | 288.1 |
| 0.4000 | 284.7 | 284.7 |
| 0.6000 | 279.2 | 278.9 |
| 0.8000 | 269.5 | 269.2 |
| 0.8500 | 265.7 | 265.8 |
| 0.9000 | 261.6 | 261.6 |
| 0.9200 | 259.9 | 260.3 |
| 0.9400 | 264.8 | 264.9 |
| 0.9600 | 269.9 | 270.0 |
| 1.0000 | 279.8 | 279.7 |

[a] Standard uncertainties $u$ are $u(T) = 1$ K and $u(x_1) = 0.0006$.

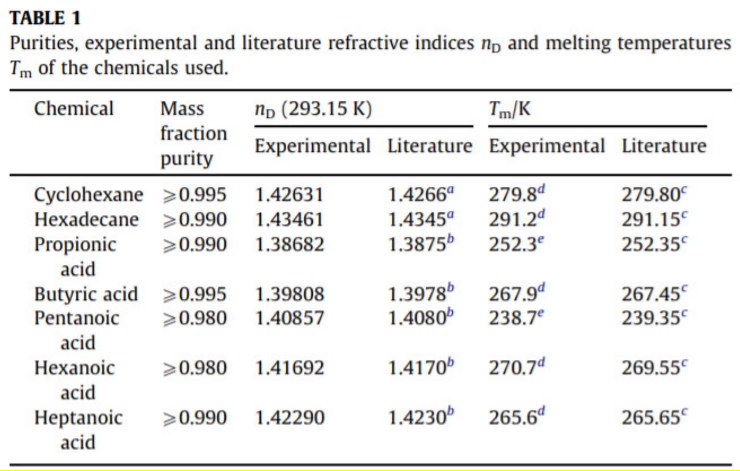


**TABLE 1**

Purities, experimental and literature refractive indices $n_D$ and melting temperatures $T_m$ of the chemicals used.

| Chemical | Mass fraction purity | $n_D$ (293.15 K) Experimental | $n_D$ (293.15 K) Literature | $T_m$/K Experimental | $T_m$/K Literature |
|---|---|---|---|---|---|
| Cyclohexane | ⩾0.995 | 1.42631 | 1.4266[a] | 279.8[d] | 279.80[c] |
| Hexadecane | ⩾0.990 | 1.43461 | 1.4345[a] | 291.2[d] | 291.15[c] |
| Propionic acid | ⩾0.990 | 1.38682 | 1.3875[b] | 252.3[e] | 252.35[c] |
| Butyric acid | ⩾0.995 | 1.39808 | 1.3978[b] | 267.9[d] | 267.45[c] |
| Pentanoic acid | ⩾0.980 | 1.40857 | 1.4080[b] | 238.7[e] | 239.35[c] |
| Hexanoic acid | ⩾0.980 | 1.41692 | 1.4170[b] | 270.7[d] | 269.55[c] |
| Heptanoic acid | ⩾0.990 | 1.42290 | 1.4230[b] | 265.6[d] | 265.65[c] |

butyric acid + propionic acid
Margreth Tadie, Indra Bahadur, Prashant Reddy, Peterson Thokozani Ngema, Paramespri Naidoo, Nirmala Deenadayalu, Deresh Ramjugernath, Solid–liquid equilibria measurements for binary systems comprising (butyric acid + propionic or pentanoic acid) and (heptanoic acid + propionic or butyric or pentanoic or hexanoic acid), J. Chem. Thermodynamics 57 (2013) 485–492

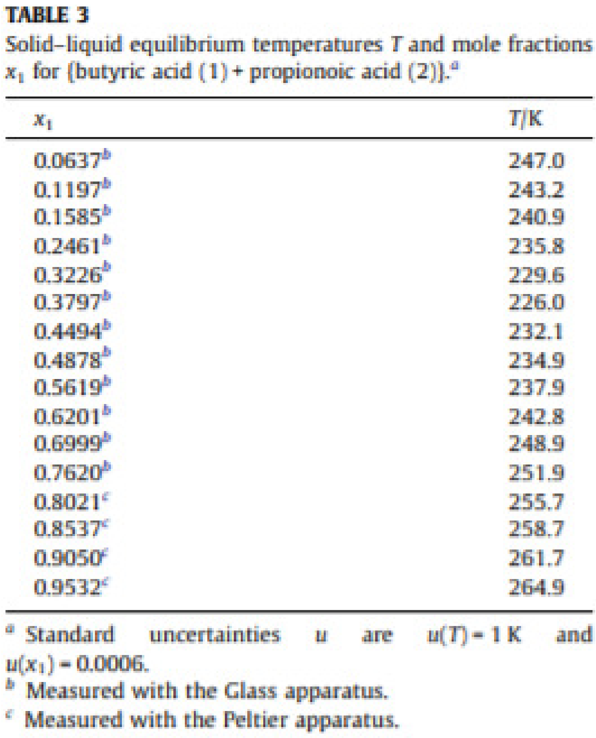


**TABLE 3**
Solid–liquid equilibrium temperatures $T$ and mole fractions $x_1$ for {butyric acid (1) + propionoic acid (2)}.[a]

| $x_1$ | $T$/K |
|---|---|
| 0.0637[b] | 247.0 |
| 0.1197[b] | 243.2 |
| 0.1585[b] | 240.9 |
| 0.2461[b] | 235.8 |
| 0.3226[b] | 229.6 |
| 0.3797[b] | 226.0 |
| 0.4494[b] | 232.1 |
| 0.4878[b] | 234.9 |
| 0.5619[b] | 237.9 |
| 0.6201[b] | 242.8 |
| 0.6999[b] | 248.9 |
| 0.7620[b] | 251.9 |
| 0.8021[c] | 255.7 |
| 0.8537[c] | 258.7 |
| 0.9050[c] | 261.7 |
| 0.9532[c] | 264.9 |

[a] Standard uncertainties $u$ are $u(T) = 1$ K and $u(x_1) = 0.0006$.
[b] Measured with the Glass apparatus.
[c] Measured with the Peltier apparatus.

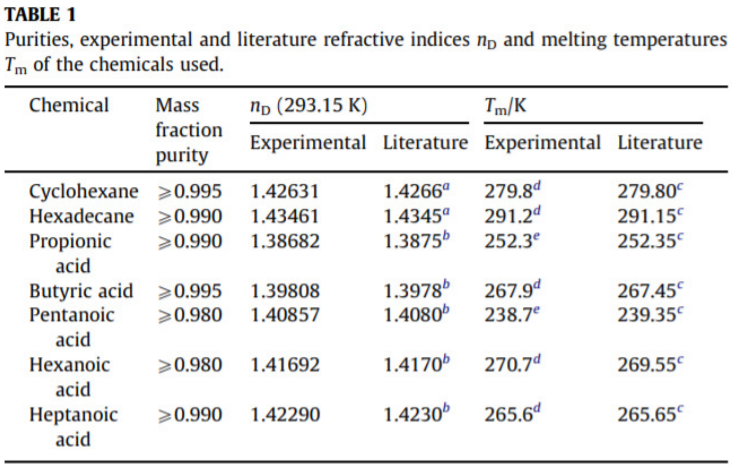


**TABLE 1**
Purities, experimental and literature refractive indices $n_D$ and melting temperatures $T_m$ of the chemicals used.

| Chemical | Mass fraction purity | $n_D$ (293.15 K) | | $T_m$/K | |
|---|---|---|---|---|---|
| | | Experimental | Literature | Experimental | Literature |
| Cyclohexane | ⩾0.995 | 1.42631 | 1.4266[a] | 279.8[d] | 279.80[c] |
| Hexadecane | ⩾0.990 | 1.43461 | 1.4345[a] | 291.2[d] | 291.15[c] |
| Propionic acid | ⩾0.990 | 1.38682 | 1.3875[b] | 252.3[e] | 252.35[c] |
| Butyric acid | ⩾0.995 | 1.39808 | 1.3978[b] | 267.9[d] | 267.45[c] |
| Pentanoic acid | ⩾0.980 | 1.40857 | 1.4080[b] | 238.7[e] | 239.35[c] |
| Hexanoic acid | ⩾0.980 | 1.41692 | 1.4170[b] | 270.7[d] | 269.55[c] |
| Heptanoic acid | ⩾0.990 | 1.42290 | 1.4230[b] | 265.6[d] | 265.65[c] |

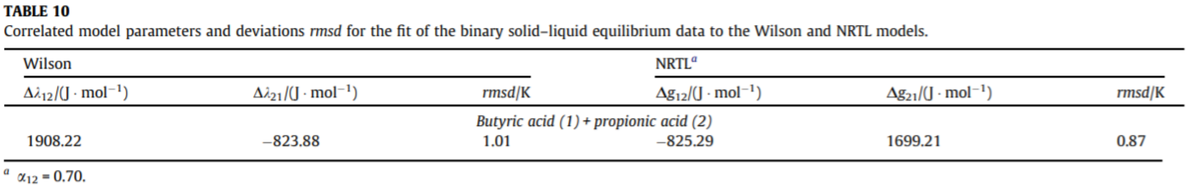


**TABLE 10**
Correlated model parameters and deviations *rmsd* for the fit of the binary solid–liquid equilibrium data to the Wilson and NRTL models.

| Wilson | | | NRTL[a] | | |
|---|---|---|---|---|---|
| $\Delta\lambda_{12}/(\mathrm{J\cdot mol^{-1}})$ | $\Delta\lambda_{21}/(\mathrm{J\cdot mol^{-1}})$ | *rmsd*/K | $\Delta g_{12}/(\mathrm{J\cdot mol^{-1}})$ | $\Delta g_{21}/(\mathrm{J\cdot mol^{-1}})$ | *rmsd*/K |
| | | *Butyric acid (1) + propionic acid (2)* | | | |
| 1908.22 | −823.88 | 1.01 | −825.29 | 1699.21 | 0.87 |

[a] $\alpha_{12} = 0.70$.

ODABRATI JEDAN MODEL

butyric acid + pentanoic acid

Margreth Tadie, Indra Bahadur, Prashant Reddy, Peterson Thokozani Ngema, Paramespri Naidoo, Nirmala Deenadayalu, Deresh Ramjugernath, Solid–liquid equilibria measurements for binary systems comprising (butyric acid + propionic or pentanoic acid) and (heptanoic acid + propionic or butyric or pentanoic or hexanoic acid), J. Chem. Thermodynamics 57 (2013) 485–492

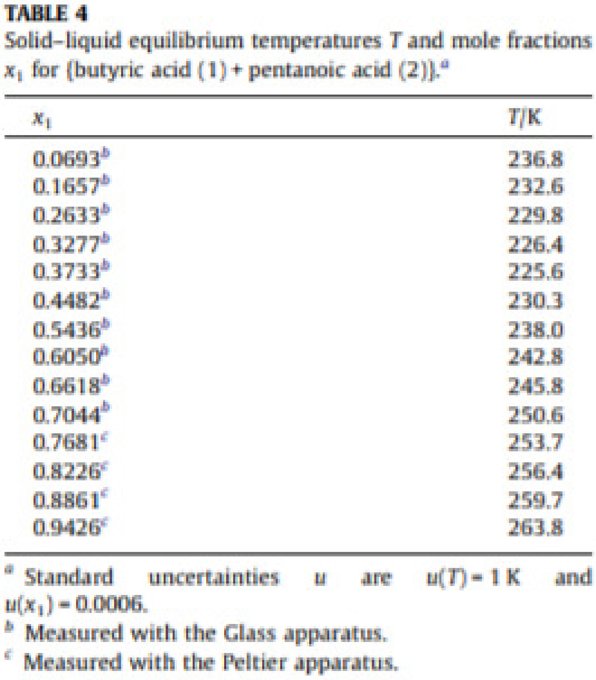


**TABLE 4**

Solid–liquid equilibrium temperatures $T$ and mole fractions $x_1$ for {butyric acid (1) + pentanoic acid (2)}.[a]

| $x_1$ | $T$/K |
|---|---|
| 0.0693[b] | 236.8 |
| 0.1657[b] | 232.6 |
| 0.2633[b] | 229.8 |
| 0.3277[b] | 226.4 |
| 0.3733[b] | 225.6 |
| 0.4482[b] | 230.3 |
| 0.5436[b] | 238.0 |
| 0.6050[b] | 242.8 |
| 0.6618[b] | 245.8 |
| 0.7044[b] | 250.6 |
| 0.7681[c] | 253.7 |
| 0.8226[c] | 256.4 |
| 0.8861[c] | 259.7 |
| 0.9426[c] | 263.8 |

[a] Standard uncertainties $u$ are $u(T) = 1$ K and $u(x_1) = 0.0006$.

[b] Measured with the Glass apparatus.

[c] Measured with the Peltier apparatus.

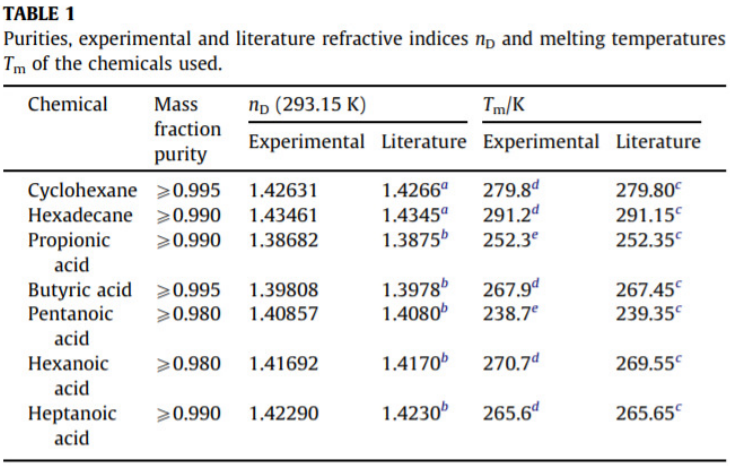


**TABLE 1**

Purities, experimental and literature refractive indices $n_D$ and melting temperatures $T_m$ of the chemicals used.

| Chemical | Mass fraction purity | $n_D$ (293.15 K) | | $T_m$/K | |
|---|---|---|---|---|---|
| | | Experimental | Literature | Experimental | Literature |
| Cyclohexane | ⩾0.995 | 1.42631 | 1.4266[a] | 279.8[d] | 279.80[c] |
| Hexadecane | ⩾0.990 | 1.43461 | 1.4345[a] | 291.2[d] | 291.15[c] |
| Propionic acid | ⩾0.990 | 1.38682 | 1.3875[b] | 252.3[e] | 252.35[c] |
| Butyric acid | ⩾0.995 | 1.39808 | 1.3978[b] | 267.9[d] | 267.45[c] |
| Pentanoic acid | ⩾0.980 | 1.40857 | 1.4080[b] | 238.7[e] | 239.35[c] |
| Hexanoic acid | ⩾0.980 | 1.41692 | 1.4170[b] | 270.7[d] | 269.55[c] |
| Heptanoic acid | ⩾0.990 | 1.42290 | 1.4230[b] | 265.6[d] | 265.65[c] |

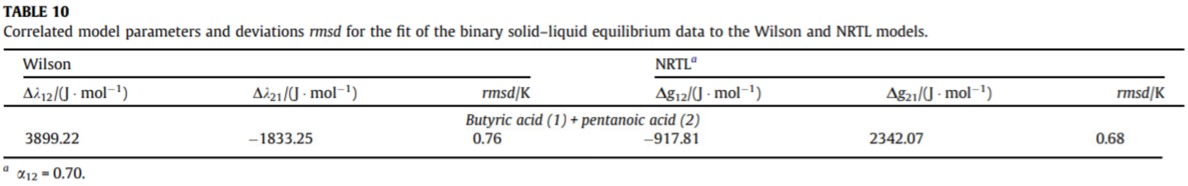


**TABLE 10**

Correlated model parameters and deviations *rmsd* for the fit of the binary solid–liquid equilibrium data to the Wilson and NRTL models.

| Wilson | | | NRTL[a] | | |
|---|---|---|---|---|---|
| $\Delta\lambda_{12}/(\text{J}\cdot\text{mol}^{-1})$ | $\Delta\lambda_{21}/(\text{J}\cdot\text{mol}^{-1})$ | *rmsd*/K | $\Delta g_{12}/(\text{J}\cdot\text{mol}^{-1})$ | $\Delta g_{21}/(\text{J}\cdot\text{mol}^{-1})$ | *rmsd*/K |
| | | *Butyric acid (1) + pentanoic acid (2)* | | | |
| 3899.22 | −1833.25 | 0.76 | −917.81 | 2342.07 | 0.68 |

[a] $\alpha_{12} = 0.70$.

ODABRATI JEDAN MODEL

heptanoic acid + pentanoic acid

Margreth Tadie, Indra Bahadur, Prashant Reddy, Peterson Thokozani Ngema, Paramespri Naidoo, Nirmala Deenadayalu, Deresh Ramjugernath, Solid–liquid equilibria measurements for binary systems comprising (butyric acid + propionic or pentanoic acid) and (heptanoic acid + propionic or butyric or pentanoic or hexanoic acid), J. Chem. Thermodynamics 57 (2013) 485–492

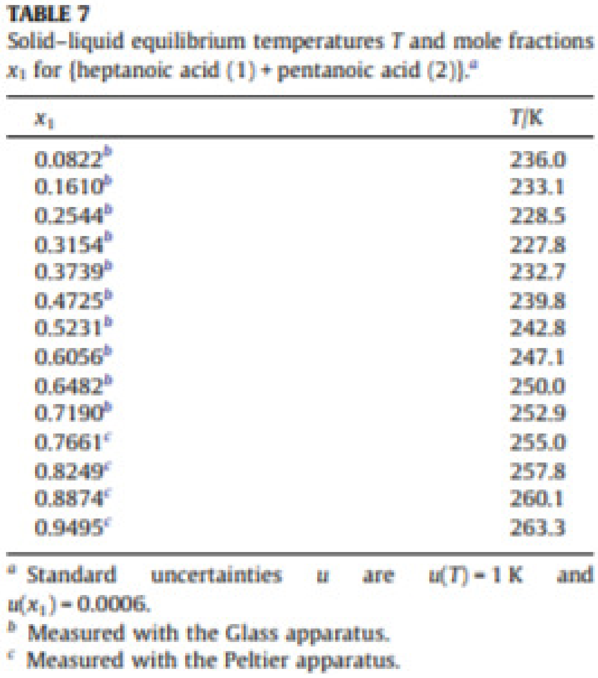


**TABLE 7**

Solid–liquid equilibrium temperatures $T$ and mole fractions $x_1$ for {heptanoic acid (1) + pentanoic acid (2)}.[a]

| $x_1$ | $T$/K |
|---|---|
| 0.0822[b] | 236.0 |
| 0.1610[b] | 233.1 |
| 0.2544[b] | 228.5 |
| 0.3154[b] | 227.8 |
| 0.3739[b] | 232.7 |
| 0.4725[b] | 239.8 |
| 0.5231[b] | 242.8 |
| 0.6056[b] | 247.1 |
| 0.6482[b] | 250.0 |
| 0.7190[b] | 252.9 |
| 0.7661[c] | 255.0 |
| 0.8249[c] | 257.8 |
| 0.8874[c] | 260.1 |
| 0.9495[c] | 263.3 |

[a] Standard uncertainties $u$ are $u(T) = 1$ K and $u(x_1) = 0.0006$.

[b] Measured with the Glass apparatus.

[c] Measured with the Peltier apparatus.

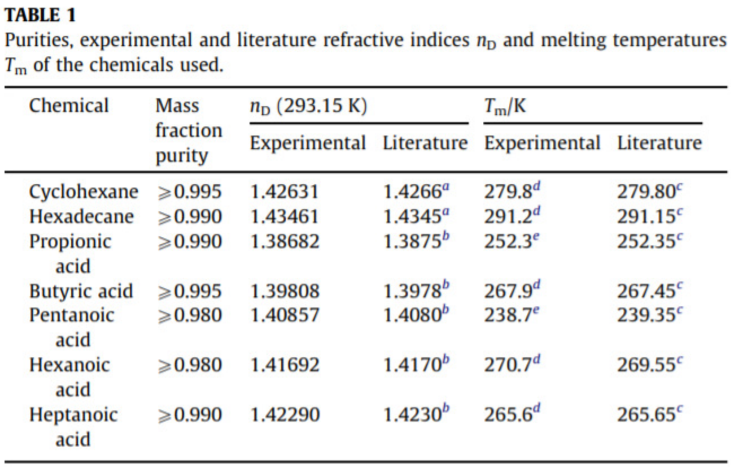


**TABLE 1**

Purities, experimental and literature refractive indices $n_D$ and melting temperatures $T_m$ of the chemicals used.

| Chemical | Mass fraction purity | $n_D$ (293.15 K) | | $T_m$/K | |
|---|---|---|---|---|---|
| | | Experimental | Literature | Experimental | Literature |
| Cyclohexane | ⩾0.995 | 1.42631 | 1.4266[a] | 279.8[d] | 279.80[c] |
| Hexadecane | ⩾0.990 | 1.43461 | 1.4345[a] | 291.2[d] | 291.15[c] |
| Propionic acid | ⩾0.990 | 1.38682 | 1.3875[b] | 252.3[e] | 252.35[c] |
| Butyric acid | ⩾0.995 | 1.39808 | 1.3978[b] | 267.9[d] | 267.45[c] |
| Pentanoic acid | ⩾0.980 | 1.40857 | 1.4080[b] | 238.7[e] | 239.35[c] |
| Hexanoic acid | ⩾0.980 | 1.41692 | 1.4170[b] | 270.7[d] | 269.55[c] |
| Heptanoic acid | ⩾0.990 | 1.42290 | 1.4230[b] | 265.6[d] | 265.65[c] |

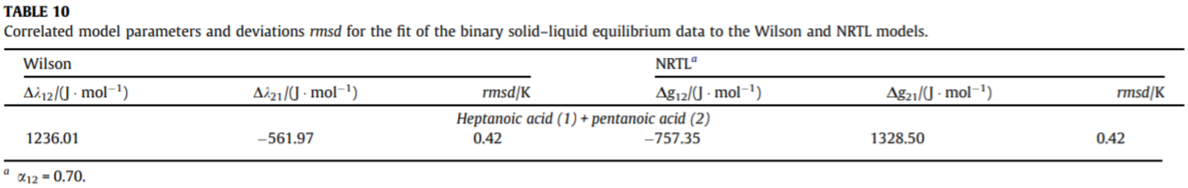


**TABLE 10**

Correlated model parameters and deviations *rmsd* for the fit of the binary solid–liquid equilibrium data to the Wilson and NRTL models.

| Wilson | | | NRTL[a] | | |
|---|---|---|---|---|---|
| $\Delta\lambda_{12}/(\mathrm{J \cdot mol^{-1}})$ | $\Delta\lambda_{21}/(\mathrm{J \cdot mol^{-1}})$ | *rmsd*/K | $\Delta g_{12}/(\mathrm{J \cdot mol^{-1}})$ | $\Delta g_{21}/(\mathrm{J \cdot mol^{-1}})$ | *rmsd*/K |
| | | *Heptanoic acid (1) + pentanoic acid (2)* | | | |
| 1236.01 | −561.97 | 0.42 | −757.35 | 1328.50 | 0.42 |

[a] $\alpha_{12} = 0.70$.

ODABRATI JEDAN MODEL

heptanoic acid + butyric acid
Margreth Tadie, Indra Bahadur, Prashant Reddy, Peterson Thokozani Ngema, Paramespri Naidoo, Nirmala Deenadayalu, Deresh Ramjugernath, Solid–liquid equilibria measurements for binary systems comprising (butyric acid + propionic or pentanoic acid) and (heptanoic acid + propionic or butyric or pentanoic or hexanoic acid), J. Chem. Thermodynamics 57 (2013) 485–492

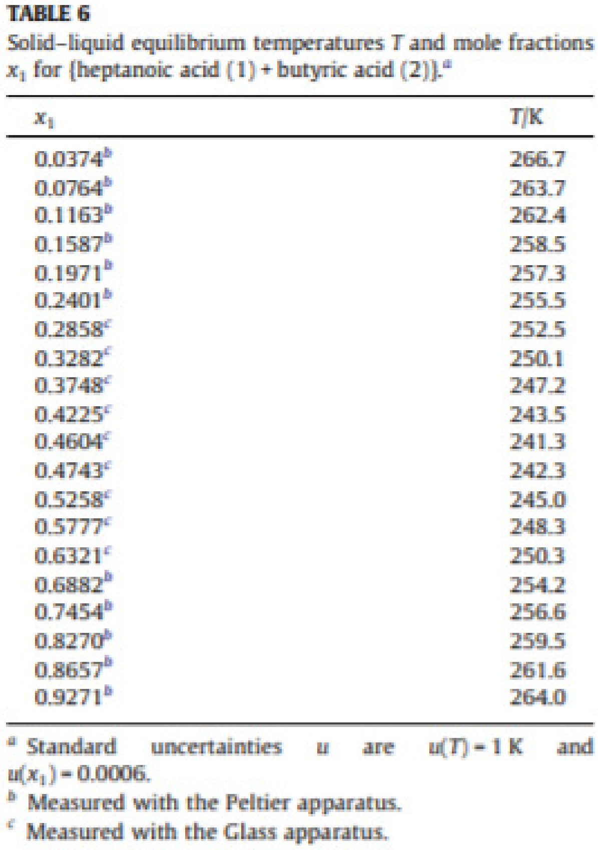


**TABLE 6**

Solid–liquid equilibrium temperatures *T* and mole fractions $x_1$ for {heptanoic acid (1) + butyric acid (2)}.[a]

| $x_1$ | T/K |
|---|---|
| 0.0374$^{b}$ | 266.7 |
| 0.0764$^{b}$ | 263.7 |
| 0.1163$^{b}$ | 262.4 |
| 0.1587$^{b}$ | 258.5 |
| 0.1971$^{b}$ | 257.3 |
| 0.2401$^{b}$ | 255.5 |
| 0.2858$^{c}$ | 252.5 |
| 0.3282$^{c}$ | 250.1 |
| 0.3748$^{c}$ | 247.2 |
| 0.4225$^{c}$ | 243.5 |
| 0.4604$^{c}$ | 241.3 |
| 0.4743$^{c}$ | 242.3 |
| 0.5258$^{c}$ | 245.0 |
| 0.5777$^{c}$ | 248.3 |
| 0.6321$^{c}$ | 250.3 |
| 0.6882$^{b}$ | 254.2 |
| 0.7454$^{b}$ | 256.6 |
| 0.8270$^{b}$ | 259.5 |
| 0.8657$^{b}$ | 261.6 |
| 0.9271$^{b}$ | 264.0 |

[a] Standard uncertainties *u* are $u(T) = 1$ K and $u(x_1) = 0.0006$.

[b] Measured with the Peltier apparatus.

[c] Measured with the Glass apparatus.

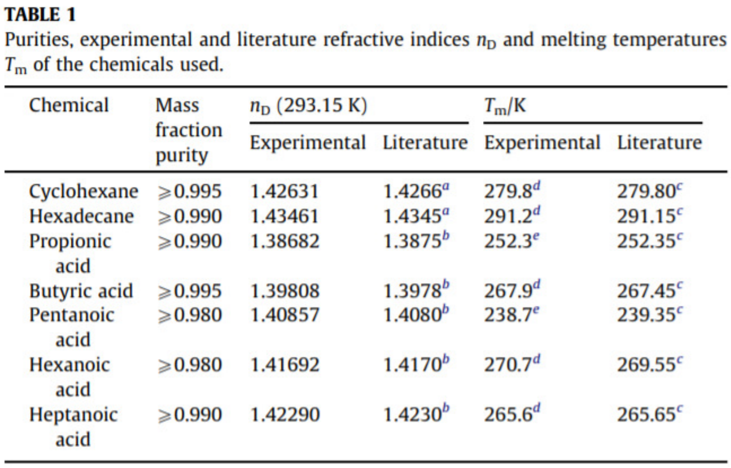


**TABLE 1**

Purities, experimental and literature refractive indices $n_D$ and melting temperatures $T_m$ of the chemicals used.

| Chemical | Mass fraction purity | $n_D$ (293.15 K) | | $T_m$/K | |
|---|---|---|---|---|---|
| | | Experimental | Literature | Experimental | Literature |
| Cyclohexane | ⩾0.995 | 1.42631 | 1.4266$^{a}$ | 279.8$^{d}$ | 279.80$^{c}$ |
| Hexadecane | ⩾0.990 | 1.43461 | 1.4345$^{a}$ | 291.2$^{d}$ | 291.15$^{c}$ |
| Propionic acid | ⩾0.990 | 1.38682 | 1.3875$^{b}$ | 252.3$^{e}$ | 252.35$^{c}$ |
| Butyric acid | ⩾0.995 | 1.39808 | 1.3978$^{b}$ | 267.9$^{d}$ | 267.45$^{c}$ |
| Pentanoic acid | ⩾0.980 | 1.40857 | 1.4080$^{b}$ | 238.7$^{e}$ | 239.35$^{c}$ |
| Hexanoic acid | ⩾0.980 | 1.41692 | 1.4170$^{b}$ | 270.7$^{d}$ | 269.55$^{c}$ |
| Heptanoic acid | ⩾0.990 | 1.42290 | 1.4230$^{b}$ | 265.6$^{d}$ | 265.65$^{c}$ |

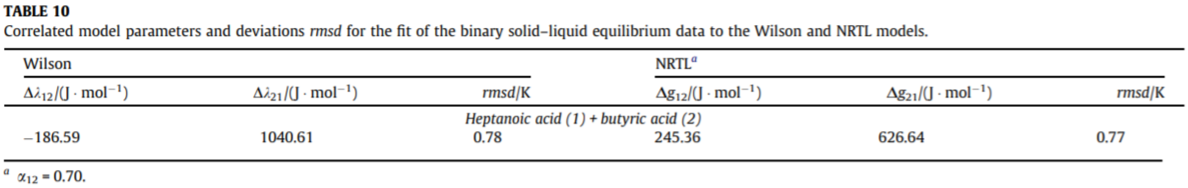


**TABLE 10**

Correlated model parameters and deviations *rmsd* for the fit of the binary solid–liquid equilibrium data to the Wilson and NRTL models.

| Wilson | | | NRTL[a] | | |
|---|---|---|---|---|---|
| $\Delta\lambda_{12}/(\mathrm{J\cdot mol^{-1}})$ | $\Delta\lambda_{21}/(\mathrm{J\cdot mol^{-1}})$ | *rmsd*/K | $\Delta g_{12}/(\mathrm{J\cdot mol^{-1}})$ | $\Delta g_{21}/(\mathrm{J\cdot mol^{-1}})$ | *rmsd*/K |
| | | *Heptanoic acid (1) + butyric acid (2)* | | | |
| −186.59 | 1040.61 | 0.78 | 245.36 | 626.64 | 0.77 |

[a] $\alpha_{12} = 0.70$.

ODABRATI JEDAN MODEL

heptanoic acid + propionic acid

Margreth Tadie, Indra Bahadur, Prashant Reddy, Peterson Thokozani Ngema, Paramespri Naidoo, Nirmala Deenadayalu, Deresh Ramjugernath, Solid–liquid equilibria measurements for binary systems comprising (butyric acid + propionic or pentanoic acid) and (heptanoic acid + propionic or butyric or pentanoic or hexanoic acid), J. Chem. Thermodynamics 57 (2013) 485–492

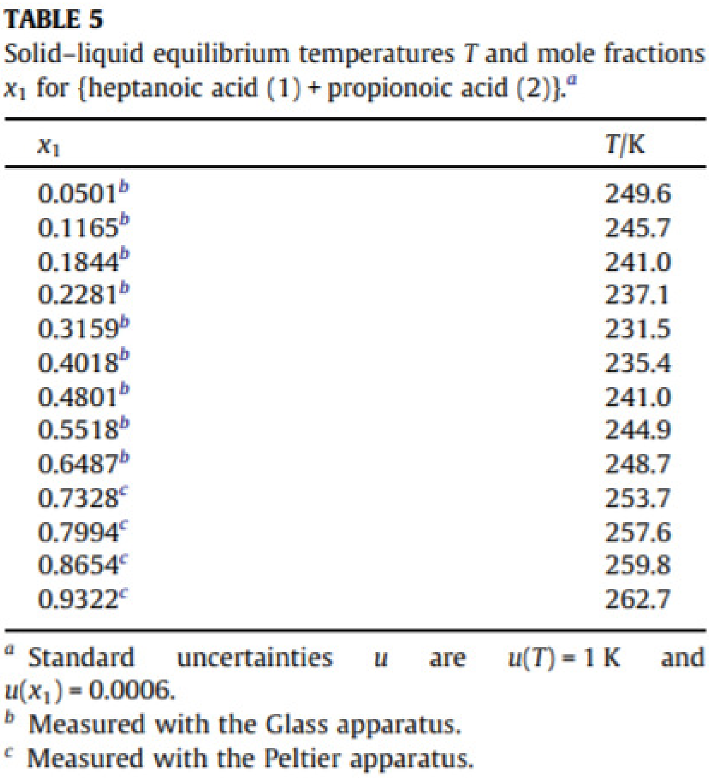


**TABLE 5**

Solid–liquid equilibrium temperatures $T$ and mole fractions $x_1$ for {heptanoic acid (1) + propionoic acid (2)}.[a]

| $x_1$ | $T$/K |
|---|---|
| 0.0501[b] | 249.6 |
| 0.1165[b] | 245.7 |
| 0.1844[b] | 241.0 |
| 0.2281[b] | 237.1 |
| 0.3159[b] | 231.5 |
| 0.4018[b] | 235.4 |
| 0.4801[b] | 241.0 |
| 0.5518[b] | 244.9 |
| 0.6487[b] | 248.7 |
| 0.7328[c] | 253.7 |
| 0.7994[c] | 257.6 |
| 0.8654[c] | 259.8 |
| 0.9322[c] | 262.7 |

[a] Standard uncertainties $u$ are $u(T) = 1$ K and $u(x_1) = 0.0006$.

[b] Measured with the Glass apparatus.

[c] Measured with the Peltier apparatus.

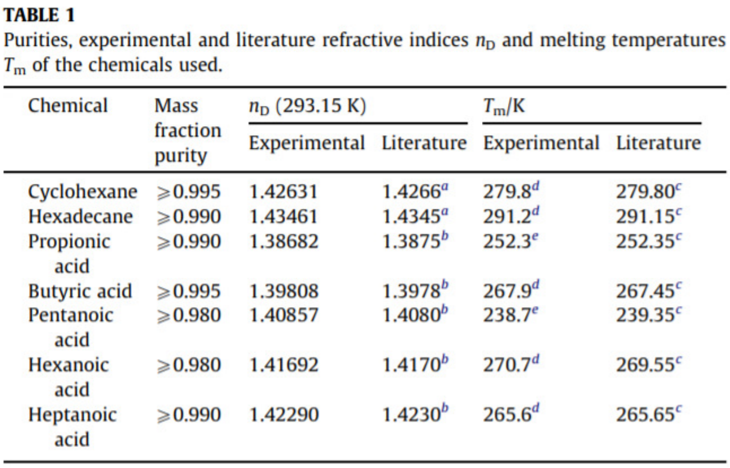


**TABLE 1**

Purities, experimental and literature refractive indices $n_D$ and melting temperatures $T_m$ of the chemicals used.

| Chemical | Mass fraction purity | $n_D$ (293.15 K) | | $T_m$/K | |
|---|---|---|---|---|---|
| | | Experimental | Literature | Experimental | Literature |
| Cyclohexane | ⩾0.995 | 1.42631 | 1.4266[a] | 279.8[d] | 279.80[c] |
| Hexadecane | ⩾0.990 | 1.43461 | 1.4345[a] | 291.2[d] | 291.15[c] |
| Propionic acid | ⩾0.990 | 1.38682 | 1.3875[b] | 252.3[e] | 252.35[c] |
| Butyric acid | ⩾0.995 | 1.39808 | 1.3978[b] | 267.9[d] | 267.45[c] |
| Pentanoic acid | ⩾0.980 | 1.40857 | 1.4080[b] | 238.7[e] | 239.35[c] |
| Hexanoic acid | ⩾0.980 | 1.41692 | 1.4170[b] | 270.7[d] | 269.55[c] |
| Heptanoic acid | ⩾0.990 | 1.42290 | 1.4230[b] | 265.6[d] | 265.65[c] |

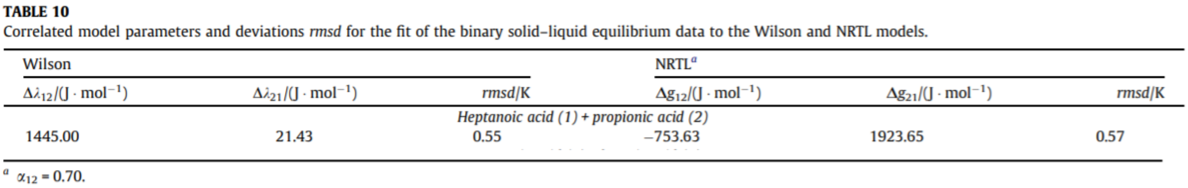


**TABLE 10**

Correlated model parameters and deviations *rmsd* for the fit of the binary solid–liquid equilibrium data to the Wilson and NRTL models.

| Wilson | | | NRTL[a] | | |
|---|---|---|---|---|---|
| $\Delta\lambda_{12}/(\text{J}\cdot\text{mol}^{-1})$ | $\Delta\lambda_{21}/(\text{J}\cdot\text{mol}^{-1})$ | *rmsd*/K | $\Delta g_{12}/(\text{J}\cdot\text{mol}^{-1})$ | $\Delta g_{21}/(\text{J}\cdot\text{mol}^{-1})$ | *rmsd*/K |
| *Heptanoic acid (1) + propionic acid (2)* | | | | | |
| 1445.00 | 21.43 | 0.55 | −753.63 | 1923.65 | 0.57 |

[a] $\alpha_{12} = 0.70$.

ODABRATI JEDAN MODEL

heptanoic acid + hexanoic acid

Margreth Tadie, Indra Bahadur, Prashant Reddy, Peterson Thokozani Ngema, Paramespri Naidoo, Nirmala Deenadayalu, Deresh Ramjugernath, Solid–liquid equilibria measurements for binary systems comprising (butyric acid + propionic or pentanoic acid) and (heptanoic acid + propionic or butyric or pentanoic or hexanoic acid), J. Chem. Thermodynamics 57 (2013) 485–492

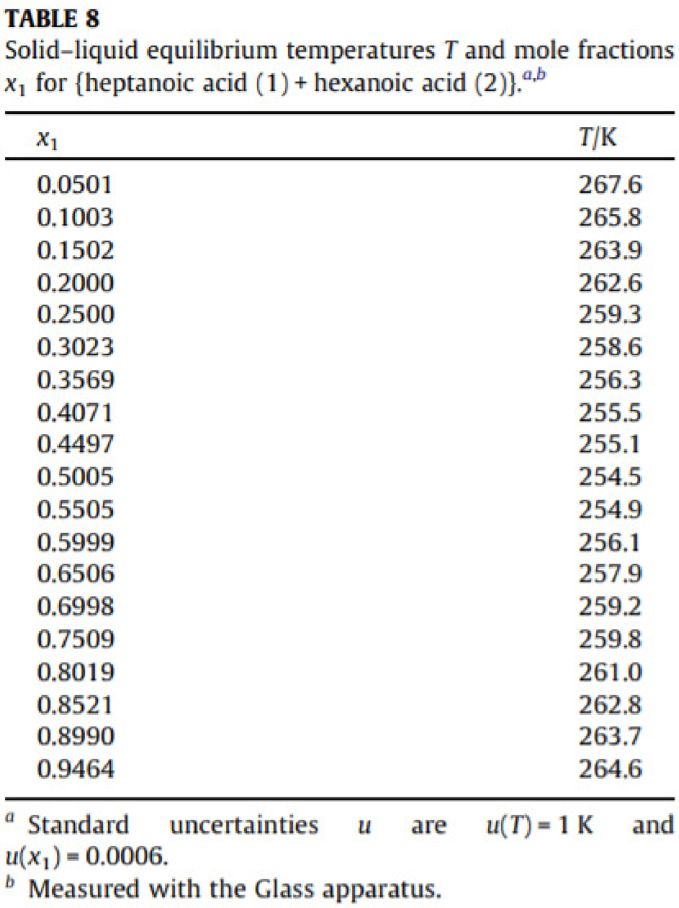


**TABLE 8**

Solid–liquid equilibrium temperatures $T$ and mole fractions $x_1$ for {heptanoic acid (1) + hexanoic acid (2)}.[a,b]

| $x_1$ | $T$/K |
|---|---|
| 0.0501 | 267.6 |
| 0.1003 | 265.8 |
| 0.1502 | 263.9 |
| 0.2000 | 262.6 |
| 0.2500 | 259.3 |
| 0.3023 | 258.6 |
| 0.3569 | 256.3 |
| 0.4071 | 255.5 |
| 0.4497 | 255.1 |
| 0.5005 | 254.5 |
| 0.5505 | 254.9 |
| 0.5999 | 256.1 |
| 0.6506 | 257.9 |
| 0.6998 | 259.2 |
| 0.7509 | 259.8 |
| 0.8019 | 261.0 |
| 0.8521 | 262.8 |
| 0.8990 | 263.7 |
| 0.9464 | 264.6 |

[a] Standard uncertainties $u$ are $u(T) = 1$ K and $u(x_1) = 0.0006$.

[b] Measured with the Glass apparatus.

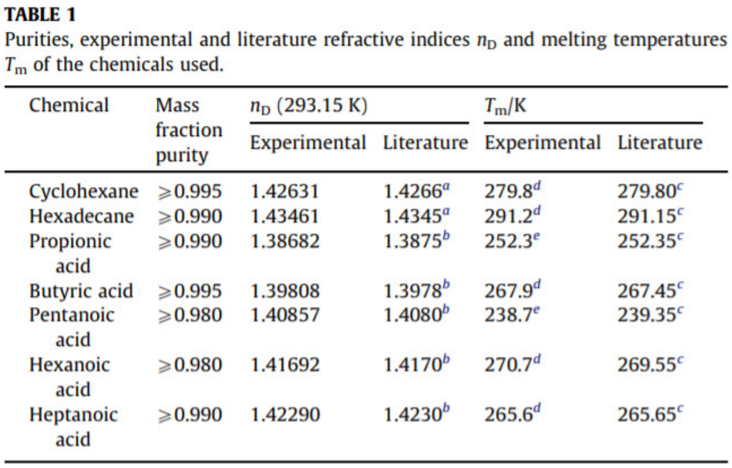


**TABLE 1**

Purities, experimental and literature refractive indices $n_D$ and melting temperatures $T_m$ of the chemicals used.

| Chemical | Mass fraction purity | $n_D$ (293.15 K) | | $T_m$/K | |
|---|---|---|---|---|---|
| | | Experimental | Literature | Experimental | Literature |
| Cyclohexane | ⩾0.995 | 1.42631 | 1.4266[a] | 279.8[d] | 279.80[c] |
| Hexadecane | ⩾0.990 | 1.43461 | 1.4345[a] | 291.2[d] | 291.15[c] |
| Propionic acid | ⩾0.990 | 1.38682 | 1.3875[b] | 252.3[e] | 252.35[c] |
| Butyric acid | ⩾0.995 | 1.39808 | 1.3978[b] | 267.9[d] | 267.45[c] |
| Pentanoic acid | ⩾0.980 | 1.40857 | 1.4080[b] | 238.7[e] | 239.35[c] |
| Hexanoic acid | ⩾0.980 | 1.41692 | 1.4170[b] | 270.7[d] | 269.55[c] |
| Heptanoic acid | ⩾0.990 | 1.42290 | 1.4230[b] | 265.6[d] | 265.65[c] |

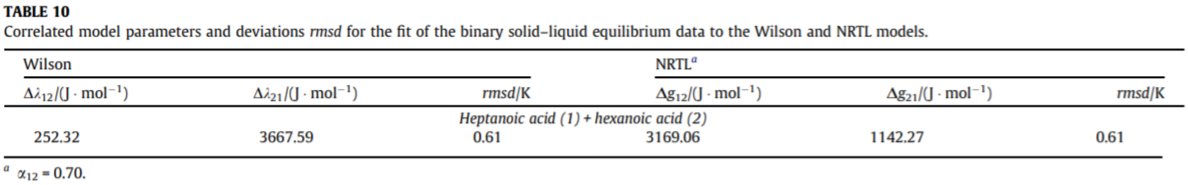


**TABLE 10**

Correlated model parameters and deviations *rmsd* for the fit of the binary solid–liquid equilibrium data to the Wilson and NRTL models.

| Wilson | | | NRTL[a] | | |
|---|---|---|---|---|---|
| $\Delta\lambda_{12}/(J \cdot mol^{-1})$ | $\Delta\lambda_{21}/(J \cdot mol^{-1})$ | *rmsd*/K | $\Delta g_{12}/(J \cdot mol^{-1})$ | $\Delta g_{21}/(J \cdot mol^{-1})$ | *rmsd*/K |
| | | *Heptanoic acid (1) + hexanoic acid (2)* | | | |
| 252.32 | 3667.59 | 0.61 | 3169.06 | 1142.27 | 0.61 |

[a] $\alpha_{12} = 0.70$.

ODABRATI JEDAN MODEL

stearic acid + adipic acid

Guixiang Ma, Jinhe Sun, Shaolei Xie, Zhao Wang, Yan Jing, Yongzhong Jia, Solid-liquid phase equilibria of stearic acid and dicarboxylic acids binary mixtures as low temperature thermal energy storage materials, The Journal of Chemical Thermodynamics, Volume 120, May 2018, Pages 60-71

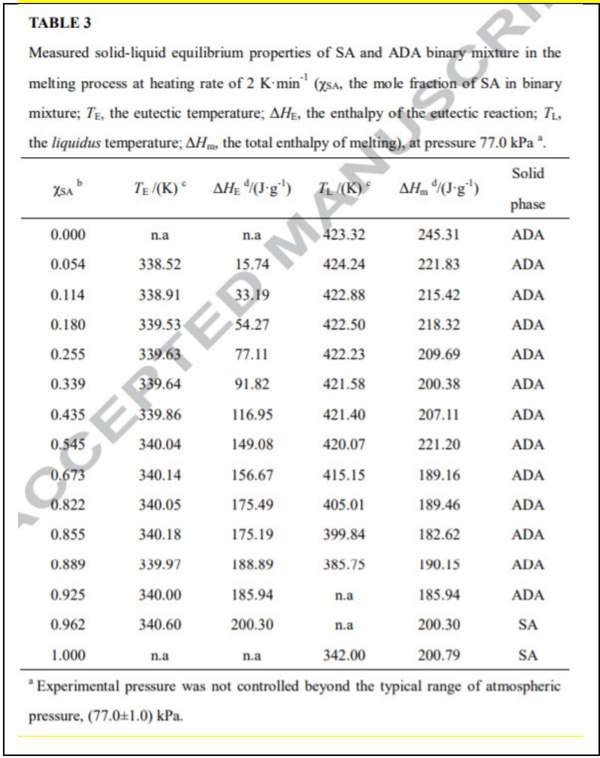


**TABLE 3**

Measured solid-liquid equilibrium properties of SA and ADA binary mixture in the melting process at heating rate of 2 K·min$^{-1}$ ($\chi_{SA}$, the mole fraction of SA in binary mixture; $T_E$, the eutectic temperature; $\Delta H_E$, the enthalpy of the eutectic reaction; $T_L$, the *liquidus* temperature; $\Delta H_m$, the total enthalpy of melting), at pressure 77.0 kPa [a].

| $\chi_{SA}$ [b] | $T_E$ /(K) [c] | $\Delta H_E$ [d]/(J·g$^{-1}$) | $T_L$ /(K) [c] | $\Delta H_m$ [d]/(J·g$^{-1}$) | Solid phase |
|---|---|---|---|---|---|
| 0.000 | n.a | n.a | 423.32 | 245.31 | ADA |
| 0.054 | 338.52 | 15.74 | 424.24 | 221.83 | ADA |
| 0.114 | 338.91 | 33.19 | 422.88 | 215.42 | ADA |
| 0.180 | 339.53 | 54.27 | 422.50 | 218.32 | ADA |
| 0.255 | 339.63 | 77.11 | 422.23 | 209.69 | ADA |
| 0.339 | 339.64 | 91.82 | 421.58 | 200.38 | ADA |
| 0.435 | 339.86 | 116.95 | 421.40 | 207.11 | ADA |
| 0.545 | 340.04 | 149.08 | 420.07 | 221.20 | ADA |
| 0.673 | 340.14 | 156.67 | 415.15 | 189.16 | ADA |
| 0.822 | 340.05 | 175.49 | 405.01 | 189.46 | ADA |
| 0.855 | 340.18 | 175.19 | 399.84 | 182.62 | ADA |
| 0.889 | 339.97 | 188.89 | 385.75 | 190.15 | ADA |
| 0.925 | 340.00 | 185.94 | n.a | 185.94 | ADA |
| 0.962 | 340.60 | 200.30 | n.a | 200.30 | SA |
| 1.000 | n.a | n.a | 342.00 | 200.79 | SA |

[a] Experimental pressure was not controlled beyond the typical range of atmospheric pressure, (77.0±1.0) kPa.

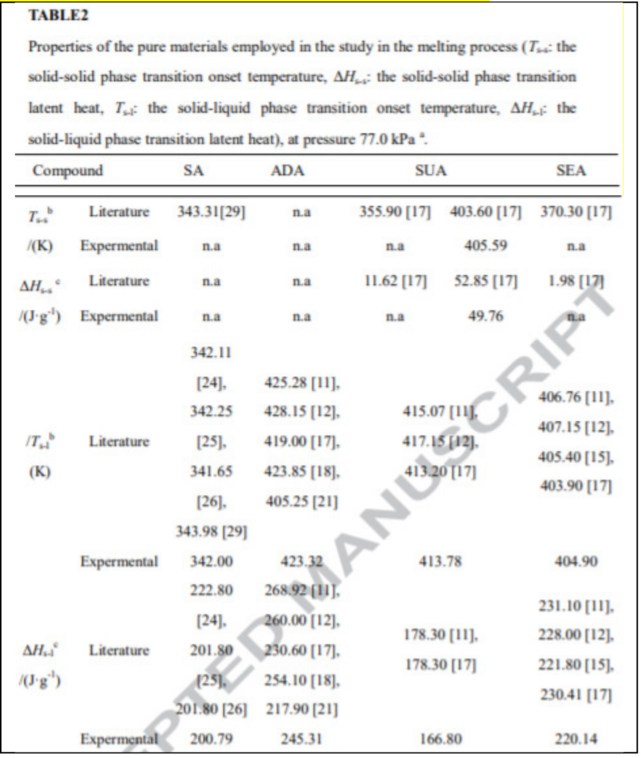


**TABLE2**

Properties of the pure materials employed in the study in the melting process ($T_{s\text{-}s}$: the solid-solid phase transition onset temperature, $\Delta H_{s\text{-}s}$: the solid-solid phase transition latent heat, $T_{s\text{-}l}$: the solid-liquid phase transition onset temperature, $\Delta H_{s\text{-}l}$: the solid-liquid phase transition latent heat), at pressure 77.0 kPa [a].

| Compound | | SA | ADA | SUA | | SEA |
|---|---|---|---|---|---|---|
| $T_{s\text{-}s}$ [b] /(K) | Literature | 343.31[29] | n.a | 355.90 [17] | 403.60 [17] | 370.30 [17] |
| | Expermental | n.a | n.a | n.a | 405.59 | n.a |
| $\Delta H_{s\text{-}s}$ [c] /(J·g$^{-1}$) | Literature | n.a | n.a | 11.62 [17] | 52.85 [17] | 1.98 [17] |
| | Expermental | n.a | n.a | n.a | 49.76 | n.a |
| /$T_{s\text{-}l}$ [b] (K) | Literature | 342.11 [24],<br>342.25 [25],<br>341.65 [26],<br>343.98 [29] | 425.28 [11],<br>428.15 [12],<br>419.00 [17],<br>423.85 [18],<br>405.25 [21] | 415.07 [11],<br>417.15 [12],<br>413.20 [17] | | 406.76 [11],<br>407.15 [12],<br>405.40 [15],<br>403.90 [17] |
| | Expermental | 342.00 | 423.32 | 413.78 | | 404.90 |
| $\Delta H_{s\text{-}l}$ [c] /(J·g$^{-1}$) | Literature | 222.80 [24],<br>201.80 [25],<br>201.80 [26] | 268.92 [11],<br>260.00 [12],<br>230.60 [17],<br>254.10 [18],<br>217.90 [21] | 178.30 [11],<br>178.30 [17] | | 231.10 [11],<br>228.00 [12],<br>221.80 [15],<br>230.41 [17] |
| | Expermental | 200.79 | 245.31 | 166.80 | | 220.14 |

stearic acid + suberic acid

Guixiang Ma, Jinhe Sun, Shaolei Xie, Zhao Wang, Yan Jing, Yongzhong Jia, Solid-liquid phase equilibria of stearic acid and dicarboxylic acids binary mixtures as low temperature thermal energy storage materials, The Journal of Chemical Thermodynamics, Volume 120, May 2018, Pages 60-71

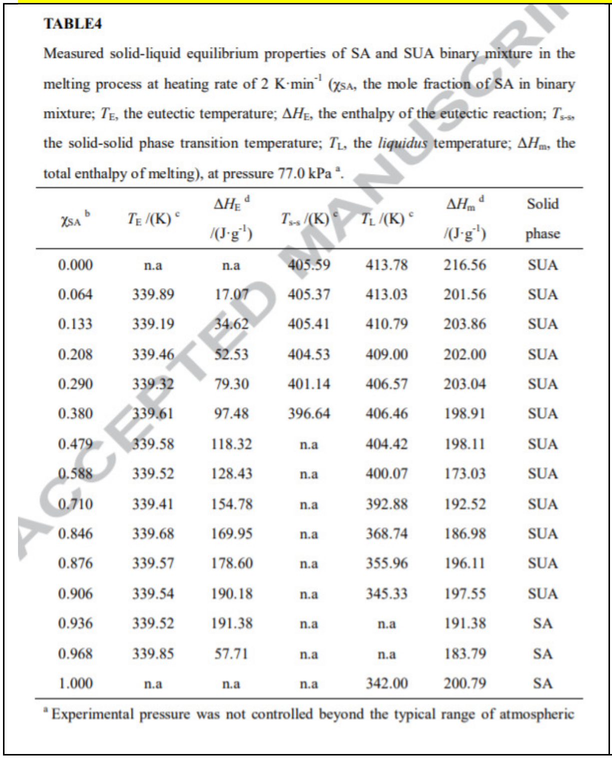


**TABLE4**

Measured solid-liquid equilibrium properties of SA and SUA binary mixture in the melting process at heating rate of 2 K·min$^{-1}$ ($\chi_{SA}$, the mole fraction of SA in binary mixture; $T_E$, the eutectic temperature; $\Delta H_E$, the enthalpy of the eutectic reaction; $T_{s\text{-}s}$, the solid-solid phase transition temperature; $T_L$, the *liquidus* temperature; $\Delta H_m$, the total enthalpy of melting), at pressure 77.0 kPa [a].

| $\chi_{SA}$ [b] | $T_E$ /(K) [c] | $\Delta H_E$ [d] /(J·g$^{-1}$) | $T_{s\text{-}s}$ /(K) [c] | $T_L$ /(K) [c] | $\Delta H_m$ [d] /(J·g$^{-1}$) | Solid phase |
|---|---|---|---|---|---|---|
| 0.000 | n.a | n.a | 405.59 | 413.78 | 216.56 | SUA |
| 0.064 | 339.89 | 17.07 | 405.37 | 413.03 | 201.56 | SUA |
| 0.133 | 339.19 | 34.62 | 405.41 | 410.79 | 203.86 | SUA |
| 0.208 | 339.46 | 52.53 | 404.53 | 409.00 | 202.00 | SUA |
| 0.290 | 339.32 | 79.30 | 401.14 | 406.57 | 203.04 | SUA |
| 0.380 | 339.61 | 97.48 | 396.64 | 406.46 | 198.91 | SUA |
| 0.479 | 339.58 | 118.32 | n.a | 404.42 | 198.11 | SUA |
| 0.588 | 339.52 | 128.43 | n.a | 400.07 | 173.03 | SUA |
| 0.710 | 339.41 | 154.78 | n.a | 392.88 | 192.52 | SUA |
| 0.846 | 339.68 | 169.95 | n.a | 368.74 | 186.98 | SUA |
| 0.876 | 339.57 | 178.60 | n.a | 355.96 | 196.11 | SUA |
| 0.906 | 339.54 | 190.18 | n.a | 345.33 | 197.55 | SUA |
| 0.936 | 339.52 | 191.38 | n.a | n.a | 191.38 | SA |
| 0.968 | 339.85 | 57.71 | n.a | n.a | 183.79 | SA |
| 1.000 | n.a | n.a | n.a | 342.00 | 200.79 | SA |

[a] Experimental pressure was not controlled beyond the typical range of atmospheric

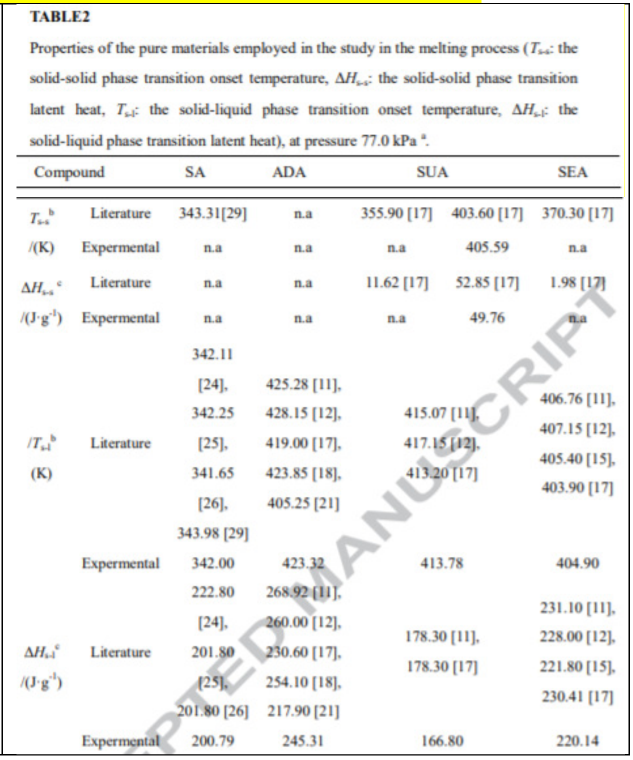


**TABLE2**

Properties of the pure materials employed in the study in the melting process ($T_{s\text{-}s}$: the solid-solid phase transition onset temperature, $\Delta H_{s\text{-}s}$: the solid-solid phase transition latent heat, $T_{s\text{-}l}$: the solid-liquid phase transition onset temperature, $\Delta H_{s\text{-}l}$: the solid-liquid phase transition latent heat), at pressure 77.0 kPa [a].

| Compound | | SA | ADA | SUA | | SEA |
|---|---|---|---|---|---|---|
| $T_{s\text{-}s}$ [b] /(K) | Literature | 343.31[29] | n.a | 355.90 [17] | 403.60 [17] | 370.30 [17] |
| | Expermental | n.a | n.a | n.a | 405.59 | n.a |
| $\Delta H_{s\text{-}s}$ [c] /(J·g$^{-1}$) | Literature | n.a | n.a | 11.62 [17] | 52.85 [17] | 1.98 [17] |
| | Expermental | n.a | n.a | n.a | 49.76 | n.a |
| /$T_{s\text{-}l}$ [b] (K) | Literature | 342.11 [24], 342.25 [25], 341.65 [26], 343.98 [29] | 425.28 [11],<br>428.15 [12],<br>419.00 [17],<br>423.85 [18],<br>405.25 [21] | 415.07 [11],<br>417.15 [12],<br>413.20 [17] | | 406.76 [11],<br>407.15 [12],<br>405.40 [15],<br>403.90 [17] |
| | Expermental | 342.00 | 423.32 | 413.78 | | 404.90 |
| $\Delta H_{s\text{-}l}$ [c] /(J·g$^{-1}$) | Literature | 222.80 [24], 201.80 [25], 201.80 [26] | 268.92 [11],<br>260.00 [12],<br>230.60 [17],<br>254.10 [18],<br>217.90 [21] | 178.30 [11],<br>178.30 [17] | | 231.10 [11],<br>228.00 [12],<br>221.80 [15],<br>230.41 [17] |
| | Expermental | 200.79 | 245.31 | 166.80 | | 220.14 |

stearic acid + sebacic acid
Guixiang Ma, Jinhe Sun, Shaolei Xie, Zhao Wang, Yan Jing, Yongzhong Jia, Solid-liquid phase equilibria of stearic acid and dicarboxylic acids binary mixtures as low temperature thermal energy storage materials, The Journal of Chemical Thermodynamics, Volume 120, May 2018, Pages 60-71

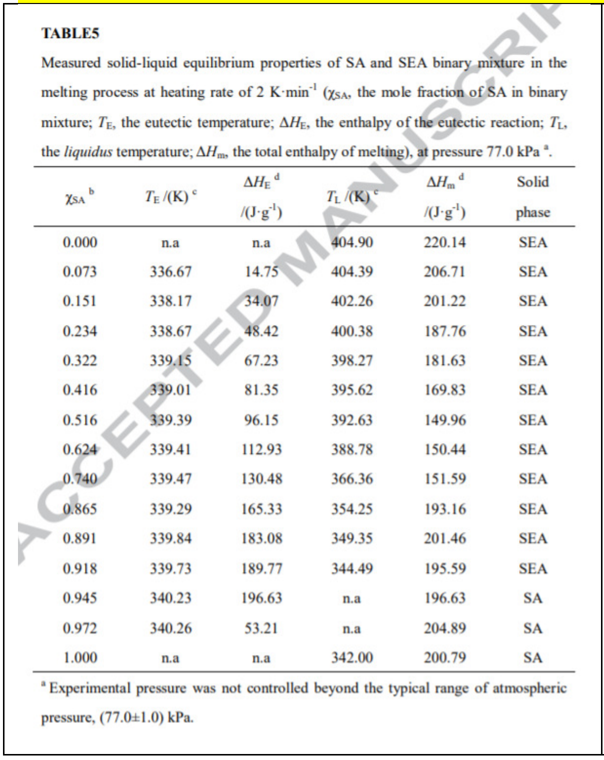


**TABLE5**

Measured solid-liquid equilibrium properties of SA and SEA binary mixture in the melting process at heating rate of 2 K·min$^{-1}$ ($\chi_{SA}$, the mole fraction of SA in binary mixture; $T_E$, the eutectic temperature; $\Delta H_E$, the enthalpy of the eutectic reaction; $T_L$, the *liquidus* temperature; $\Delta H_m$, the total enthalpy of melting), at pressure 77.0 kPa [a].

| $\chi_{SA}$ [b] | $T_E$ /(K) [c] | $\Delta H_E$ [d] /(J·g$^{-1}$) | $T_L$ /(K) [c] | $\Delta H_m$ [d] /(J·g$^{-1}$) | Solid phase |
|---|---|---|---|---|---|
| 0.000 | n.a | n.a | 404.90 | 220.14 | SEA |
| 0.073 | 336.67 | 14.75 | 404.39 | 206.71 | SEA |
| 0.151 | 338.17 | 34.07 | 402.26 | 201.22 | SEA |
| 0.234 | 338.67 | 48.42 | 400.38 | 187.76 | SEA |
| 0.322 | 339.15 | 67.23 | 398.27 | 181.63 | SEA |
| 0.416 | 339.01 | 81.35 | 395.62 | 169.83 | SEA |
| 0.516 | 339.39 | 96.15 | 392.63 | 149.96 | SEA |
| 0.624 | 339.41 | 112.93 | 388.78 | 150.44 | SEA |
| 0.740 | 339.47 | 130.48 | 366.36 | 151.59 | SEA |
| 0.865 | 339.29 | 165.33 | 354.25 | 193.16 | SEA |
| 0.891 | 339.84 | 183.08 | 349.35 | 201.46 | SEA |
| 0.918 | 339.73 | 189.77 | 344.49 | 195.59 | SEA |
| 0.945 | 340.23 | 196.63 | n.a | 196.63 | SA |
| 0.972 | 340.26 | 53.21 | n.a | 204.89 | SA |
| 1.000 | n.a | n.a | 342.00 | 200.79 | SA |

[a] Experimental pressure was not controlled beyond the typical range of atmospheric pressure, (77.0±1.0) kPa.

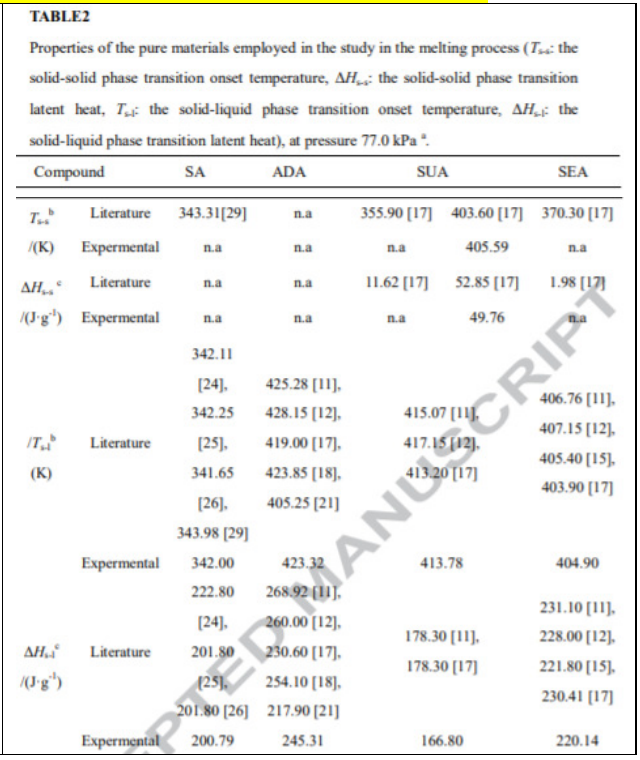


**TABLE2**

Properties of the pure materials employed in the study in the melting process ($T_{s\text{-}s}$: the solid-solid phase transition onset temperature, $\Delta H_{s\text{-}s}$: the solid-solid phase transition latent heat, $T_{s\text{-}l}$: the solid-liquid phase transition onset temperature, $\Delta H_{s\text{-}l}$: the solid-liquid phase transition latent heat), at pressure 77.0 kPa [a].

| Compound | | SA | ADA | SUA | | SEA |
|---|---|---|---|---|---|---|
| $T_{s\text{-}s}$ [b] /(K) | Literature | 343.31[29] | n.a | 355.90 [17] | 403.60 [17] | 370.30 [17] |
| | Expermental | n.a | n.a | n.a | 405.59 | n.a |
| $\Delta H_{s\text{-}s}$ [c] /(J·g$^{-1}$) | Literature | n.a | n.a | 11.62 [17] | 52.85 [17] | 1.98 [17] |
| | Expermental | n.a | n.a | n.a | 49.76 | n.a |
| /$T_{s\text{-}l}$ [b] (K) | Literature | 342.11 [24],<br>342.25 [25],<br>341.65 [26],<br>343.98 [29] | 425.28 [11],<br>428.15 [12],<br>419.00 [17],<br>423.85 [18],<br>405.25 [21] | 415.07 [11],<br>417.15 [12],<br>413.20 [17] | | 406.76 [11],<br>407.15 [12],<br>405.40 [15],<br>403.90 [17] |
| | Expermental | 342.00 | 423.32 | 413.78 | | 404.90 |
| $\Delta H_{s\text{-}l}$ [c] /(J·g$^{-1}$) | Literature | 222.80 [24],<br>201.80 [25],<br>201.80 [26] | 268.92 [11],<br>260.00 [12],<br>230.60 [17],<br>254.10 [18],<br>217.90 [21] | 178.30 [11],<br>178.30 [17] | | 231.10 [11],<br>228.00 [12],<br>221.80 [15],<br>230.41 [17] |
| | Expermental | 200.79 | 245.31 | 166.80 | | 220.14 |

phenantrene + *o*-dichlorobenzene
Dongwei Wei, (Solid+liquid) equilibria of (phenanthrene+dichlorobenzenes), Thermochimica Acta 479 (2008) 32–36

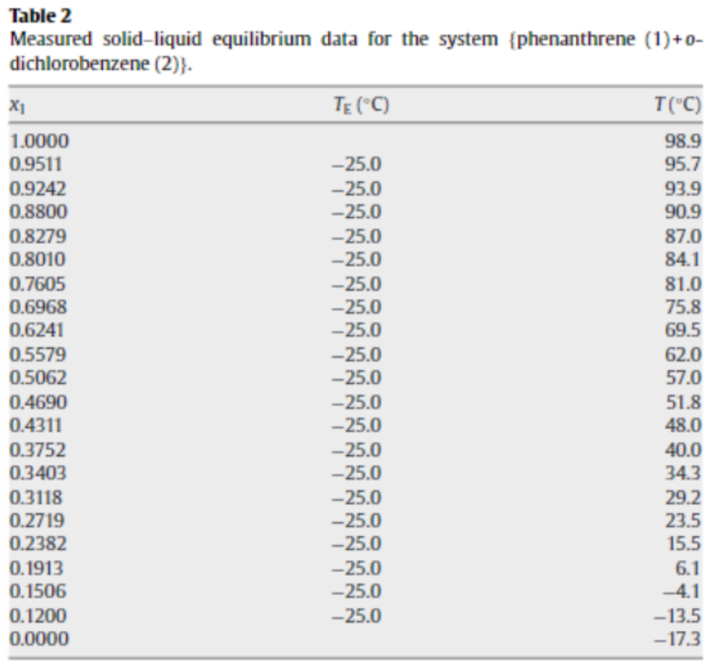


**Table 2**
Measured solid–liquid equilibrium data for the system {phenanthrene (1) + *o*-dichlorobenzene (2)}.

| $x_1$ | $T_E$ (°C) | $T$ (°C) |
|---|---|---|
| 1.0000 | | 98.9 |
| 0.9511 | −25.0 | 95.7 |
| 0.9242 | −25.0 | 93.9 |
| 0.8800 | −25.0 | 90.9 |
| 0.8279 | −25.0 | 87.0 |
| 0.8010 | −25.0 | 84.1 |
| 0.7605 | −25.0 | 81.0 |
| 0.6968 | −25.0 | 75.8 |
| 0.6241 | −25.0 | 69.5 |
| 0.5579 | −25.0 | 62.0 |
| 0.5062 | −25.0 | 57.0 |
| 0.4690 | −25.0 | 51.8 |
| 0.4311 | −25.0 | 48.0 |
| 0.3752 | −25.0 | 40.0 |
| 0.3403 | −25.0 | 34.3 |
| 0.3118 | −25.0 | 29.2 |
| 0.2719 | −25.0 | 23.5 |
| 0.2382 | −25.0 | 15.5 |
| 0.1913 | −25.0 | 6.1 |
| 0.1506 | −25.0 | −4.1 |
| 0.1200 | −25.0 | −13.5 |
| 0.0000 | | −17.3 |

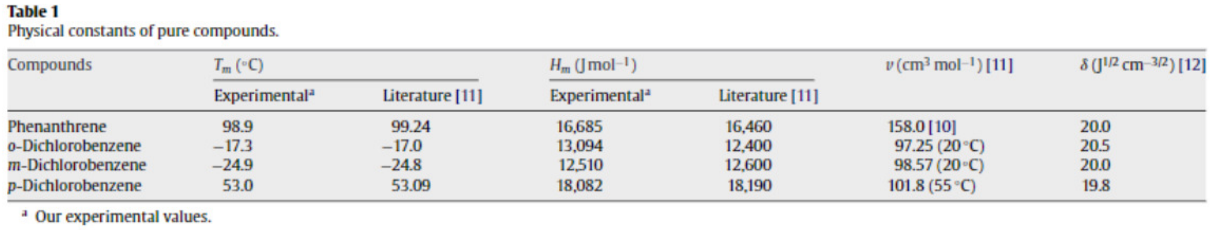


**Table 1**
Physical constants of pure compounds.

| Compounds | $T_m$ (°C) | | $H_m$ (J mol$^{-1}$) | | $v$ (cm$^3$ mol$^{-1}$) [11] | $\delta$ (J$^{1/2}$ cm$^{-3/2}$) [12] |
|---|---|---|---|---|---|---|
| | Experimental[a] | Literature [11] | Experimental[a] | Literature [11] | | |
| Phenanthrene | 98.9 | 99.24 | 16,685 | 16,460 | 158.0 [10] | 20.0 |
| *o*-Dichlorobenzene | −17.3 | −17.0 | 13,094 | 12,400 | 97.25 (20 °C) | 20.5 |
| *m*-Dichlorobenzene | −24.9 | −24.8 | 12,510 | 12,600 | 98.57 (20 °C) | 20.0 |
| *p*-Dichlorobenzene | 53.0 | 53.09 | 18,082 | 18,190 | 101.8 (55 °C) | 19.8 |

[a] Our experimental values.

phenantrene + *p*-dichlorobenzene
Dongwei Wei, (Solid+liquid) equilibria of (phenanthrene+dichlorobenzenes), Thermochimica Acta 479 (2008) 32–36

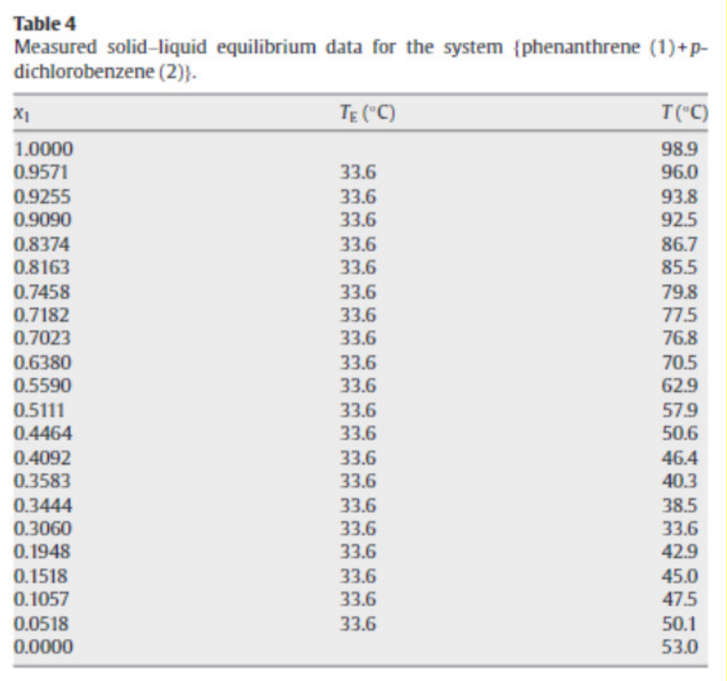


**Table 4**
Measured solid–liquid equilibrium data for the system {phenanthrene (1) + *p*-dichlorobenzene (2)}.

| $x_1$ | $T_E$ (°C) | $T$ (°C) |
|---|---|---|
| 1.0000 | | 98.9 |
| 0.9571 | 33.6 | 96.0 |
| 0.9255 | 33.6 | 93.8 |
| 0.9090 | 33.6 | 92.5 |
| 0.8374 | 33.6 | 86.7 |
| 0.8163 | 33.6 | 85.5 |
| 0.7458 | 33.6 | 79.8 |
| 0.7182 | 33.6 | 77.5 |
| 0.7023 | 33.6 | 76.8 |
| 0.6380 | 33.6 | 70.5 |
| 0.5590 | 33.6 | 62.9 |
| 0.5111 | 33.6 | 57.9 |
| 0.4464 | 33.6 | 50.6 |
| 0.4092 | 33.6 | 46.4 |
| 0.3583 | 33.6 | 40.3 |
| 0.3444 | 33.6 | 38.5 |
| 0.3060 | 33.6 | 33.6 |
| 0.1948 | 33.6 | 42.9 |
| 0.1518 | 33.6 | 45.0 |
| 0.1057 | 33.6 | 47.5 |
| 0.0518 | 33.6 | 50.1 |
| 0.0000 | | 53.0 |

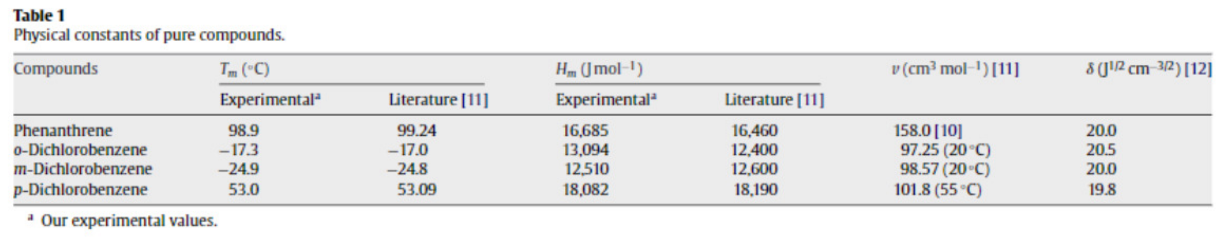


**Table 1**
Physical constants of pure compounds.

| Compounds | $T_m$ (°C) | | $H_m$ (J mol$^{-1}$) | | $v$ (cm$^3$ mol$^{-1}$) [11] | $\delta$ (J$^{1/2}$ cm$^{-3/2}$) [12] |
|---|---|---|---|---|---|---|
| | Experimental[a] | Literature [11] | Experimental[a] | Literature [11] | | |
| Phenanthrene | 98.9 | 99.24 | 16,685 | 16,460 | 158.0 [10] | 20.0 |
| *o*-Dichlorobenzene | −17.3 | −17.0 | 13,094 | 12,400 | 97.25 (20 °C) | 20.5 |
| *m*-Dichlorobenzene | −24.9 | −24.8 | 12,510 | 12,600 | 98.57 (20 °C) | 20.0 |
| *p*-Dichlorobenzene | 53.0 | 53.09 | 18,082 | 18,190 | 101.8 (55 °C) | 19.8 |

[a] Our experimental values.

phenantrene + *m*-dichlorobenzene
Dongwei Wei, (Solid+liquid) equilibria of (phenanthrene+dichlorobenzenes), Thermochimica Acta 479 (2008) 32–36

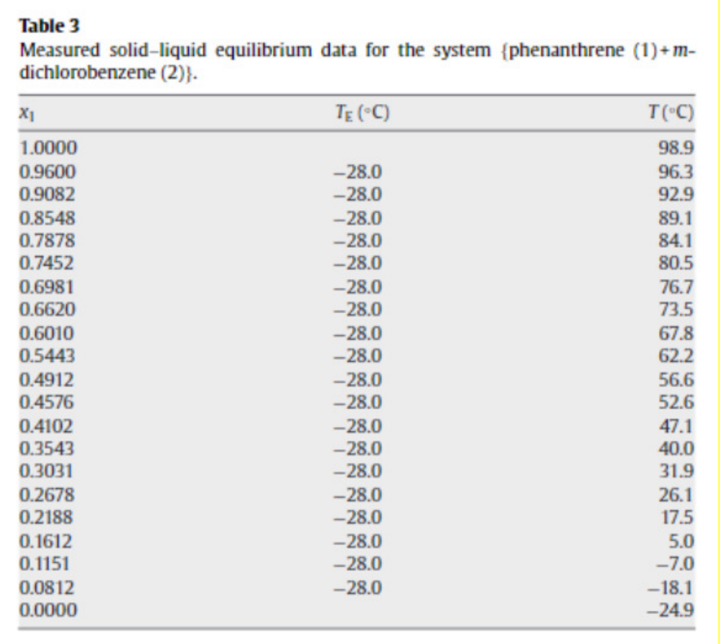


**Table 3**
Measured solid–liquid equilibrium data for the system {phenanthrene (1) + *m*-dichlorobenzene (2)}.

| $x_1$ | $T_E$ (°C) | $T$ (°C) |
|---|---|---|
| 1.0000 | | 98.9 |
| 0.9600 | −28.0 | 96.3 |
| 0.9082 | −28.0 | 92.9 |
| 0.8548 | −28.0 | 89.1 |
| 0.7878 | −28.0 | 84.1 |
| 0.7452 | −28.0 | 80.5 |
| 0.6981 | −28.0 | 76.7 |
| 0.6620 | −28.0 | 73.5 |
| 0.6010 | −28.0 | 67.8 |
| 0.5443 | −28.0 | 62.2 |
| 0.4912 | −28.0 | 56.6 |
| 0.4576 | −28.0 | 52.6 |
| 0.4102 | −28.0 | 47.1 |
| 0.3543 | −28.0 | 40.0 |
| 0.3031 | −28.0 | 31.9 |
| 0.2678 | −28.0 | 26.1 |
| 0.2188 | −28.0 | 17.5 |
| 0.1612 | −28.0 | 5.0 |
| 0.1151 | −28.0 | −7.0 |
| 0.0812 | −28.0 | −18.1 |
| 0.0000 | | −24.9 |

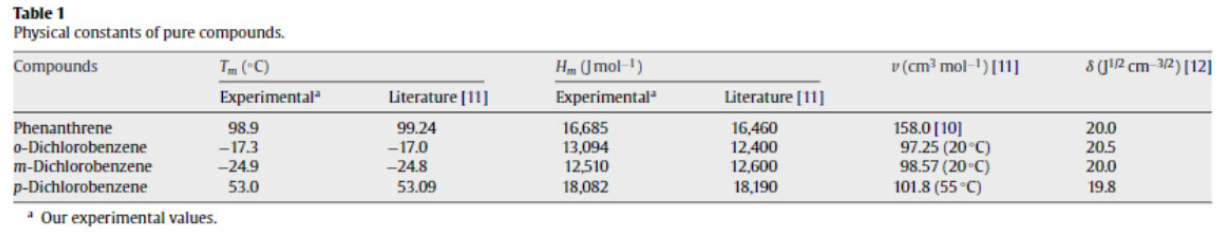


**Table 1**
Physical constants of pure compounds.

| Compounds | $T_m$ (°C) | | $H_m$ (J mol$^{-1}$) | | $v$ (cm$^3$ mol$^{-1}$) [11] | $\delta$ (J$^{1/2}$ cm$^{-3/2}$) [12] |
|---|---|---|---|---|---|---|
| | Experimental[a] | Literature [11] | Experimental[a] | Literature [11] | | |
| Phenanthrene | 98.9 | 99.24 | 16,685 | 16,460 | 158.0 [10] | 20.0 |
| *o*-Dichlorobenzene | −17.3 | −17.0 | 13,094 | 12,400 | 97.25 (20 °C) | 20.5 |
| *m*-Dichlorobenzene | −24.9 | −24.8 | 12,510 | 12,600 | 98.57 (20 °C) | 20.0 |
| *p*-Dichlorobenzene | 53.0 | 53.09 | 18,082 | 18,190 | 101.8 (55 °C) | 19.8 |

[a] Our experimental values.

*N*,*N*,*N'*,*N'*-tetramethylethylenediamine + *n*-heptane

Farida AllalAbdallah Dahmani, Measurement and prediction of solid–liquid phase equilibriafor diamine+*n*-heptane, or cyclohexane, Fluid Phase Equilibria 190 (2001) 33–45

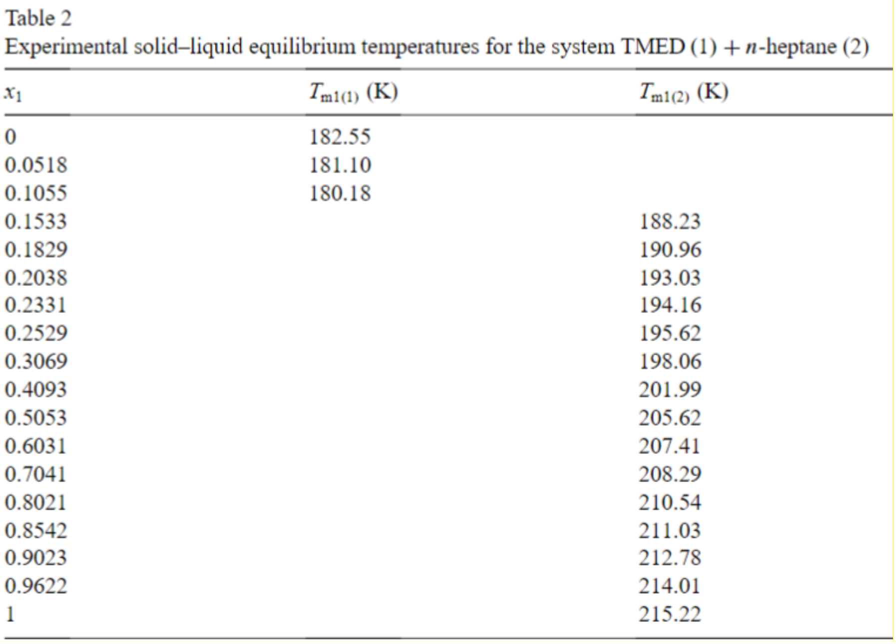


Table 2

Experimental solid–liquid equilibrium temperatures for the system TMED (1) + *n*-heptane (2)

| $x_1$ | $T_{m1(1)}$ (K) | $T_{m1(2)}$ (K) |
|---|---|---|
| 0 | 182.55 | |
| 0.0518 | 181.10 | |
| 0.1055 | 180.18 | |
| 0.1533 | | 188.23 |
| 0.1829 | | 190.96 |
| 0.2038 | | 193.03 |
| 0.2331 | | 194.16 |
| 0.2529 | | 195.62 |
| 0.3069 | | 198.06 |
| 0.4093 | | 201.99 |
| 0.5053 | | 205.62 |
| 0.6031 | | 207.41 |
| 0.7041 | | 208.29 |
| 0.8021 | | 210.54 |
| 0.8542 | | 211.03 |
| 0.9023 | | 212.78 |
| 0.9622 | | 214.01 |
| 1 | | 215.22 |

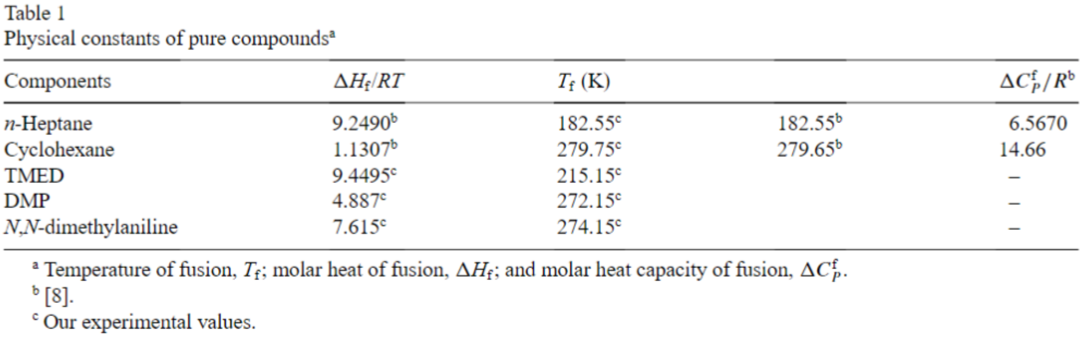


Table 1

Physical constants of pure compounds[a]

| Components | $\Delta H_f/RT$ | $T_f$ (K) | | $\Delta C_P^f/R$[b] |
|---|---|---|---|---|
| *n*-Heptane | 9.2490[b] | 182.55[c] | 182.55[b] | 6.5670 |
| Cyclohexane | 1.1307[b] | 279.75[c] | 279.65[b] | 14.66 |
| TMED | 9.4495[c] | 215.15[c] | | – |
| DMP | 4.887[c] | 272.15[c] | | – |
| *N*,*N*-dimethylaniline | 7.615[c] | 274.15[c] | | – |

[a] Temperature of fusion, $T_f$; molar heat of fusion, $\Delta H_f$; and molar heat capacity of fusion, $\Delta C_P^f$.

[b] [8].

[c] Our experimental values.

*N*,*N*,*N*’,*N*’-tetramethylethylenediamine + cyclohexane
Farida AllalAbdallah Dahmani, Measurement and prediction of solid–liquid phase equilibriafor diamine+*n*-heptane, or cyclohexane, Fluid Phase Equilibria 190 (2001) 33–45

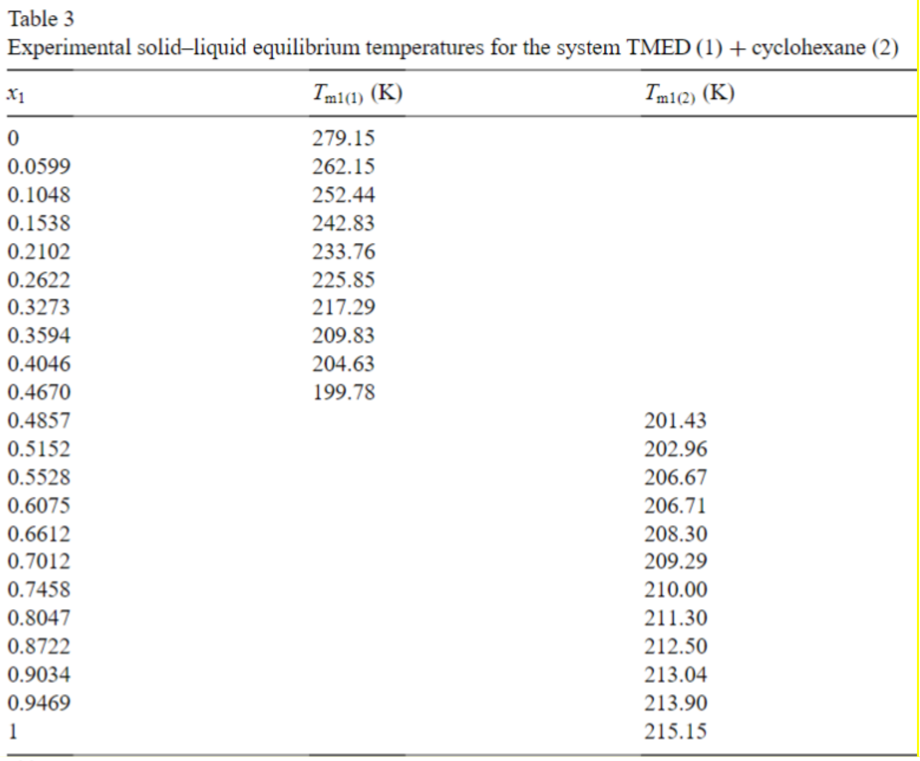


Table 3
Experimental solid–liquid equilibrium temperatures for the system TMED (1) + cyclohexane (2)

| $x_1$ | $T_{m1(1)}$ (K) | $T_{m1(2)}$ (K) |
|---|---|---|
| 0 | 279.15 | |
| 0.0599 | 262.15 | |
| 0.1048 | 252.44 | |
| 0.1538 | 242.83 | |
| 0.2102 | 233.76 | |
| 0.2622 | 225.85 | |
| 0.3273 | 217.29 | |
| 0.3594 | 209.83 | |
| 0.4046 | 204.63 | |
| 0.4670 | 199.78 | |
| 0.4857 | | 201.43 |
| 0.5152 | | 202.96 |
| 0.5528 | | 206.67 |
| 0.6075 | | 206.71 |
| 0.6612 | | 208.30 |
| 0.7012 | | 209.29 |
| 0.7458 | | 210.00 |
| 0.8047 | | 211.30 |
| 0.8722 | | 212.50 |
| 0.9034 | | 213.04 |
| 0.9469 | | 213.90 |
| 1 | | 215.15 |

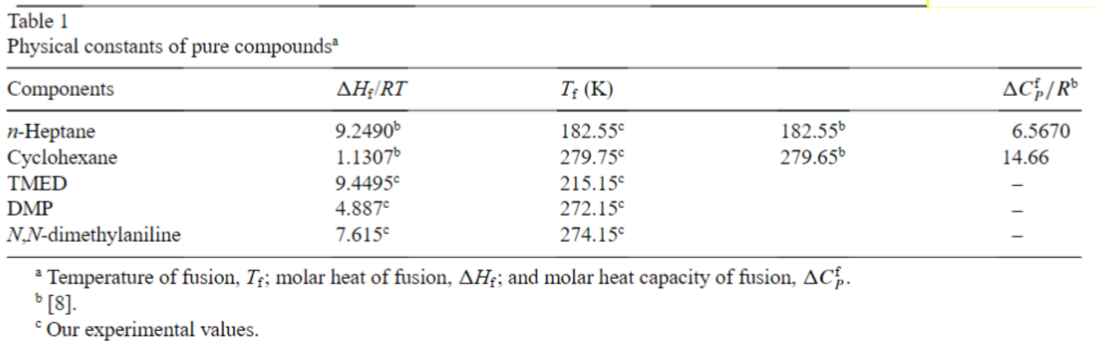


Table 1
Physical constants of pure compounds[a]

| Components | $\Delta H_f/RT$ | $T_f$ (K) | | $\Delta C_P^f/R$[b] |
|---|---|---|---|---|
| *n*-Heptane | 9.2490[b] | 182.55[c] | 182.55[b] | 6.5670 |
| Cyclohexane | 1.1307[b] | 279.75[c] | 279.65[b] | 14.66 |
| TMED | 9.4495[c] | 215.15[c] | | – |
| DMP | 4.887[c] | 272.15[c] | | – |
| *N*,*N*-dimethylaniline | 7.615[c] | 274.15[c] | | – |

[a] Temperature of fusion, $T_f$; molar heat of fusion, $\Delta H_f$; and molar heat capacity of fusion, $\Delta C_P^f$.
[b] [8].
[c] Our experimental values.

1,4-dimethylpiperazine + *n*-heptane
Farida AllalAbdallah Dahmani, Measurement and prediction of solid–liquid phase equilibriafor diamine+*n*-heptane, or cyclohexane, Fluid Phase Equilibria 190 (2001) 33–45

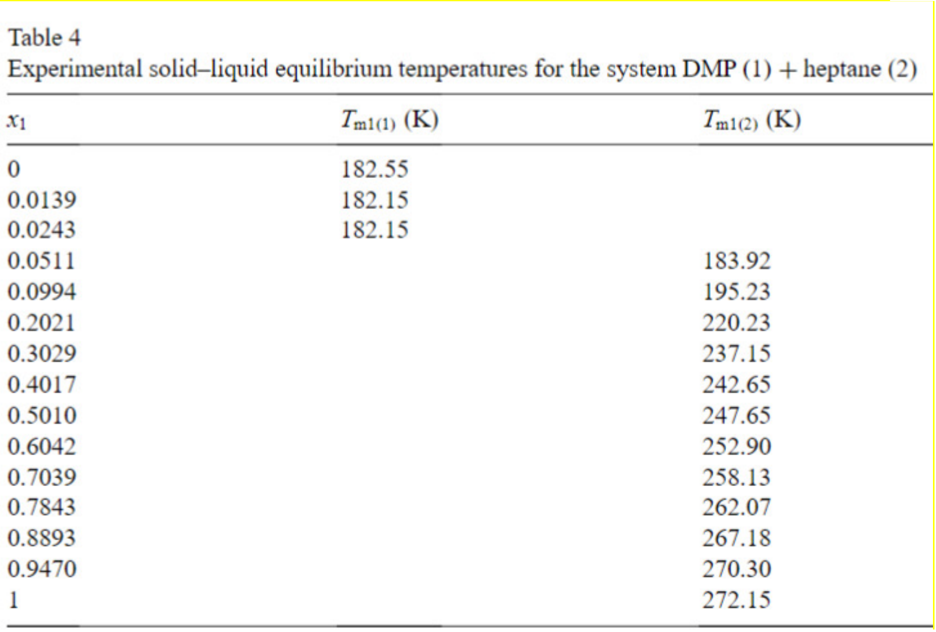


Table 4
Experimental solid–liquid equilibrium temperatures for the system DMP (1) + heptane (2)

| $x_1$ | $T_{m1(1)}$ (K) | $T_{m1(2)}$ (K) |
|---|---|---|
| 0 | 182.55 | |
| 0.0139 | 182.15 | |
| 0.0243 | 182.15 | |
| 0.0511 | | 183.92 |
| 0.0994 | | 195.23 |
| 0.2021 | | 220.23 |
| 0.3029 | | 237.15 |
| 0.4017 | | 242.65 |
| 0.5010 | | 247.65 |
| 0.6042 | | 252.90 |
| 0.7039 | | 258.13 |
| 0.7843 | | 262.07 |
| 0.8893 | | 267.18 |
| 0.9470 | | 270.30 |
| 1 | | 272.15 |

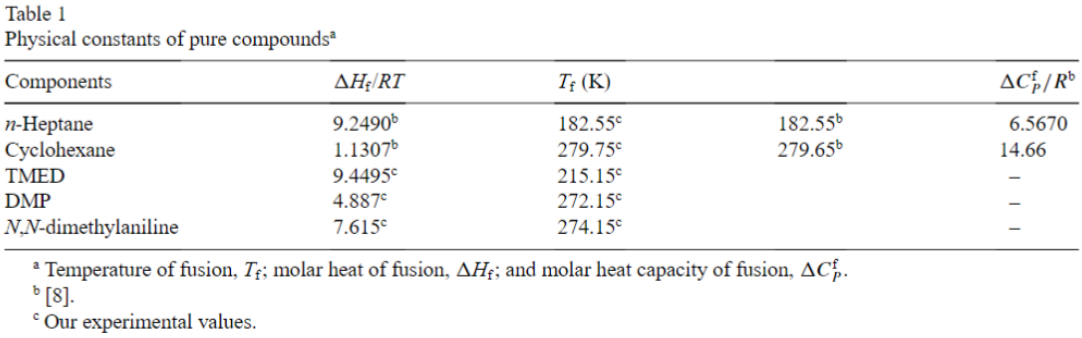


Table 1
Physical constants of pure compounds[a]

| Components | $\Delta H_f/RT$ | $T_f$ (K) | | $\Delta C_P^f/R$[b] |
|---|---|---|---|---|
| *n*-Heptane | 9.2490[b] | 182.55[c] | 182.55[b] | 6.5670 |
| Cyclohexane | 1.1307[b] | 279.75[c] | 279.65[b] | 14.66 |
| TMED | 9.4495[c] | 215.15[c] | | – |
| DMP | 4.887[c] | 272.15[c] | | – |
| *N*,*N*-dimethylaniline | 7.615[c] | 274.15[c] | | – |

[a] Temperature of fusion, $T_f$; molar heat of fusion, $\Delta H_f$; and molar heat capacity of fusion, $\Delta C_P^f$.
[b] [8].
[c] Our experimental values.

1,4-dimethylpiperazine + cyclohexane

Farida AllalAbdallah Dahmani, Measurement and prediction of solid–liquid phase equilibriafor diamine+*n*-heptane, or cyclohexane, Fluid Phase Equilibria 190 (2001) 33–45

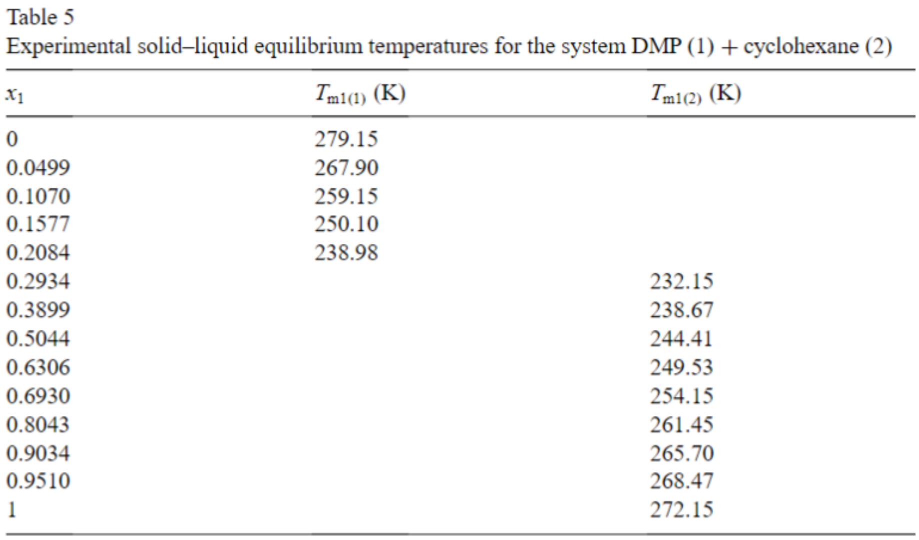


Table 5

Experimental solid–liquid equilibrium temperatures for the system DMP (1) + cyclohexane (2)

| $x_1$ | $T_{m1(1)}$ (K) | $T_{m1(2)}$ (K) |
|---|---|---|
| 0 | 279.15 | |
| 0.0499 | 267.90 | |
| 0.1070 | 259.15 | |
| 0.1577 | 250.10 | |
| 0.2084 | 238.98 | |
| 0.2934 | | 232.15 |
| 0.3899 | | 238.67 |
| 0.5044 | | 244.41 |
| 0.6306 | | 249.53 |
| 0.6930 | | 254.15 |
| 0.8043 | | 261.45 |
| 0.9034 | | 265.70 |
| 0.9510 | | 268.47 |
| 1 | | 272.15 |

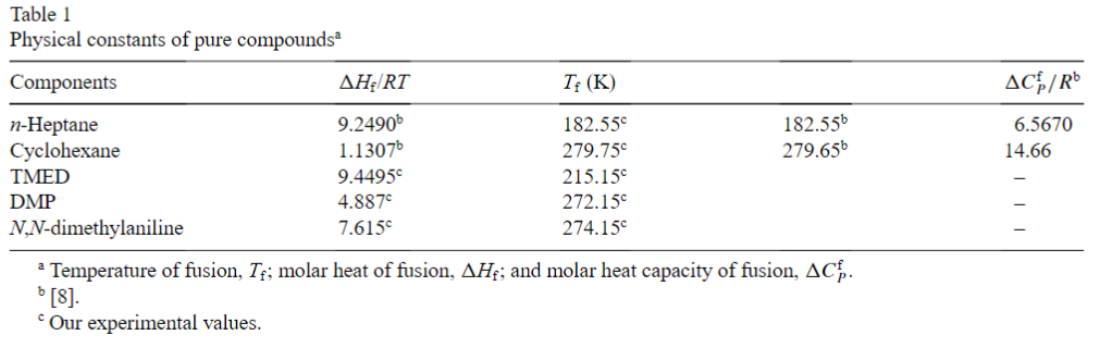


Table 1

Physical constants of pure compounds[a]

| Components | $\Delta H_f/RT$ | $T_f$ (K) | | $\Delta C_P^f/R$[b] |
|---|---|---|---|---|
| *n*-Heptane | 9.2490[b] | 182.55[c] | 182.55[b] | 6.5670 |
| Cyclohexane | 1.1307[b] | 279.75[c] | 279.65[b] | 14.66 |
| TMED | 9.4495[c] | 215.15[c] | | – |
| DMP | 4.887[c] | 272.15[c] | | – |
| *N*,*N*-dimethylaniline | 7.615[c] | 274.15[c] | | – |

[a] Temperature of fusion, $T_f$; molar heat of fusion, $\Delta H_f$; and molar heat capacity of fusion, $\Delta C_P^f$.

[b] [8].

[c] Our experimental values.

*N*,*N*-dimethylaniline + *n*-heptane
Farida AllalAbdallah Dahmani, Measurement and prediction of solid–liquid phase equilibriafor diamine+*n*-heptane, or cyclohexane, Fluid Phase Equilibria 190 (2001) 33–45

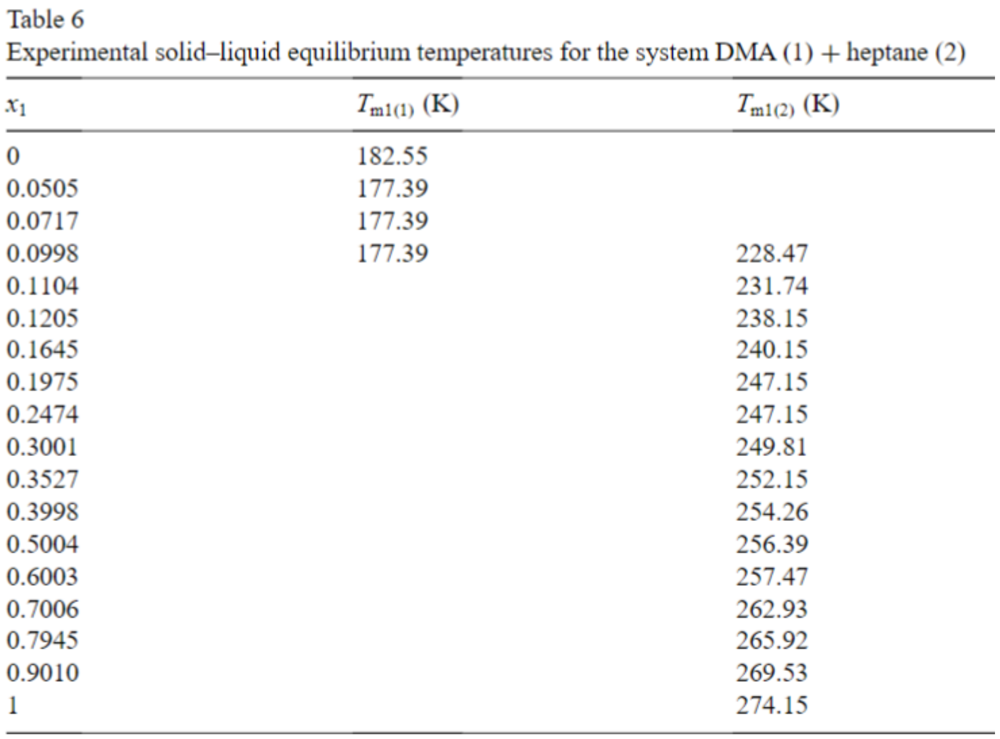


Table 6
Experimental solid–liquid equilibrium temperatures for the system DMA (1) + heptane (2)

| $x_1$ | $T_{m1(1)}$ (K) | $T_{m1(2)}$ (K) |
|---|---|---|
| 0 | 182.55 | |
| 0.0505 | 177.39 | |
| 0.0717 | 177.39 | |
| 0.0998 | 177.39 | 228.47 |
| 0.1104 | | 231.74 |
| 0.1205 | | 238.15 |
| 0.1645 | | 240.15 |
| 0.1975 | | 247.15 |
| 0.2474 | | 247.15 |
| 0.3001 | | 249.81 |
| 0.3527 | | 252.15 |
| 0.3998 | | 254.26 |
| 0.5004 | | 256.39 |
| 0.6003 | | 257.47 |
| 0.7006 | | 262.93 |
| 0.7945 | | 265.92 |
| 0.9010 | | 269.53 |
| 1 | | 274.15 |

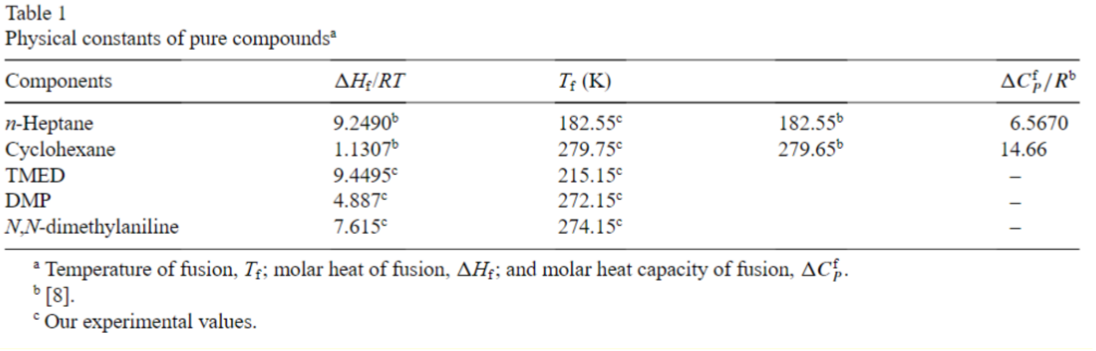


Table 1
Physical constants of pure compounds[a]

| Components | $\Delta H_f/RT$ | $T_f$ (K) | | $\Delta C_P^f/R$[b] |
|---|---|---|---|---|
| *n*-Heptane | 9.2490[b] | 182.55[c] | 182.55[b] | 6.5670 |
| Cyclohexane | 1.1307[b] | 279.75[c] | 279.65[b] | 14.66 |
| TMED | 9.4495[c] | 215.15[c] | | – |
| DMP | 4.887[c] | 272.15[c] | | – |
| *N*,*N*-dimethylaniline | 7.615[c] | 274.15[c] | | – |

[a] Temperature of fusion, $T_f$; molar heat of fusion, $\Delta H_f$; and molar heat capacity of fusion, $\Delta C_P^f$.
[b] [8].
[c] Our experimental values.

*N*,*N*-dimethylaniline + cyclohexane

Farida AllalAbdallah Dahmani, Measurement and prediction of solid–liquid phase equilibriafor diamine+*n*-heptane, or cyclohexane, Fluid Phase Equilibria 190 (2001) 33–45

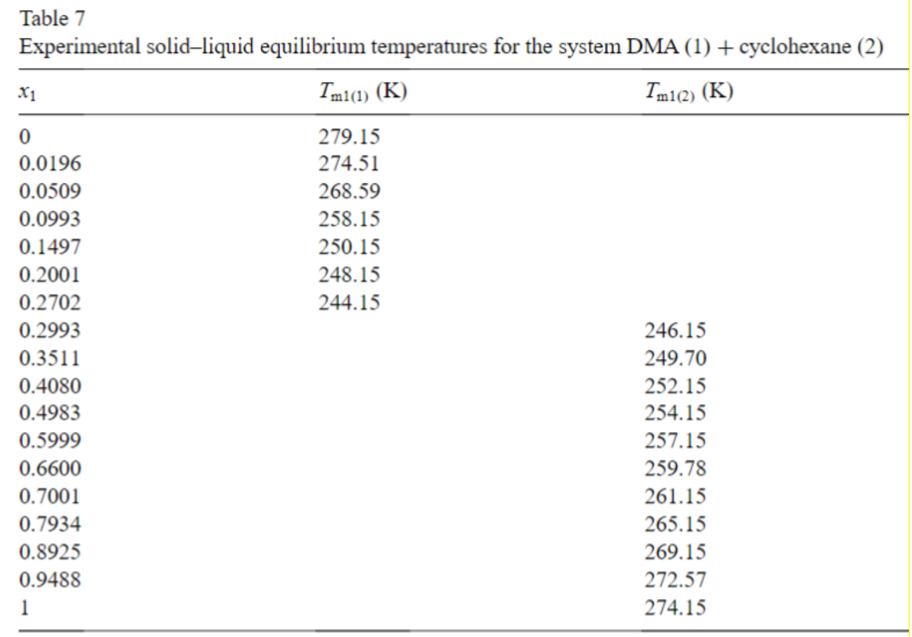


Table 7
Experimental solid–liquid equilibrium temperatures for the system DMA (1) + cyclohexane (2)

| $x_1$ | $T_{m1(1)}$ (K) | $T_{m1(2)}$ (K) |
|---|---|---|
| 0 | 279.15 | |
| 0.0196 | 274.51 | |
| 0.0509 | 268.59 | |
| 0.0993 | 258.15 | |
| 0.1497 | 250.15 | |
| 0.2001 | 248.15 | |
| 0.2702 | 244.15 | |
| 0.2993 | | 246.15 |
| 0.3511 | | 249.70 |
| 0.4080 | | 252.15 |
| 0.4983 | | 254.15 |
| 0.5999 | | 257.15 |
| 0.6600 | | 259.78 |
| 0.7001 | | 261.15 |
| 0.7934 | | 265.15 |
| 0.8925 | | 269.15 |
| 0.9488 | | 272.57 |
| 1 | | 274.15 |

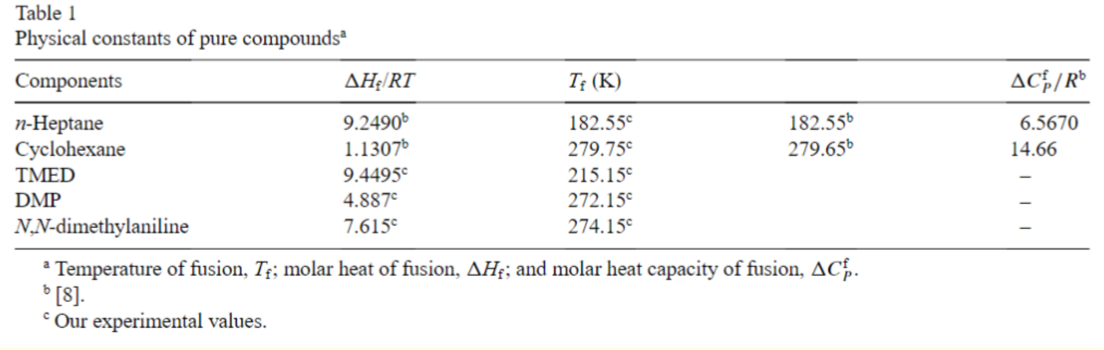


Table 1
Physical constants of pure compounds[a]

| Components | $\Delta H_f/RT$ | $T_f$ (K) | | $\Delta C_P^f/R$[b] |
|---|---|---|---|---|
| *n*-Heptane | 9.2490[b] | 182.55[c] | 182.55[b] | 6.5670 |
| Cyclohexane | 1.1307[b] | 279.75[c] | 279.65[b] | 14.66 |
| TMED | 9.4495[c] | 215.15[c] | | – |
| DMP | 4.887[c] | 272.15[c] | | – |
| *N*,*N*-dimethylaniline | 7.615[c] | 274.15[c] | | – |

[a] Temperature of fusion, $T_f$; molar heat of fusion, $\Delta H_f$; and molar heat capacity of fusion, $\Delta C_P^f$.
[b] [8].
[c] Our experimental values.

*n*-octadecane + myristic acid

Dongwei Wei, Sainan Han, Xiao Shen, Solid–liquid phase equilibria of (n-octadecane with myristic, and palmitic acid) binary mixtures used as phase change materials (PCMs), J. Chem. Thermodynamics 101 (2016) 7–11

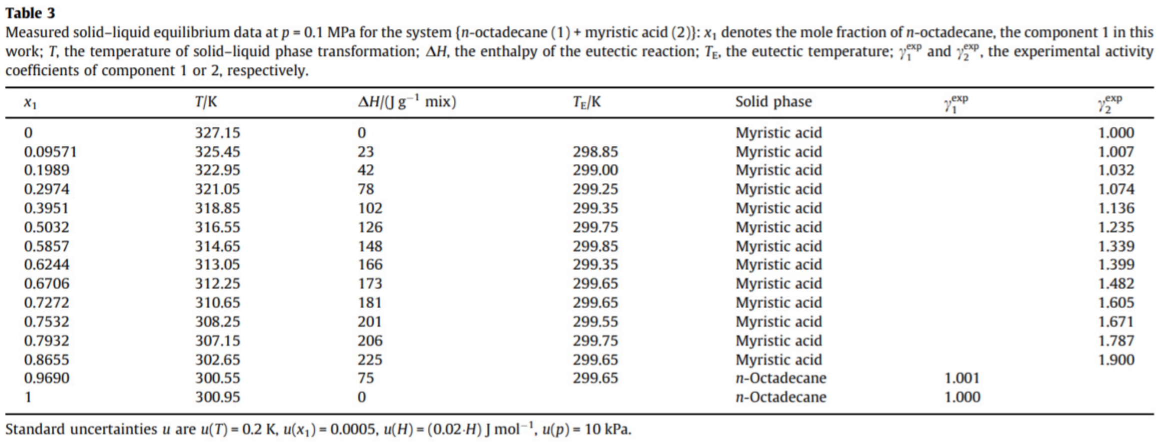


**Table 3**
Measured solid–liquid equilibrium data at $p = 0.1$ MPa for the system {*n*-octadecane (1) + myristic acid (2)}: $x_1$ denotes the mole fraction of *n*-octadecane, the component 1 in this work; *T*, the temperature of solid–liquid phase transformation; $\Delta H$, the enthalpy of the eutectic reaction; $T_E$, the eutectic temperature; $\gamma_1^{exp}$ and $\gamma_2^{exp}$, the experimental activity coefficients of component 1 or 2, respectively.

| $x_1$ | $T$/K | $\Delta H$/(J g$^{-1}$ mix) | $T_E$/K | Solid phase | $\gamma_1^{exp}$ | $\gamma_2^{exp}$ |
|---|---|---|---|---|---|---|
| 0 | 327.15 | 0 | | Myristic acid | | 1.000 |
| 0.09571 | 325.45 | 23 | 298.85 | Myristic acid | | 1.007 |
| 0.1989 | 322.95 | 42 | 299.00 | Myristic acid | | 1.032 |
| 0.2974 | 321.05 | 78 | 299.25 | Myristic acid | | 1.074 |
| 0.3951 | 318.85 | 102 | 299.35 | Myristic acid | | 1.136 |
| 0.5032 | 316.55 | 126 | 299.75 | Myristic acid | | 1.235 |
| 0.5857 | 314.65 | 148 | 299.85 | Myristic acid | | 1.339 |
| 0.6244 | 313.05 | 166 | 299.35 | Myristic acid | | 1.399 |
| 0.6706 | 312.25 | 173 | 299.65 | Myristic acid | | 1.482 |
| 0.7272 | 310.65 | 181 | 299.65 | Myristic acid | | 1.605 |
| 0.7532 | 308.25 | 201 | 299.55 | Myristic acid | | 1.671 |
| 0.7932 | 307.15 | 206 | 299.75 | Myristic acid | | 1.787 |
| 0.8655 | 302.65 | 225 | 299.65 | Myristic acid | | 1.900 |
| 0.9690 | 300.55 | 75 | 299.65 | *n*-Octadecane | 1.001 | |
| 1 | 300.95 | 0 | | *n*-Octadecane | 1.000 | |

Standard uncertainties *u* are $u(T) = 0.2$ K, $u(x_1) = 0.0005$, $u(H) = (0.02 \cdot H)$ J mol$^{-1}$, $u(p) = 10$ kPa.

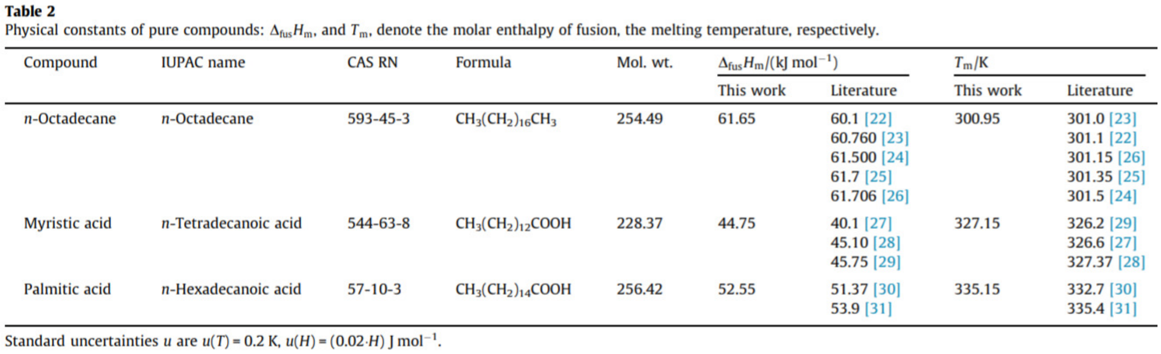


**Table 2**
Physical constants of pure compounds: $\Delta_{fus}H_m$, and $T_m$, denote the molar enthalpy of fusion, the melting temperature, respectively.

| Compound | IUPAC name | CAS RN | Formula | Mol. wt. | $\Delta_{fus}H_m$/(kJ mol$^{-1}$) | | $T_m$/K | |
|---|---|---|---|---|---|---|---|---|
| | | | | | This work | Literature | This work | Literature |
| *n*-Octadecane | *n*-Octadecane | 593-45-3 | $CH_3(CH_2)_{16}CH_3$ | 254.49 | 61.65 | 60.1 [22]<br>60.760 [23]<br>61.500 [24]<br>61.7 [25]<br>61.706 [26] | 300.95 | 301.0 [23]<br>301.1 [22]<br>301.15 [26]<br>301.35 [25]<br>301.5 [24] |
| Myristic acid | *n*-Tetradecanoic acid | 544-63-8 | $CH_3(CH_2)_{12}COOH$ | 228.37 | 44.75 | 40.1 [27]<br>45.10 [28]<br>45.75 [29] | 327.15 | 326.2 [29]<br>326.6 [27]<br>327.37 [28] |
| Palmitic acid | *n*-Hexadecanoic acid | 57-10-3 | $CH_3(CH_2)_{14}COOH$ | 256.42 | 52.55 | 51.37 [30]<br>53.9 [31] | 335.15 | 332.7 [30]<br>335.4 [31] |

Standard uncertainties *u* are $u(T) = 0.2$ K, $u(H) = (0.02 \cdot H)$ J mol$^{-1}$.

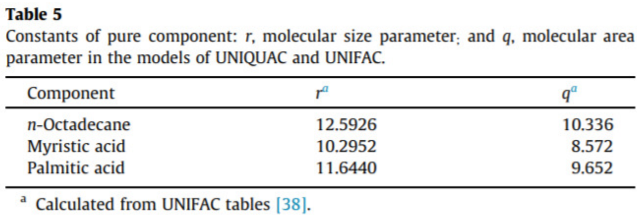


**Table 5**
Constants of pure component: *r*, molecular size parameter; and *q*, molecular area parameter in the models of UNIQUAC and UNIFAC.

| Component | $r^a$ | $q^a$ |
|---|---|---|
| *n*-Octadecane | 12.5926 | 10.336 |
| Myristic acid | 10.2952 | 8.572 |
| Palmitic acid | 11.6440 | 9.652 |

[a] Calculated from UNIFAC tables [38].

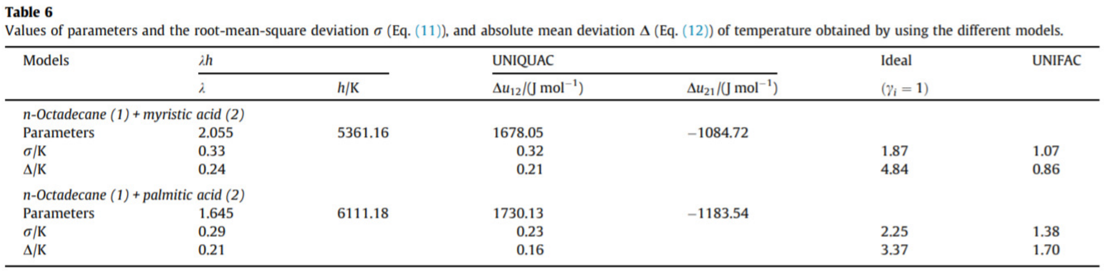


**Table 6**
Values of parameters and the root-mean-square deviation $\sigma$ (Eq. (11)), and absolute mean deviation $\Delta$ (Eq. (12)) of temperature obtained by using the different models.

| Models | $\lambda h$ | | UNIQUAC | | Ideal | UNIFAC |
|---|---|---|---|---|---|---|
| | $\lambda$ | $h$/K | $\Delta u_{12}$/(J mol$^{-1}$) | $\Delta u_{21}$/(J mol$^{-1}$) | ($\gamma_i = 1$) | |
| *n-Octadecane (1) + myristic acid (2)* | | | | | | |
| Parameters | 2.055 | 5361.16 | 1678.05 | −1084.72 | | |
| $\sigma$/K | 0.33 | | 0.32 | | 1.87 | 1.07 |
| $\Delta$/K | 0.24 | | 0.21 | | 4.84 | 0.86 |
| *n-Octadecane (1) + palmitic acid (2)* | | | | | | |
| Parameters | 1.645 | 6111.18 | 1730.13 | −1183.54 | | |
| $\sigma$/K | 0.29 | | 0.23 | | 2.25 | 1.38 |
| $\Delta$/K | 0.21 | | 0.16 | | 3.37 | 1.70 |

ODABRATI UNIQUAC

*n*-octadecane + palmitic acid

Dongwei Wei, Sainan Han, Xiao Shen, Solid–liquid phase equilibria of (n-octadecane with myristic, and palmitic acid) binary mixtures used as phase change materials (PCMs), J. Chem. Thermodynamics 101 (2016) 7–11

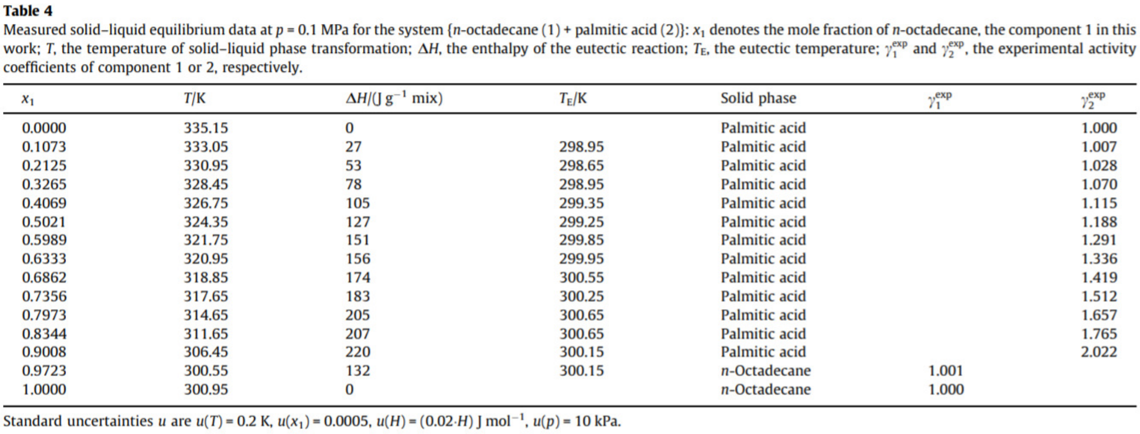


**Table 4**
Measured solid–liquid equilibrium data at $p$ = 0.1 MPa for the system {*n*-octadecane (1) + palmitic acid (2)}: $x_1$ denotes the mole fraction of *n*-octadecane, the component 1 in this work; $T$, the temperature of solid–liquid phase transformation; $\Delta H$, the enthalpy of the eutectic reaction; $T_E$, the eutectic temperature; $\gamma_1^{exp}$ and $\gamma_2^{exp}$, the experimental activity coefficients of component 1 or 2, respectively.

| $x_1$ | $T$/K | $\Delta H$/(J g$^{-1}$ mix) | $T_E$/K | Solid phase | $\gamma_1^{exp}$ | $\gamma_2^{exp}$ |
|---|---|---|---|---|---|---|
| 0.0000 | 335.15 | 0 | | Palmitic acid | | 1.000 |
| 0.1073 | 333.05 | 27 | 298.95 | Palmitic acid | | 1.007 |
| 0.2125 | 330.95 | 53 | 298.65 | Palmitic acid | | 1.028 |
| 0.3265 | 328.45 | 78 | 298.95 | Palmitic acid | | 1.070 |
| 0.4069 | 326.75 | 105 | 299.35 | Palmitic acid | | 1.115 |
| 0.5021 | 324.35 | 127 | 299.25 | Palmitic acid | | 1.188 |
| 0.5989 | 321.75 | 151 | 299.85 | Palmitic acid | | 1.291 |
| 0.6333 | 320.95 | 156 | 299.95 | Palmitic acid | | 1.336 |
| 0.6862 | 318.85 | 174 | 300.55 | Palmitic acid | | 1.419 |
| 0.7356 | 317.65 | 183 | 300.25 | Palmitic acid | | 1.512 |
| 0.7973 | 314.65 | 205 | 300.65 | Palmitic acid | | 1.657 |
| 0.8344 | 311.65 | 207 | 300.65 | Palmitic acid | | 1.765 |
| 0.9008 | 306.45 | 220 | 300.15 | Palmitic acid | | 2.022 |
| 0.9723 | 300.55 | 132 | 300.15 | *n*-Octadecane | 1.001 | |
| 1.0000 | 300.95 | 0 | | *n*-Octadecane | 1.000 | |

Standard uncertainties $u$ are $u(T)$ = 0.2 K, $u(x_1)$ = 0.0005, $u(H)$ = (0.02·$H$) J mol$^{-1}$, $u(p)$ = 10 kPa.

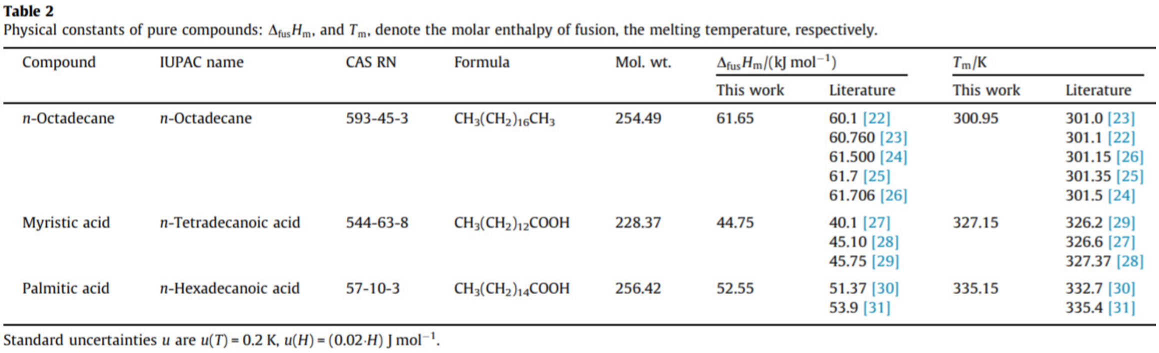


**Table 2**
Physical constants of pure compounds: $\Delta_{fus}H_m$, and $T_m$, denote the molar enthalpy of fusion, the melting temperature, respectively.

| Compound | IUPAC name | CAS RN | Formula | Mol. wt. | $\Delta_{fus}H_m$/(kJ mol$^{-1}$) | | $T_m$/K | |
|---|---|---|---|---|---|---|---|---|
| | | | | | This work | Literature | This work | Literature |
| *n*-Octadecane | *n*-Octadecane | 593-45-3 | $CH_3(CH_2)_{16}CH_3$ | 254.49 | 61.65 | 60.1 [22]<br>60.760 [23]<br>61.500 [24]<br>61.7 [25]<br>61.706 [26] | 300.95 | 301.0 [23]<br>301.1 [22]<br>301.15 [26]<br>301.35 [25]<br>301.5 [24] |
| Myristic acid | *n*-Tetradecanoic acid | 544-63-8 | $CH_3(CH_2)_{12}COOH$ | 228.37 | 44.75 | 40.1 [27]<br>45.10 [28]<br>45.75 [29] | 327.15 | 326.2 [29]<br>326.6 [27]<br>327.37 [28] |
| Palmitic acid | *n*-Hexadecanoic acid | 57-10-3 | $CH_3(CH_2)_{14}COOH$ | 256.42 | 52.55 | 51.37 [30]<br>53.9 [31] | 335.15 | 332.7 [30]<br>335.4 [31] |

Standard uncertainties $u$ are $u(T)$ = 0.2 K, $u(H)$ = (0.02·$H$) J mol$^{-1}$.

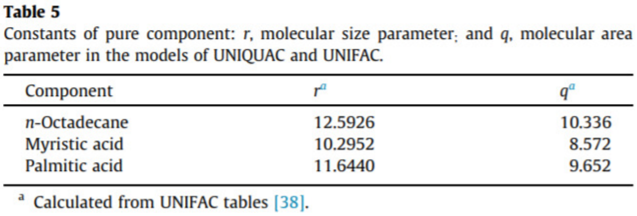


**Table 5**
Constants of pure component: $r$, molecular size parameter; and $q$, molecular area parameter in the models of UNIQUAC and UNIFAC.

| Component | $r$[a] | $q$[a] |
|---|---|---|
| *n*-Octadecane | 12.5926 | 10.336 |
| Myristic acid | 10.2952 | 8.572 |
| Palmitic acid | 11.6440 | 9.652 |

[a] Calculated from UNIFAC tables [38].

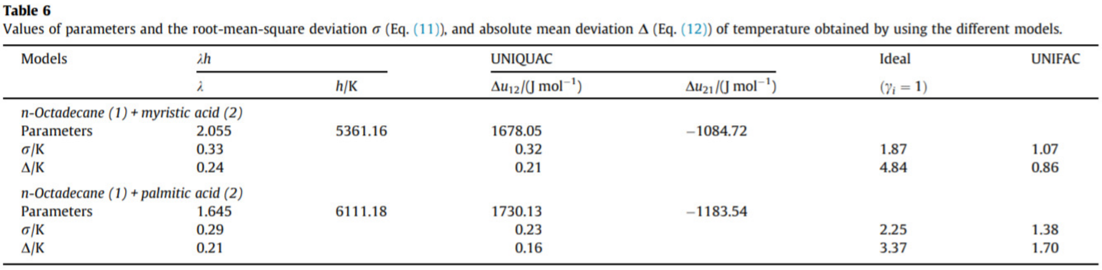


**Table 6**
Values of parameters and the root-mean-square deviation $\sigma$ (Eq. (11)), and absolute mean deviation $\Delta$ (Eq. (12)) of temperature obtained by using the different models.

| Models | $\lambda h$ | | UNIQUAC | | Ideal | UNIFAC |
|---|---|---|---|---|---|---|
| | $\lambda$ | $h$/K | $\Delta u_{12}$/(J mol$^{-1}$) | $\Delta u_{21}$/(J mol$^{-1}$) | ($\gamma_i = 1$) | |
| *n-Octadecane (1) + myristic acid (2)* | | | | | | |
| Parameters | 2.055 | 5361.16 | 1678.05 | −1084.72 | | |
| $\sigma$/K | 0.33 | | 0.32 | | 1.87 | 1.07 |
| $\Delta$/K | 0.24 | | 0.21 | | 4.84 | 0.86 |
| *n-Octadecane (1) + palmitic acid (2)* | | | | | | |
| Parameters | 1.645 | 6111.18 | 1730.13 | −1183.54 | | |
| $\sigma$/K | 0.29 | | 0.23 | | 2.25 | 1.38 |
| $\Delta$/K | 0.21 | | 0.16 | | 3.37 | 1.70 |

ODABRATI UNIQUAC

naphthalene + *o*-dichlorobenzene

Dongwei Wei, Kexin Jin, (Solid + liquid) equilibria of (naphthalene + isomeric dichlorobenzenes), J. Chem. Thermodynamics 41 (2009) 145–149

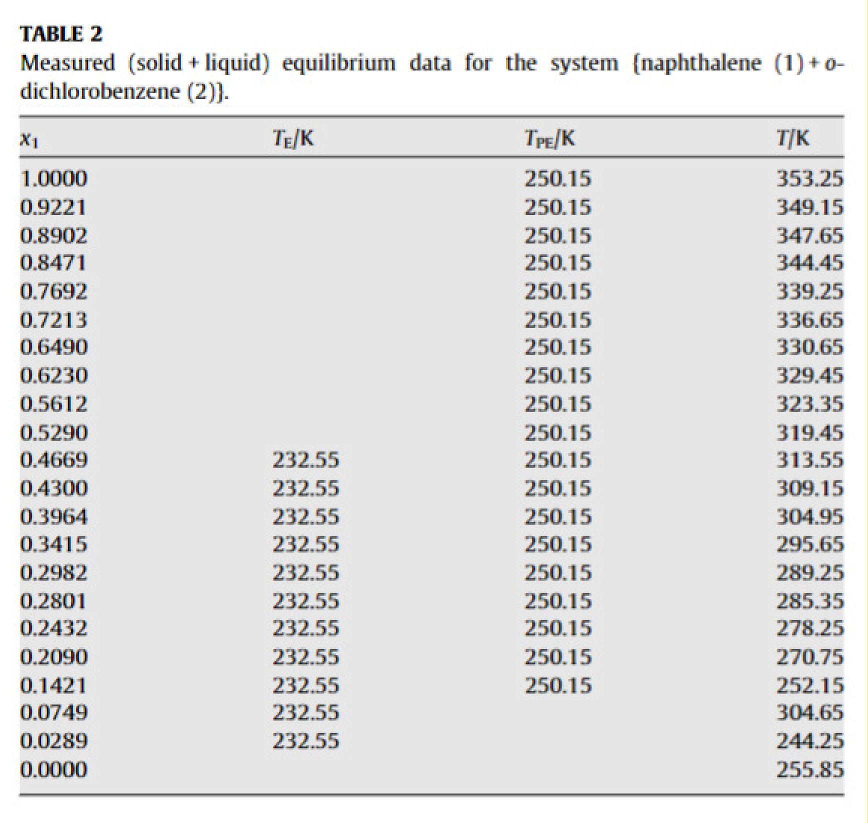


**TABLE 2**

Measured (solid + liquid) equilibrium data for the system {naphthalene (1) + *o*-dichlorobenzene (2)}.

| $x_1$ | $T_E$/K | $T_{PE}$/K | $T$/K |
|---|---|---|---|
| 1.0000 | | 250.15 | 353.25 |
| 0.9221 | | 250.15 | 349.15 |
| 0.8902 | | 250.15 | 347.65 |
| 0.8471 | | 250.15 | 344.45 |
| 0.7692 | | 250.15 | 339.25 |
| 0.7213 | | 250.15 | 336.65 |
| 0.6490 | | 250.15 | 330.65 |
| 0.6230 | | 250.15 | 329.45 |
| 0.5612 | | 250.15 | 323.35 |
| 0.5290 | | 250.15 | 319.45 |
| 0.4669 | 232.55 | 250.15 | 313.55 |
| 0.4300 | 232.55 | 250.15 | 309.15 |
| 0.3964 | 232.55 | 250.15 | 304.95 |
| 0.3415 | 232.55 | 250.15 | 295.65 |
| 0.2982 | 232.55 | 250.15 | 289.25 |
| 0.2801 | 232.55 | 250.15 | 285.35 |
| 0.2432 | 232.55 | 250.15 | 278.25 |
| 0.2090 | 232.55 | 250.15 | 270.75 |
| 0.1421 | 232.55 | 250.15 | 252.15 |
| 0.0749 | 232.55 | | 304.65 |
| 0.0289 | 232.55 | | 244.25 |
| 0.0000 | | | 255.85 |

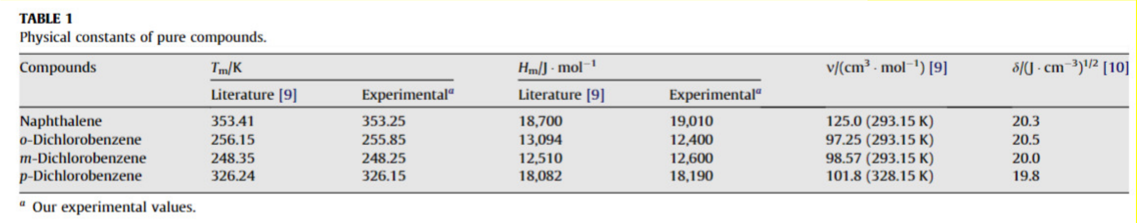


**TABLE 1**

Physical constants of pure compounds.

| Compounds | $T_m$/K | | $H_m$/J · mol$^{-1}$ | | v/(cm$^3$ · mol$^{-1}$) [9] | $\delta$/(J · cm$^{-3}$)$^{1/2}$ [10] |
|---|---|---|---|---|---|---|
| | Literature [9] | Experimental[a] | Literature [9] | Experimental[a] | | |
| Naphthalene | 353.41 | 353.25 | 18,700 | 19,010 | 125.0 (293.15 K) | 20.3 |
| *o*-Dichlorobenzene | 256.15 | 255.85 | 13,094 | 12,400 | 97.25 (293.15 K) | 20.5 |
| *m*-Dichlorobenzene | 248.35 | 248.25 | 12,510 | 12,600 | 98.57 (293.15 K) | 20.0 |
| *p*-Dichlorobenzene | 326.24 | 326.15 | 18,082 | 18,190 | 101.8 (328.15 K) | 19.8 |

[a] Our experimental values.

naphthalene + *p*-dichlorobenzene

Dongwei Wei, Kexin Jin, (Solid + liquid) equilibria of (naphthalene + isomeric dichlorobenzenes), J. Chem. Thermodynamics 41 (2009) 145–149

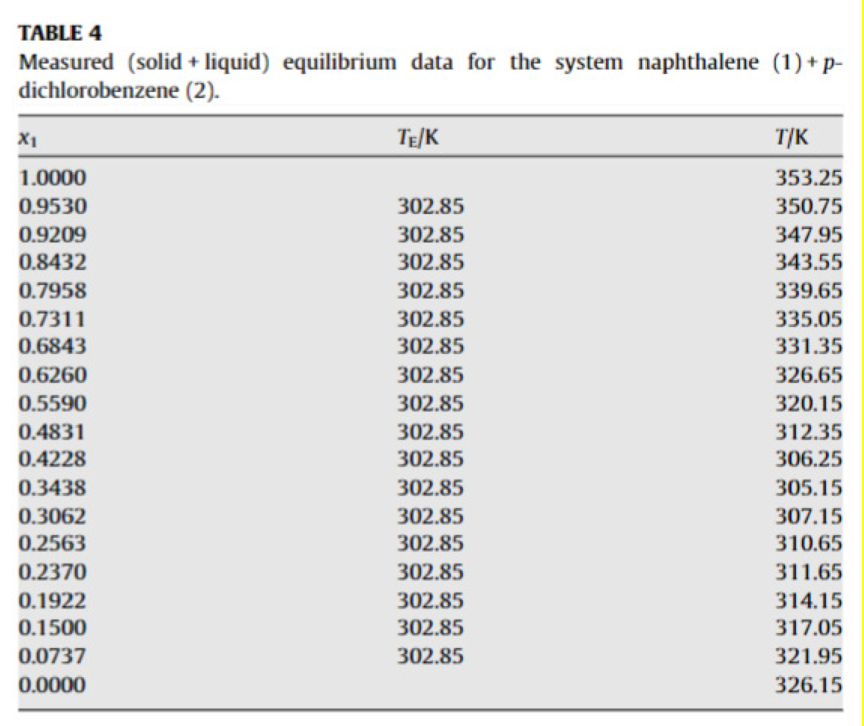


**TABLE 4**

Measured (solid + liquid) equilibrium data for the system naphthalene (1) + *p*-dichlorobenzene (2).

| $x_1$ | $T_E$/K | $T$/K |
|---|---|---|
| 1.0000 | | 353.25 |
| 0.9530 | 302.85 | 350.75 |
| 0.9209 | 302.85 | 347.95 |
| 0.8432 | 302.85 | 343.55 |
| 0.7958 | 302.85 | 339.65 |
| 0.7311 | 302.85 | 335.05 |
| 0.6843 | 302.85 | 331.35 |
| 0.6260 | 302.85 | 326.65 |
| 0.5590 | 302.85 | 320.15 |
| 0.4831 | 302.85 | 312.35 |
| 0.4228 | 302.85 | 306.25 |
| 0.3438 | 302.85 | 305.15 |
| 0.3062 | 302.85 | 307.15 |
| 0.2563 | 302.85 | 310.65 |
| 0.2370 | 302.85 | 311.65 |
| 0.1922 | 302.85 | 314.15 |
| 0.1500 | 302.85 | 317.05 |
| 0.0737 | 302.85 | 321.95 |
| 0.0000 | | 326.15 |

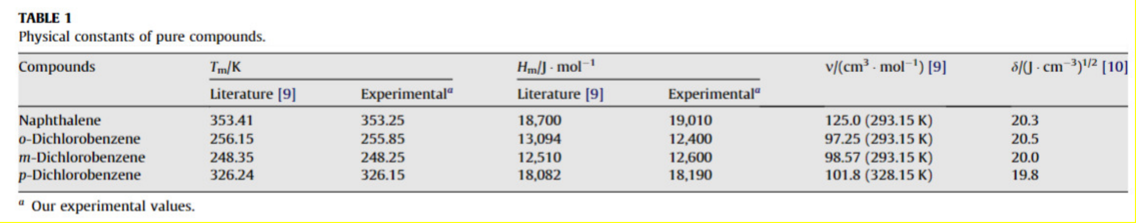


**TABLE 1**

Physical constants of pure compounds.

| Compounds | $T_m$/K | | $H_m$/J · mol$^{-1}$ | | v/(cm$^3$ · mol$^{-1}$) [9] | δ/(J · cm$^{-3}$)$^{1/2}$ [10] |
|---|---|---|---|---|---|---|
| | Literature [9] | Experimental[a] | Literature [9] | Experimental[a] | | |
| Naphthalene | 353.41 | 353.25 | 18,700 | 19,010 | 125.0 (293.15 K) | 20.3 |
| *o*-Dichlorobenzene | 256.15 | 255.85 | 13,094 | 12,400 | 97.25 (293.15 K) | 20.5 |
| *m*-Dichlorobenzene | 248.35 | 248.25 | 12,510 | 12,600 | 98.57 (293.15 K) | 20.0 |
| *p*-Dichlorobenzene | 326.24 | 326.15 | 18,082 | 18,190 | 101.8 (328.15 K) | 19.8 |

[a] Our experimental values.

naphthalene + *m*-dichlorobenzene

Dongwei Wei, Kexin Jin, (Solid + liquid) equilibria of (naphthalene + isomeric dichlorobenzenes), J. Chem. Thermodynamics 41 (2009) 145–149

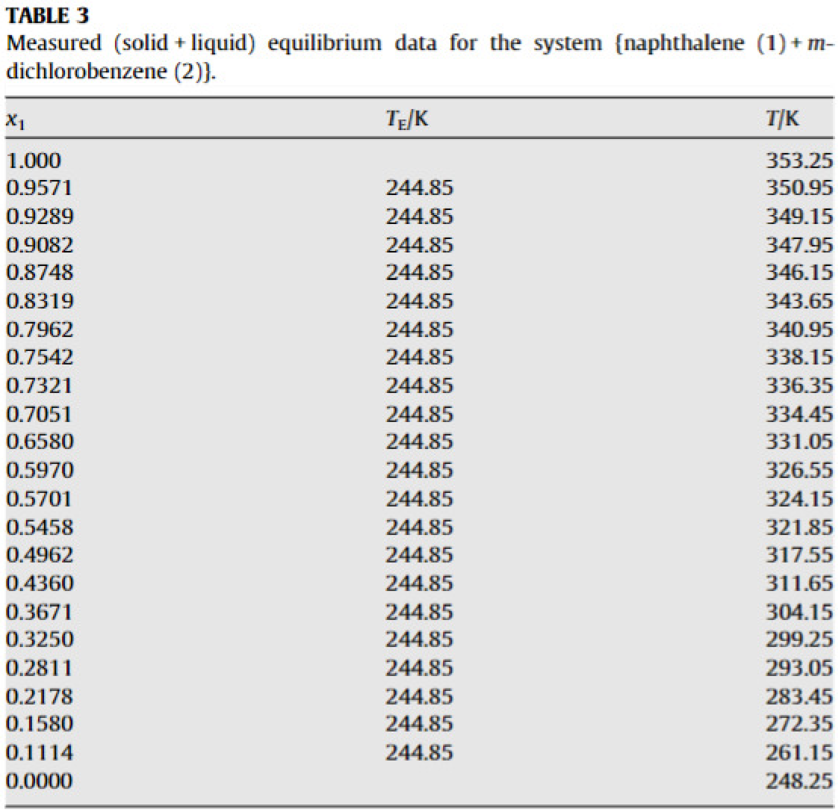


**TABLE 3**
Measured (solid + liquid) equilibrium data for the system {naphthalene (1) + *m*-dichlorobenzene (2)}.

| $x_1$ | $T_E$/K | $T$/K |
|---|---|---|
| 1.000 | | 353.25 |
| 0.9571 | 244.85 | 350.95 |
| 0.9289 | 244.85 | 349.15 |
| 0.9082 | 244.85 | 347.95 |
| 0.8748 | 244.85 | 346.15 |
| 0.8319 | 244.85 | 343.65 |
| 0.7962 | 244.85 | 340.95 |
| 0.7542 | 244.85 | 338.15 |
| 0.7321 | 244.85 | 336.35 |
| 0.7051 | 244.85 | 334.45 |
| 0.6580 | 244.85 | 331.05 |
| 0.5970 | 244.85 | 326.55 |
| 0.5701 | 244.85 | 324.15 |
| 0.5458 | 244.85 | 321.85 |
| 0.4962 | 244.85 | 317.55 |
| 0.4360 | 244.85 | 311.65 |
| 0.3671 | 244.85 | 304.15 |
| 0.3250 | 244.85 | 299.25 |
| 0.2811 | 244.85 | 293.05 |
| 0.2178 | 244.85 | 283.45 |
| 0.1580 | 244.85 | 272.35 |
| 0.1114 | 244.85 | 261.15 |
| 0.0000 | | 248.25 |

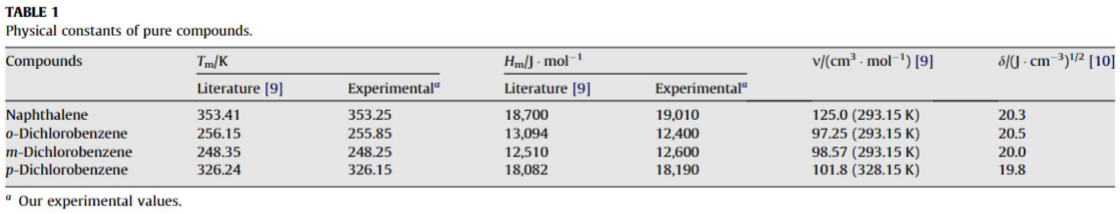


**TABLE 1**
Physical constants of pure compounds.

| Compounds | $T_m$/K | | $H_m$/J · mol$^{-1}$ | | v/(cm$^3$ · mol$^{-1}$) [9] | $\delta$/(J · cm$^{-3}$)$^{1/2}$ [10] |
|---|---|---|---|---|---|---|
| | Literature [9] | Experimental[a] | Literature [9] | Experimental[a] | | |
| Naphthalene | 353.41 | 353.25 | 18,700 | 19,010 | 125.0 (293.15 K) | 20.3 |
| *o*-Dichlorobenzene | 256.15 | 255.85 | 13,094 | 12,400 | 97.25 (293.15 K) | 20.5 |
| *m*-Dichlorobenzene | 248.35 | 248.25 | 12,510 | 12,600 | 98.57 (293.15 K) | 20.0 |
| *p*-Dichlorobenzene | 326.24 | 326.15 | 18,082 | 18,190 | 101.8 (328.15 K) | 19.8 |

[a] Our experimental values.

octan-1-ol + benzonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) phase equilibria of (alkan-1-ol +benzonitrile), (amine + benzonitrile) binary mixtures, and(decan-1-ol + decylamine + benzonitrile) ternary mixtures, Fluid Phase Equilibria 251 (2007) 161–166

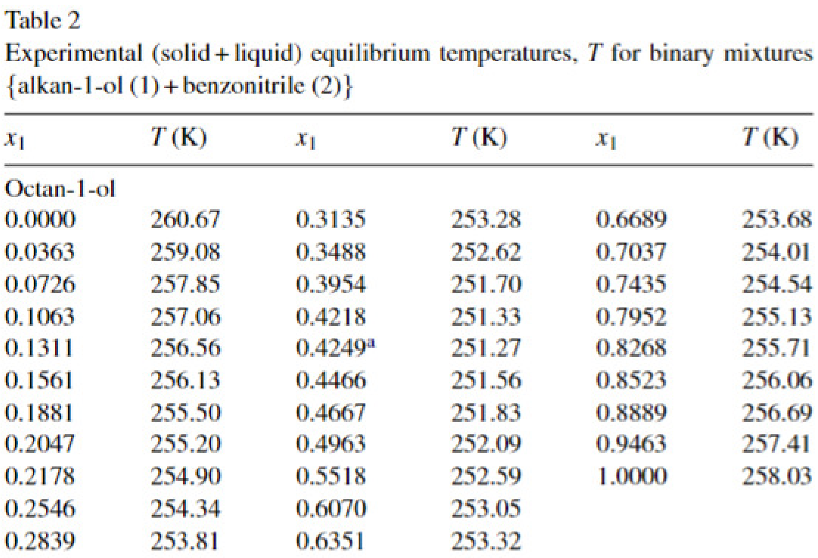


Table 2

Experimental (solid + liquid) equilibrium temperatures, $T$ for binary mixtures {alkan-1-ol (1) + benzonitrile (2)}

| $x_1$ | $T$ (K) | $x_1$ | $T$ (K) | $x_1$ | $T$ (K) |
|---|---|---|---|---|---|
| Octan-1-ol | | | | | |
| 0.0000 | 260.67 | 0.3135 | 253.28 | 0.6689 | 253.68 |
| 0.0363 | 259.08 | 0.3488 | 252.62 | 0.7037 | 254.01 |
| 0.0726 | 257.85 | 0.3954 | 251.70 | 0.7435 | 254.54 |
| 0.1063 | 257.06 | 0.4218 | 251.33 | 0.7952 | 255.13 |
| 0.1311 | 256.56 | 0.4249[a] | 251.27 | 0.8268 | 255.71 |
| 0.1561 | 256.13 | 0.4466 | 251.56 | 0.8523 | 256.06 |
| 0.1881 | 255.50 | 0.4667 | 251.83 | 0.8889 | 256.69 |
| 0.2047 | 255.20 | 0.4963 | 252.09 | 0.9463 | 257.41 |
| 0.2178 | 254.90 | 0.5518 | 252.59 | 1.0000 | 258.03 |
| 0.2546 | 254.34 | 0.6070 | 253.05 | | |
| 0.2839 | 253.81 | 0.6351 | 253.32 | | |

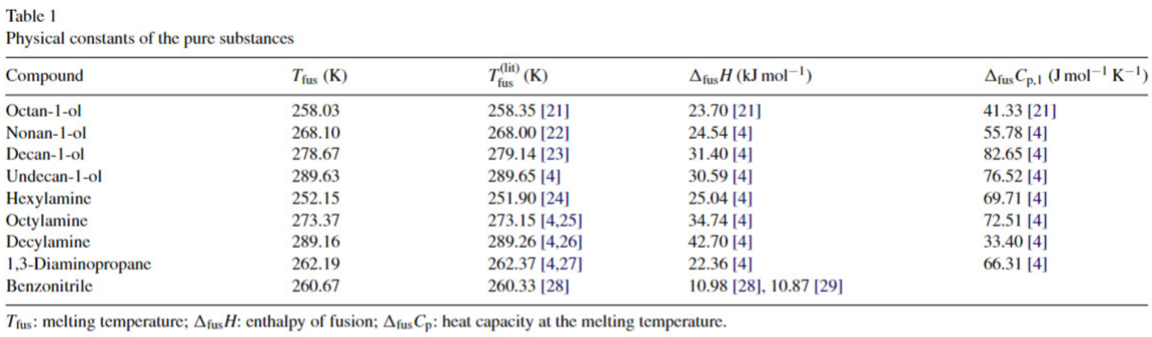


Table 1

Physical constants of the pure substances

| Compound | $T_{fus}$ (K) | $T_{fus}^{(lit)}$ (K) | $\Delta_{fus}H$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35 [21] | 23.70 [21] | 41.33 [21] |
| Nonan-1-ol | 268.10 | 268.00 [22] | 24.54 [4] | 55.78 [4] |
| Decan-1-ol | 278.67 | 279.14 [23] | 31.40 [4] | 82.65 [4] |
| Undecan-1-ol | 289.63 | 289.65 [4] | 30.59 [4] | 76.52 [4] |
| Hexylamine | 252.15 | 251.90 [24] | 25.04 [4] | 69.71 [4] |
| Octylamine | 273.37 | 273.15 [4,25] | 34.74 [4] | 72.51 [4] |
| Decylamine | 289.16 | 289.26 [4,26] | 42.70 [4] | 33.40 [4] |
| 1,3-Diaminopropane | 262.19 | 262.37 [4,27] | 22.36 [4] | 66.31 [4] |
| Benzonitrile | 260.67 | 260.33 [28] | 10.98 [28], 10.87 [29] | |

$T_{fus}$: melting temperature; $\Delta_{fus}H$: enthalpy of fusion; $\Delta_{fus}C_p$: heat capacity at the melting temperature.

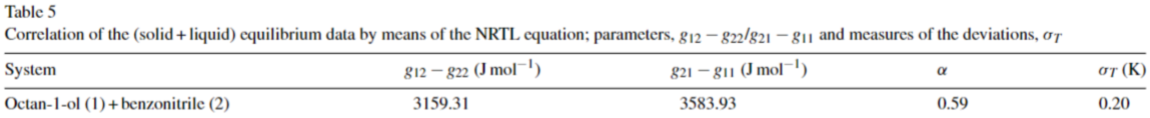


Table 5

Correlation of the (solid + liquid) equilibrium data by means of the NRTL equation; parameters, $g_{12}-g_{22}/g_{21}-g_{11}$ and measures of the deviations, $\sigma_T$

| System | $g_{12}-g_{22}$ (J mol$^{-1}$) | $g_{21}-g_{11}$ (J mol$^{-1}$) | $\alpha$ | $\sigma_T$ (K) |
|---|---|---|---|---|
| Octan-1-ol (1) + benzonitrile (2) | 3159.31 | 3583.93 | 0.59 | 0.20 |

nonan-1-ol + benzonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) phase equilibria of (alkan-1-ol +benzonitrile), (amine + benzonitrile) binary mixtures, and(decan-1-ol + decylamine + benzonitrile) ternary mixtures, Fluid Phase Equilibria 251 (2007) 161–166

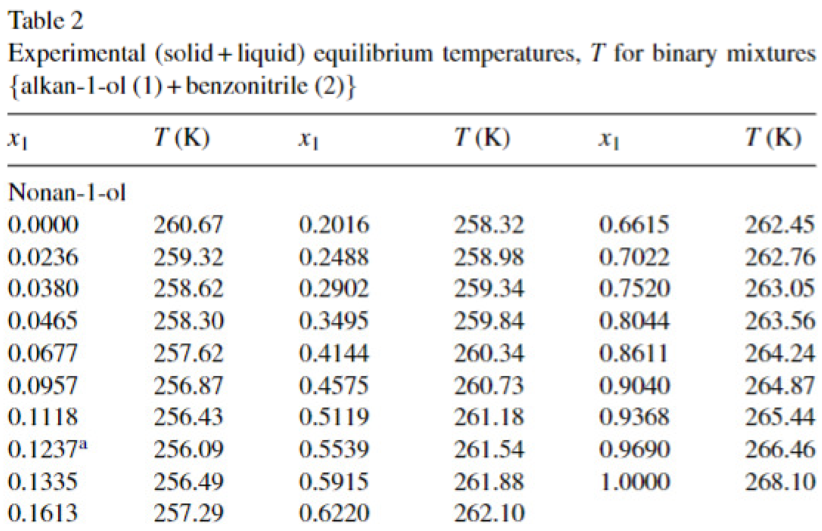


Table 2

Experimental (solid + liquid) equilibrium temperatures, $T$ for binary mixtures {alkan-1-ol (1) + benzonitrile (2)}

| $x_1$ | $T$ (K) | $x_1$ | $T$ (K) | $x_1$ | $T$ (K) |
|---|---|---|---|---|---|
| Nonan-1-ol | | | | | |
| 0.0000 | 260.67 | 0.2016 | 258.32 | 0.6615 | 262.45 |
| 0.0236 | 259.32 | 0.2488 | 258.98 | 0.7022 | 262.76 |
| 0.0380 | 258.62 | 0.2902 | 259.34 | 0.7520 | 263.05 |
| 0.0465 | 258.30 | 0.3495 | 259.84 | 0.8044 | 263.56 |
| 0.0677 | 257.62 | 0.4144 | 260.34 | 0.8611 | 264.24 |
| 0.0957 | 256.87 | 0.4575 | 260.73 | 0.9040 | 264.87 |
| 0.1118 | 256.43 | 0.5119 | 261.18 | 0.9368 | 265.44 |
| 0.1237[a] | 256.09 | 0.5539 | 261.54 | 0.9690 | 266.46 |
| 0.1335 | 256.49 | 0.5915 | 261.88 | 1.0000 | 268.10 |
| 0.1613 | 257.29 | 0.6220 | 262.10 | | |

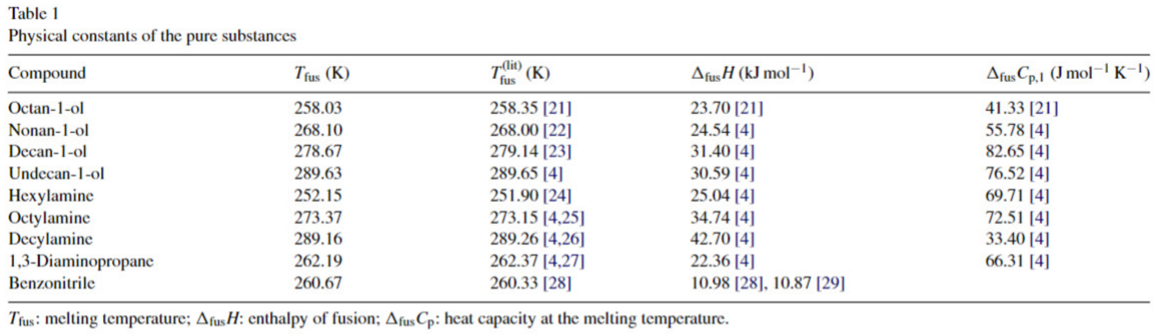


Table 1

Physical constants of the pure substances

| Compound | $T_{fus}$ (K) | $T_{fus}^{(lit)}$ (K) | $\Delta_{fus}H$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35 [21] | 23.70 [21] | 41.33 [21] |
| Nonan-1-ol | 268.10 | 268.00 [22] | 24.54 [4] | 55.78 [4] |
| Decan-1-ol | 278.67 | 279.14 [23] | 31.40 [4] | 82.65 [4] |
| Undecan-1-ol | 289.63 | 289.65 [4] | 30.59 [4] | 76.52 [4] |
| Hexylamine | 252.15 | 251.90 [24] | 25.04 [4] | 69.71 [4] |
| Octylamine | 273.37 | 273.15 [4,25] | 34.74 [4] | 72.51 [4] |
| Decylamine | 289.16 | 289.26 [4,26] | 42.70 [4] | 33.40 [4] |
| 1,3-Diaminopropane | 262.19 | 262.37 [4,27] | 22.36 [4] | 66.31 [4] |
| Benzonitrile | 260.67 | 260.33 [28] | 10.98 [28], 10.87 [29] | |

$T_{fus}$: melting temperature; $\Delta_{fus}H$: enthalpy of fusion; $\Delta_{fus}C_p$: heat capacity at the melting temperature.

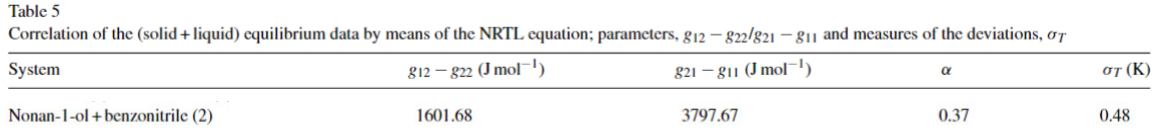


Table 5

Correlation of the (solid + liquid) equilibrium data by means of the NRTL equation; parameters, $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations, $\sigma_T$

| System | $g_{12} - g_{22}$ (J mol$^{-1}$) | $g_{21} - g_{11}$ (J mol$^{-1}$) | $\alpha$ | $\sigma_T$ (K) |
|---|---|---|---|---|
| Nonan-1-ol + benzonitrile (2) | 1601.68 | 3797.67 | 0.37 | 0.48 |

hexylamine + benzonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) phase equilibria of (alkan-1-ol +benzonitrile), (amine + benzonitrile) binary mixtures, and(decan-1-ol + decylamine + benzonitrile) ternary mixtures, Fluid Phase Equilibria 251 (2007) 161–166

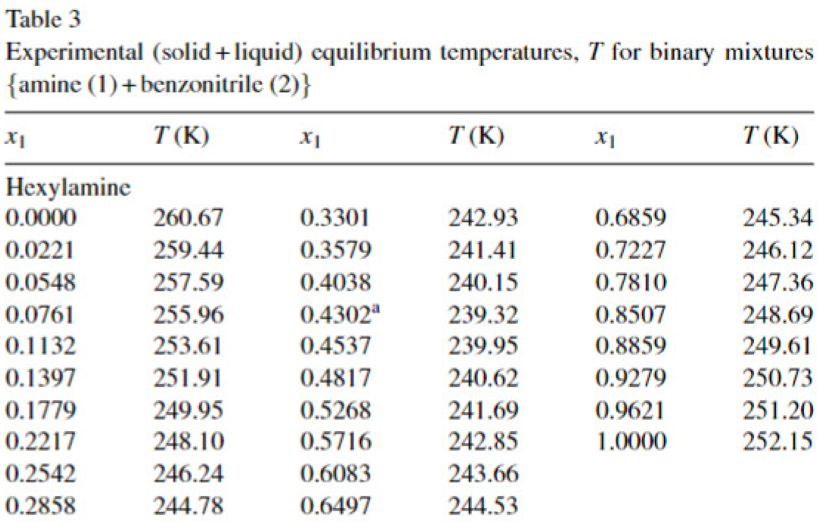


Table 3

Experimental (solid + liquid) equilibrium temperatures, $T$ for binary mixtures {amine (1) + benzonitrile (2)}

| $x_1$ | $T$ (K) | $x_1$ | $T$ (K) | $x_1$ | $T$ (K) |
|---|---|---|---|---|---|
| Hexylamine | | | | | |
| 0.0000 | 260.67 | 0.3301 | 242.93 | 0.6859 | 245.34 |
| 0.0221 | 259.44 | 0.3579 | 241.41 | 0.7227 | 246.12 |
| 0.0548 | 257.59 | 0.4038 | 240.15 | 0.7810 | 247.36 |
| 0.0761 | 255.96 | 0.4302[a] | 239.32 | 0.8507 | 248.69 |
| 0.1132 | 253.61 | 0.4537 | 239.95 | 0.8859 | 249.61 |
| 0.1397 | 251.91 | 0.4817 | 240.62 | 0.9279 | 250.73 |
| 0.1779 | 249.95 | 0.5268 | 241.69 | 0.9621 | 251.20 |
| 0.2217 | 248.10 | 0.5716 | 242.85 | 1.0000 | 252.15 |
| 0.2542 | 246.24 | 0.6083 | 243.66 | | |
| 0.2858 | 244.78 | 0.6497 | 244.53 | | |

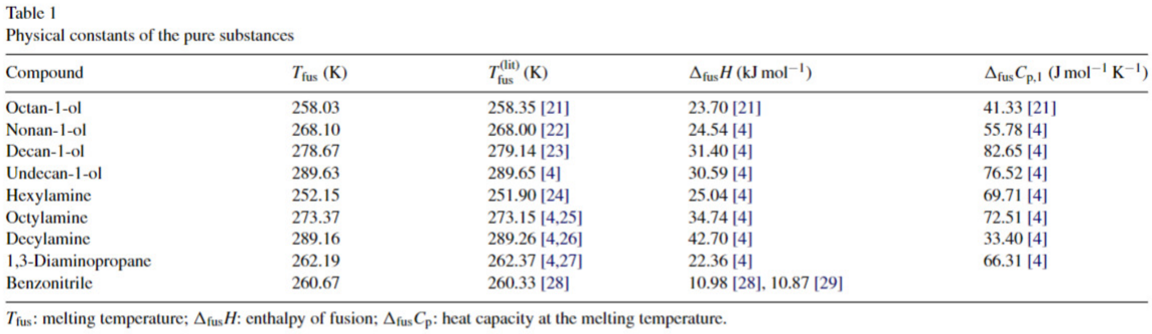


Table 1

Physical constants of the pure substances

| Compound | $T_{fus}$ (K) | $T_{fus}^{(lit)}$ (K) | $\Delta_{fus}H$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35 [21] | 23.70 [21] | 41.33 [21] |
| Nonan-1-ol | 268.10 | 268.00 [22] | 24.54 [4] | 55.78 [4] |
| Decan-1-ol | 278.67 | 279.14 [23] | 31.40 [4] | 82.65 [4] |
| Undecan-1-ol | 289.63 | 289.65 [4] | 30.59 [4] | 76.52 [4] |
| Hexylamine | 252.15 | 251.90 [24] | 25.04 [4] | 69.71 [4] |
| Octylamine | 273.37 | 273.15 [4,25] | 34.74 [4] | 72.51 [4] |
| Decylamine | 289.16 | 289.26 [4,26] | 42.70 [4] | 33.40 [4] |
| 1,3-Diaminopropane | 262.19 | 262.37 [4,27] | 22.36 [4] | 66.31 [4] |
| Benzonitrile | 260.67 | 260.33 [28] | 10.98 [28], 10.87 [29] | |

$T_{fus}$: melting temperature; $\Delta_{fus}H$: enthalpy of fusion; $\Delta_{fus}C_p$: heat capacity at the melting temperature.

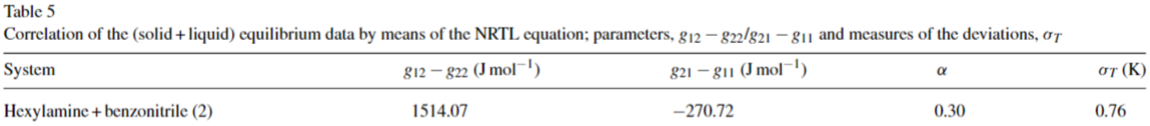


Table 5

Correlation of the (solid + liquid) equilibrium data by means of the NRTL equation; parameters, $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations, $\sigma_T$

| System | $g_{12} - g_{22}$ (J mol$^{-1}$) | $g_{21} - g_{11}$ (J mol$^{-1}$) | $\alpha$ | $\sigma_T$ (K) |
|---|---|---|---|---|
| Hexylamine + benzonitrile (2) | 1514.07 | −270.72 | 0.30 | 0.76 |

octylamine + benzonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) phase equilibria of (alkan-1-ol +benzonitrile), (amine + benzonitrile) binary mixtures, and(decan-1-ol + decylamine + benzonitrile) ternary mixtures, Fluid Phase Equilibria 251 (2007) 161–166

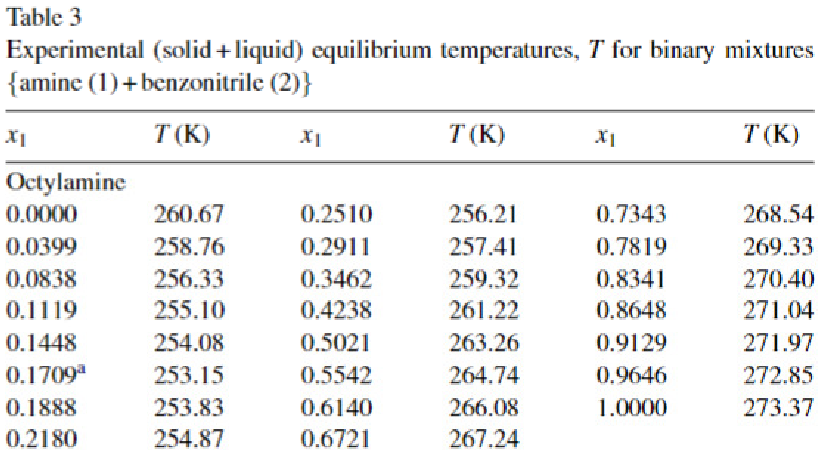


Table 3

Experimental (solid + liquid) equilibrium temperatures, $T$ for binary mixtures {amine (1) + benzonitrile (2)}

| $x_1$ | $T$ (K) | $x_1$ | $T$ (K) | $x_1$ | $T$ (K) |
|---|---|---|---|---|---|
| Octylamine | | | | | |
| 0.0000 | 260.67 | 0.2510 | 256.21 | 0.7343 | 268.54 |
| 0.0399 | 258.76 | 0.2911 | 257.41 | 0.7819 | 269.33 |
| 0.0838 | 256.33 | 0.3462 | 259.32 | 0.8341 | 270.40 |
| 0.1119 | 255.10 | 0.4238 | 261.22 | 0.8648 | 271.04 |
| 0.1448 | 254.08 | 0.5021 | 263.26 | 0.9129 | 271.97 |
| 0.1709[a] | 253.15 | 0.5542 | 264.74 | 0.9646 | 272.85 |
| 0.1888 | 253.83 | 0.6140 | 266.08 | 1.0000 | 273.37 |
| 0.2180 | 254.87 | 0.6721 | 267.24 | | |

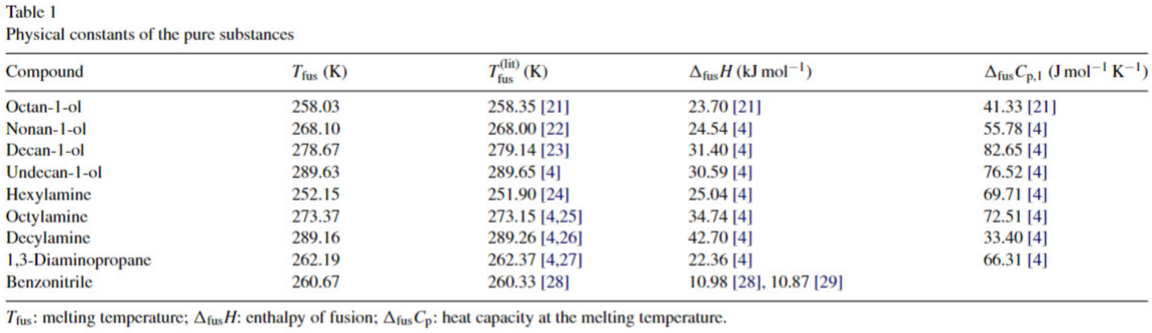


Table 1

Physical constants of the pure substances

| Compound | $T_{fus}$ (K) | $T_{fus}^{(lit)}$ (K) | $\Delta_{fus}H$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35 [21] | 23.70 [21] | 41.33 [21] |
| Nonan-1-ol | 268.10 | 268.00 [22] | 24.54 [4] | 55.78 [4] |
| Decan-1-ol | 278.67 | 279.14 [23] | 31.40 [4] | 82.65 [4] |
| Undecan-1-ol | 289.63 | 289.65 [4] | 30.59 [4] | 76.52 [4] |
| Hexylamine | 252.15 | 251.90 [24] | 25.04 [4] | 69.71 [4] |
| Octylamine | 273.37 | 273.15 [4,25] | 34.74 [4] | 72.51 [4] |
| Decylamine | 289.16 | 289.26 [4,26] | 42.70 [4] | 33.40 [4] |
| 1,3-Diaminopropane | 262.19 | 262.37 [4,27] | 22.36 [4] | 66.31 [4] |
| Benzonitrile | 260.67 | 260.33 [28] | 10.98 [28], 10.87 [29] | |

$T_{fus}$: melting temperature; $\Delta_{fus}H$: enthalpy of fusion; $\Delta_{fus}C_p$: heat capacity at the melting temperature.

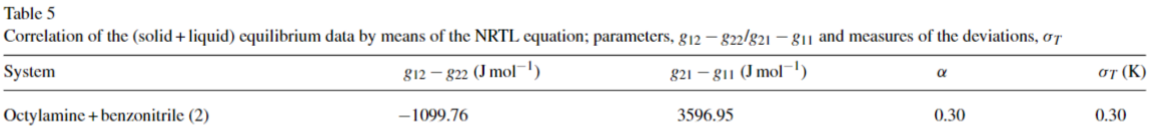


Table 5

Correlation of the (solid + liquid) equilibrium data by means of the NRTL equation; parameters, $g_{12}-g_{22}/g_{21}-g_{11}$ and measures of the deviations, $\sigma_T$

| System | $g_{12}-g_{22}$ (J mol$^{-1}$) | $g_{21}-g_{11}$ (J mol$^{-1}$) | $\alpha$ | $\sigma_T$ (K) |
|---|---|---|---|---|
| Octylamine + benzonitrile (2) | −1099.76 | 3596.95 | 0.30 | 0.30 |

decan-1-ol + benzonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) phase equilibria of (alkan-1-ol +benzonitrile), (amine + benzonitrile) binary mixtures, and(decan-1-ol + decylamine + benzonitrile) ternary mixtures, Fluid Phase Equilibria 251 (2007) 161–166

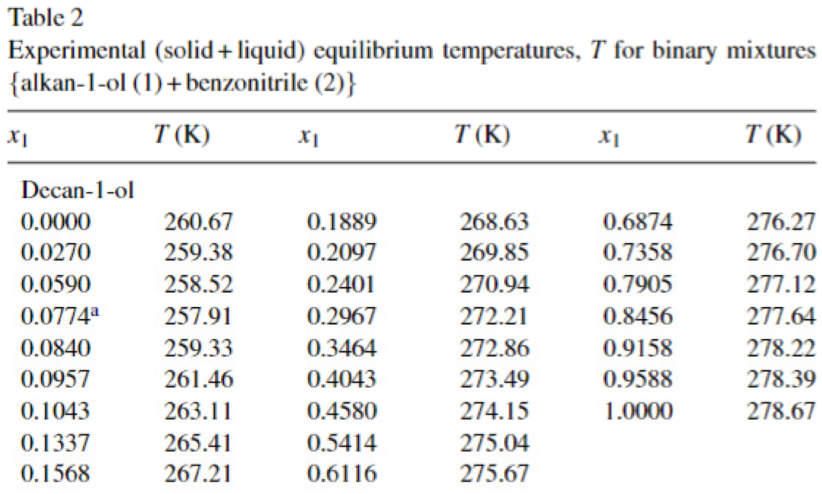


Table 2
Experimental (solid + liquid) equilibrium temperatures, $T$ for binary mixtures {alkan-1-ol (1) + benzonitrile (2)}

| $x_1$ | $T$ (K) | $x_1$ | $T$ (K) | $x_1$ | $T$ (K) |
|---|---|---|---|---|---|
| Decan-1-ol | | | | | |
| 0.0000 | 260.67 | 0.1889 | 268.63 | 0.6874 | 276.27 |
| 0.0270 | 259.38 | 0.2097 | 269.85 | 0.7358 | 276.70 |
| 0.0590 | 258.52 | 0.2401 | 270.94 | 0.7905 | 277.12 |
| $0.0774^{a}$ | 257.91 | 0.2967 | 272.21 | 0.8456 | 277.64 |
| 0.0840 | 259.33 | 0.3464 | 272.86 | 0.9158 | 278.22 |
| 0.0957 | 261.46 | 0.4043 | 273.49 | 0.9588 | 278.39 |
| 0.1043 | 263.11 | 0.4580 | 274.15 | 1.0000 | 278.67 |
| 0.1337 | 265.41 | 0.5414 | 275.04 | | |
| 0.1568 | 267.21 | 0.6116 | 275.67 | | |

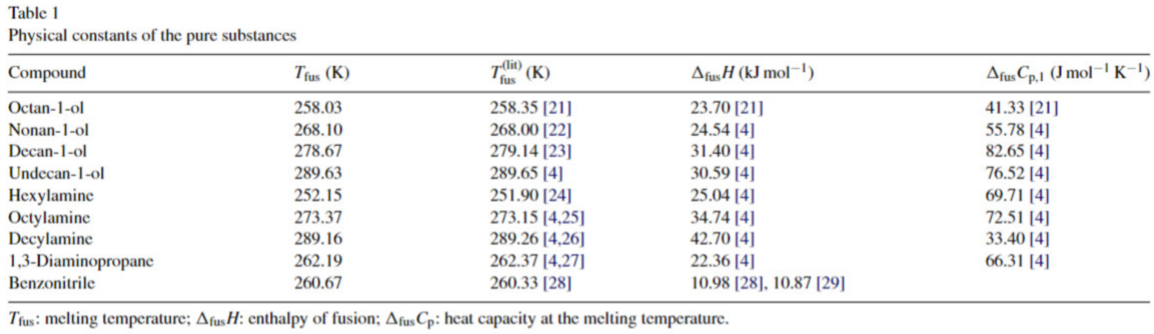


Table 1
Physical constants of the pure substances

| Compound | $T_{\mathrm{fus}}$ (K) | $T_{\mathrm{fus}}^{(\mathrm{lit})}$ (K) | $\Delta_{\mathrm{fus}}H$ (kJ mol$^{-1}$) | $\Delta_{\mathrm{fus}}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35 [21] | 23.70 [21] | 41.33 [21] |
| Nonan-1-ol | 268.10 | 268.00 [22] | 24.54 [4] | 55.78 [4] |
| Decan-1-ol | 278.67 | 279.14 [23] | 31.40 [4] | 82.65 [4] |
| Undecan-1-ol | 289.63 | 289.65 [4] | 30.59 [4] | 76.52 [4] |
| Hexylamine | 252.15 | 251.90 [24] | 25.04 [4] | 69.71 [4] |
| Octylamine | 273.37 | 273.15 [4,25] | 34.74 [4] | 72.51 [4] |
| Decylamine | 289.16 | 289.26 [4,26] | 42.70 [4] | 33.40 [4] |
| 1,3-Diaminopropane | 262.19 | 262.37 [4,27] | 22.36 [4] | 66.31 [4] |
| Benzonitrile | 260.67 | 260.33 [28] | 10.98 [28], 10.87 [29] | |

$T_{\mathrm{fus}}$: melting temperature; $\Delta_{\mathrm{fus}}H$: enthalpy of fusion; $\Delta_{\mathrm{fus}}C_p$: heat capacity at the melting temperature.

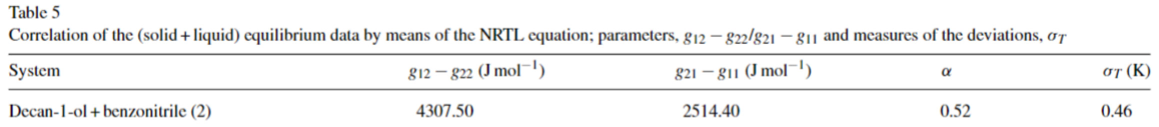


Table 5
Correlation of the (solid + liquid) equilibrium data by means of the NRTL equation; parameters, $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations, $\sigma_T$

| System | $g_{12} - g_{22}$ (J mol$^{-1}$) | $g_{21} - g_{11}$ (J mol$^{-1}$) | $\alpha$ | $\sigma_T$ (K) |
|---|---|---|---|---|
| Decan-1-ol + benzonitrile (2) | 4307.50 | 2514.40 | 0.52 | 0.46 |

undecan-1-ol + benzonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) phase equilibria of (alkan-1-ol +benzonitrile), (amine + benzonitrile) binary mixtures, and(decan-1-ol + decylamine + benzonitrile) ternary mixtures, Fluid Phase Equilibria 251 (2007) 161–166

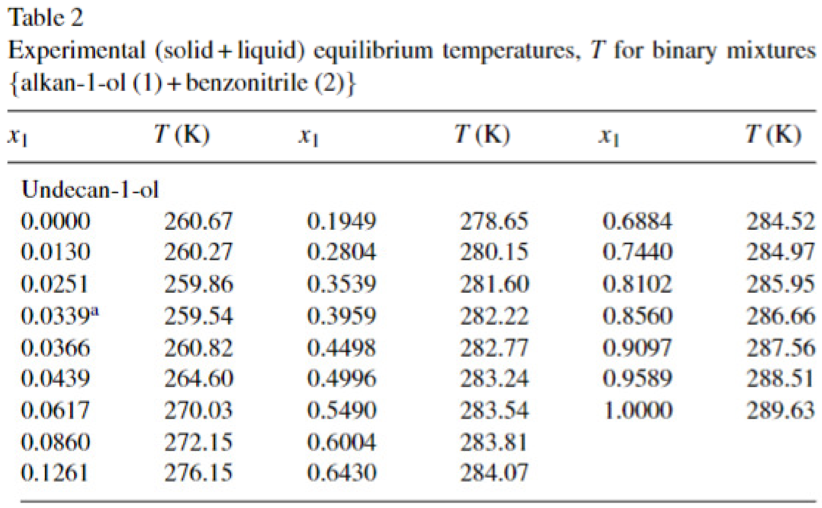


Table 2
Experimental (solid + liquid) equilibrium temperatures, $T$ for binary mixtures {alkan-1-ol (1) + benzonitrile (2)}

| $x_1$ | $T$ (K) | $x_1$ | $T$ (K) | $x_1$ | $T$ (K) |
|---|---|---|---|---|---|
| Undecan-1-ol | | | | | |
| 0.0000 | 260.67 | 0.1949 | 278.65 | 0.6884 | 284.52 |
| 0.0130 | 260.27 | 0.2804 | 280.15 | 0.7440 | 284.97 |
| 0.0251 | 259.86 | 0.3539 | 281.60 | 0.8102 | 285.95 |
| 0.0339[a] | 259.54 | 0.3959 | 282.22 | 0.8560 | 286.66 |
| 0.0366 | 260.82 | 0.4498 | 282.77 | 0.9097 | 287.56 |
| 0.0439 | 264.60 | 0.4996 | 283.24 | 0.9589 | 288.51 |
| 0.0617 | 270.03 | 0.5490 | 283.54 | 1.0000 | 289.63 |
| 0.0860 | 272.15 | 0.6004 | 283.81 | | |
| 0.1261 | 276.15 | 0.6430 | 284.07 | | |

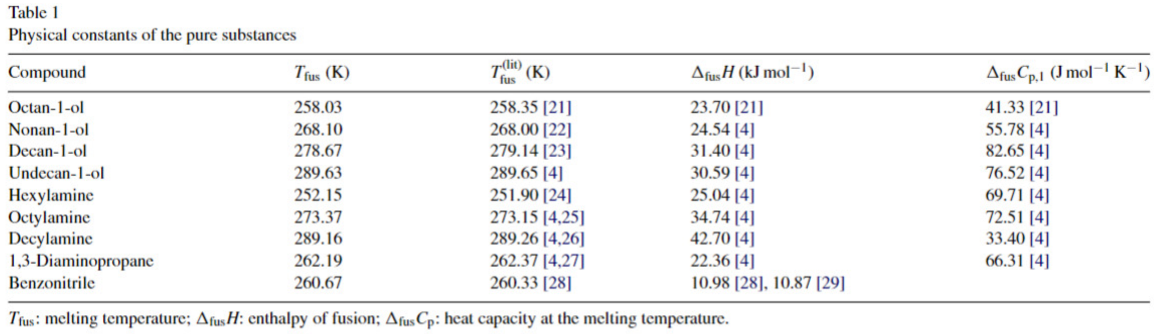


Table 1
Physical constants of the pure substances

| Compound | $T_{fus}$ (K) | $T_{fus}^{(lit)}$ (K) | $\Delta_{fus}H$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35 [21] | 23.70 [21] | 41.33 [21] |
| Nonan-1-ol | 268.10 | 268.00 [22] | 24.54 [4] | 55.78 [4] |
| Decan-1-ol | 278.67 | 279.14 [23] | 31.40 [4] | 82.65 [4] |
| Undecan-1-ol | 289.63 | 289.65 [4] | 30.59 [4] | 76.52 [4] |
| Hexylamine | 252.15 | 251.90 [24] | 25.04 [4] | 69.71 [4] |
| Octylamine | 273.37 | 273.15 [4,25] | 34.74 [4] | 72.51 [4] |
| Decylamine | 289.16 | 289.26 [4,26] | 42.70 [4] | 33.40 [4] |
| 1,3-Diaminopropane | 262.19 | 262.37 [4,27] | 22.36 [4] | 66.31 [4] |
| Benzonitrile | 260.67 | 260.33 [28] | 10.98 [28], 10.87 [29] | |

$T_{fus}$: melting temperature; $\Delta_{fus}H$: enthalpy of fusion; $\Delta_{fus}C_p$: heat capacity at the melting temperature.

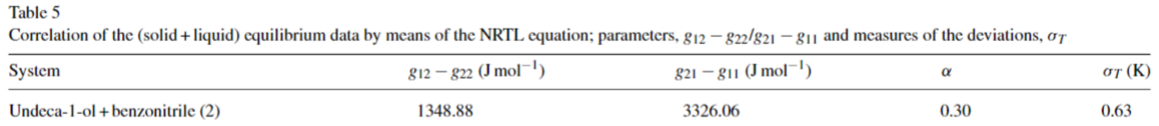


Table 5
Correlation of the (solid + liquid) equilibrium data by means of the NRTL equation; parameters, $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations, $\sigma_T$

| System | $g_{12} - g_{22}$ (J mol$^{-1}$) | $g_{21} - g_{11}$ (J mol$^{-1}$) | $\alpha$ | $\sigma_T$ (K) |
|---|---|---|---|---|
| Undeca-1-ol + benzonitrile (2) | 1348.88 | 3326.06 | 0.30 | 0.63 |

decylamine + benzonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) phase equilibria of (alkan-1-ol +benzonitrile), (amine + benzonitrile) binary mixtures, and(decan-1-ol + decylamine + benzonitrile) ternary mixtures, Fluid Phase Equilibria 251 (2007) 161–166

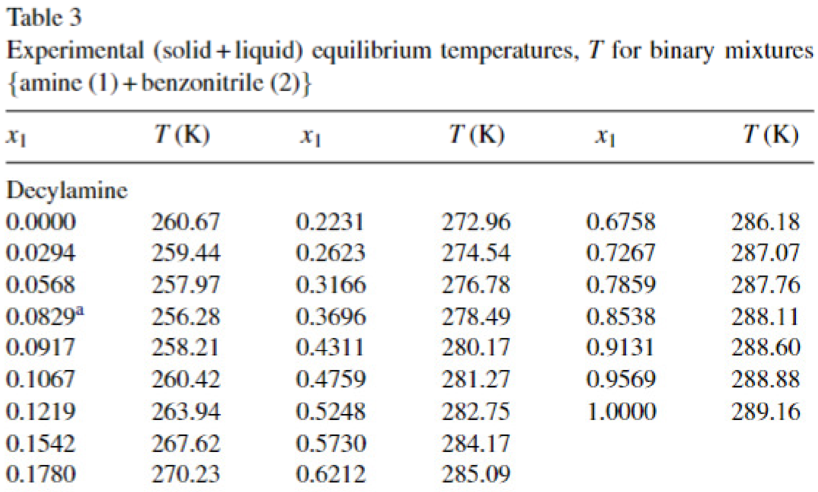


Table 3

Experimental (solid + liquid) equilibrium temperatures, $T$ for binary mixtures {amine (1) + benzonitrile (2)}

| $x_1$ | $T$ (K) | $x_1$ | $T$ (K) | $x_1$ | $T$ (K) |
|---|---|---|---|---|---|
| Decylamine | | | | | |
| 0.0000 | 260.67 | 0.2231 | 272.96 | 0.6758 | 286.18 |
| 0.0294 | 259.44 | 0.2623 | 274.54 | 0.7267 | 287.07 |
| 0.0568 | 257.97 | 0.3166 | 276.78 | 0.7859 | 287.76 |
| 0.0829[a] | 256.28 | 0.3696 | 278.49 | 0.8538 | 288.11 |
| 0.0917 | 258.21 | 0.4311 | 280.17 | 0.9131 | 288.60 |
| 0.1067 | 260.42 | 0.4759 | 281.27 | 0.9569 | 288.88 |
| 0.1219 | 263.94 | 0.5248 | 282.75 | 1.0000 | 289.16 |
| 0.1542 | 267.62 | 0.5730 | 284.17 | | |
| 0.1780 | 270.23 | 0.6212 | 285.09 | | |

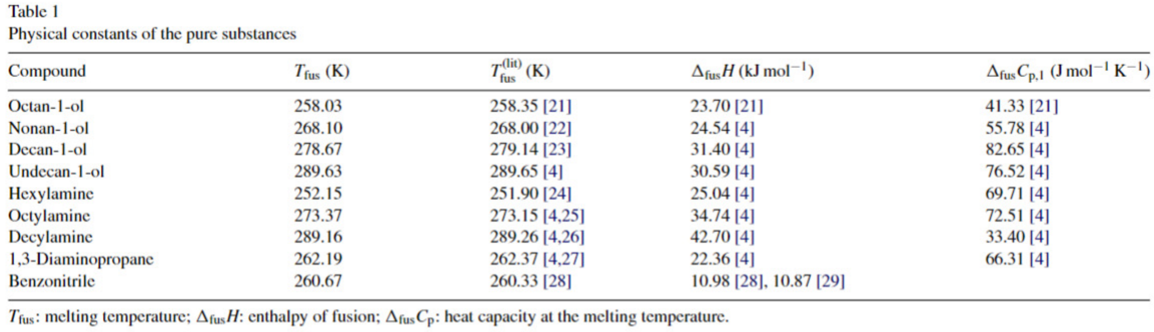


Table 1

Physical constants of the pure substances

| Compound | $T_{\text{fus}}$ (K) | $T_{\text{fus}}^{(\text{lit})}$ (K) | $\Delta_{\text{fus}}H$ (kJ mol$^{-1}$) | $\Delta_{\text{fus}}C_{\text{p},1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35 [21] | 23.70 [21] | 41.33 [21] |
| Nonan-1-ol | 268.10 | 268.00 [22] | 24.54 [4] | 55.78 [4] |
| Decan-1-ol | 278.67 | 279.14 [23] | 31.40 [4] | 82.65 [4] |
| Undecan-1-ol | 289.63 | 289.65 [4] | 30.59 [4] | 76.52 [4] |
| Hexylamine | 252.15 | 251.90 [24] | 25.04 [4] | 69.71 [4] |
| Octylamine | 273.37 | 273.15 [4,25] | 34.74 [4] | 72.51 [4] |
| Decylamine | 289.16 | 289.26 [4,26] | 42.70 [4] | 33.40 [4] |
| 1,3-Diaminopropane | 262.19 | 262.37 [4,27] | 22.36 [4] | 66.31 [4] |
| Benzonitrile | 260.67 | 260.33 [28] | 10.98 [28], 10.87 [29] | |

$T_{\text{fus}}$: melting temperature; $\Delta_{\text{fus}}H$: enthalpy of fusion; $\Delta_{\text{fus}}C_{\text{p}}$: heat capacity at the melting temperature.

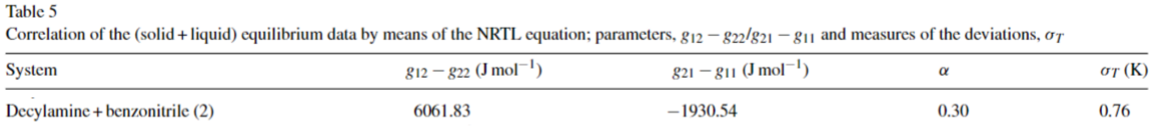


Table 5

Correlation of the (solid + liquid) equilibrium data by means of the NRTL equation; parameters, $g_{12}-g_{22}/g_{21}-g_{11}$ and measures of the deviations, $\sigma_T$

| System | $g_{12}-g_{22}$ (J mol$^{-1}$) | $g_{21}-g_{11}$ (J mol$^{-1}$) | $\alpha$ | $\sigma_T$ (K) |
|---|---|---|---|---|
| Decylamine + benzonitrile (2) | 6061.83 | −1930.54 | 0.30 | 0.76 |

1,3-diaminopropane + benzonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) phase equilibria of (alkan-1-ol +benzonitrile), (amine + benzonitrile) binary mixtures, and(decan-1-ol + decylamine + benzonitrile) ternary mixtures, Fluid Phase Equilibria 251 (2007) 161–166

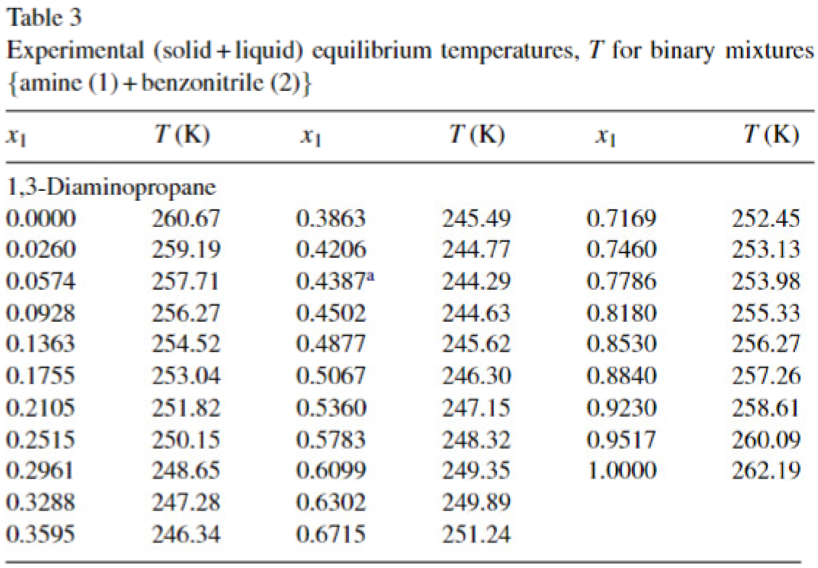


Table 3

Experimental (solid + liquid) equilibrium temperatures, $T$ for binary mixtures {amine (1) + benzonitrile (2)}

| $x_1$ | $T$ (K) | $x_1$ | $T$ (K) | $x_1$ | $T$ (K) |
|---|---|---|---|---|---|
| 1,3-Diaminopropane | | | | | |
| 0.0000 | 260.67 | 0.3863 | 245.49 | 0.7169 | 252.45 |
| 0.0260 | 259.19 | 0.4206 | 244.77 | 0.7460 | 253.13 |
| 0.0574 | 257.71 | 0.4387[a] | 244.29 | 0.7786 | 253.98 |
| 0.0928 | 256.27 | 0.4502 | 244.63 | 0.8180 | 255.33 |
| 0.1363 | 254.52 | 0.4877 | 245.62 | 0.8530 | 256.27 |
| 0.1755 | 253.04 | 0.5067 | 246.30 | 0.8840 | 257.26 |
| 0.2105 | 251.82 | 0.5360 | 247.15 | 0.9230 | 258.61 |
| 0.2515 | 250.15 | 0.5783 | 248.32 | 0.9517 | 260.09 |
| 0.2961 | 248.65 | 0.6099 | 249.35 | 1.0000 | 262.19 |
| 0.3288 | 247.28 | 0.6302 | 249.89 | | |
| 0.3595 | 246.34 | 0.6715 | 251.24 | | |

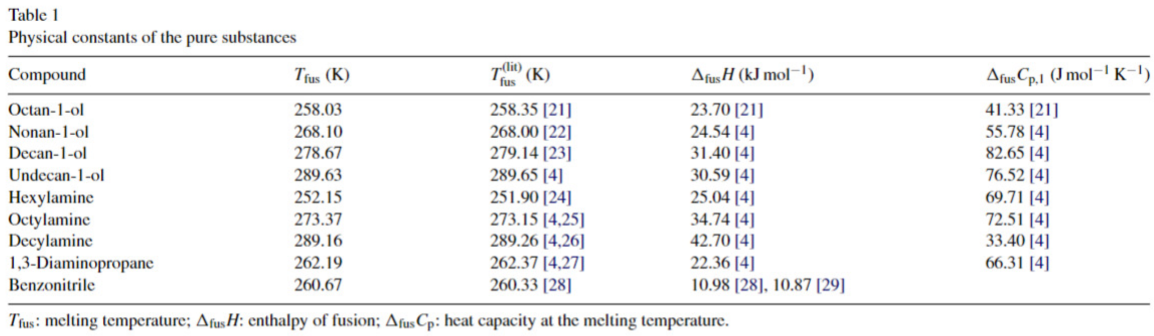


Table 1

Physical constants of the pure substances

| Compound | $T_{fus}$ (K) | $T_{fus}^{(lit)}$ (K) | $\Delta_{fus}H$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p,1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35 [21] | 23.70 [21] | 41.33 [21] |
| Nonan-1-ol | 268.10 | 268.00 [22] | 24.54 [4] | 55.78 [4] |
| Decan-1-ol | 278.67 | 279.14 [23] | 31.40 [4] | 82.65 [4] |
| Undecan-1-ol | 289.63 | 289.65 [4] | 30.59 [4] | 76.52 [4] |
| Hexylamine | 252.15 | 251.90 [24] | 25.04 [4] | 69.71 [4] |
| Octylamine | 273.37 | 273.15 [4,25] | 34.74 [4] | 72.51 [4] |
| Decylamine | 289.16 | 289.26 [4,26] | 42.70 [4] | 33.40 [4] |
| 1,3-Diaminopropane | 262.19 | 262.37 [4,27] | 22.36 [4] | 66.31 [4] |
| Benzonitrile | 260.67 | 260.33 [28] | 10.98 [28], 10.87 [29] | |

$T_{fus}$: melting temperature; $\Delta_{fus}H$: enthalpy of fusion; $\Delta_{fus}C_p$: heat capacity at the melting temperature.

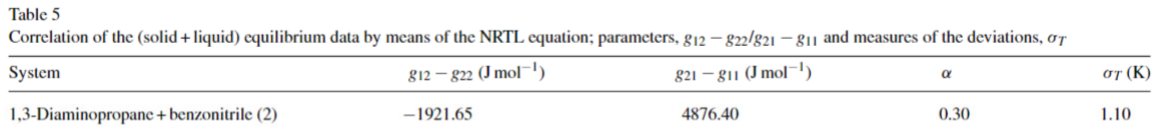


Table 5

Correlation of the (solid + liquid) equilibrium data by means of the NRTL equation; parameters, $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations, $\sigma_T$

| System | $g_{12} - g_{22}$ (J mol$^{-1}$) | $g_{21} - g_{11}$ (J mol$^{-1}$) | $\alpha$ | $\sigma_T$ (K) |
|---|---|---|---|---|
| 1,3-Diaminopropane + benzonitrile (2) | −1921.65 | 4876.40 | 0.30 | 1.10 |

hexylamine + acetonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) or (liquid + liquid) phase equilibria of (amine + nitrile) binary mixtures, J. Chem. Thermodynamics 39 (2007) 247–253

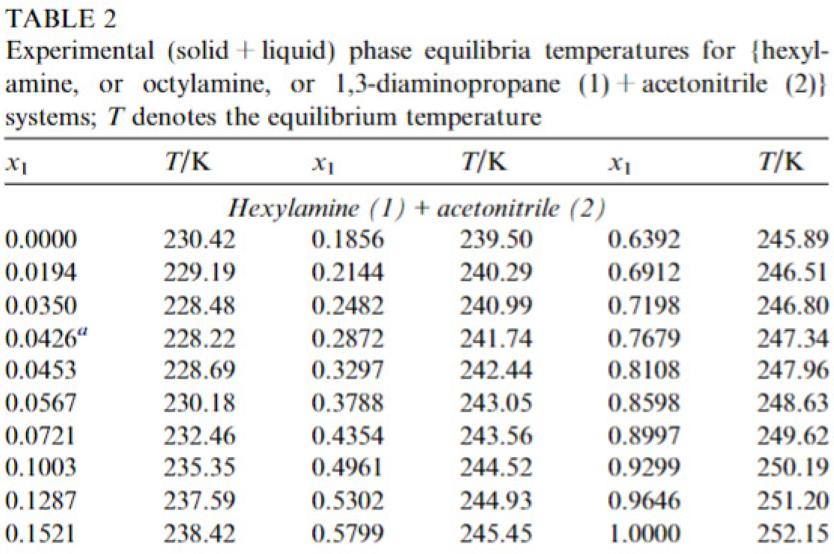


TABLE 2

Experimental (solid + liquid) phase equilibria temperatures for {hexylamine, or octylamine, or 1,3-diaminopropane (1) + acetonitrile (2)} systems; $T$ denotes the equilibrium temperature

| $x_1$ | $T$/K | $x_1$ | $T$/K | $x_1$ | $T$/K |
|---|---|---|---|---|---|
| | | *Hexylamine (1) + acetonitrile (2)* | | | |
| 0.0000 | 230.42 | 0.1856 | 239.50 | 0.6392 | 245.89 |
| 0.0194 | 229.19 | 0.2144 | 240.29 | 0.6912 | 246.51 |
| 0.0350 | 228.48 | 0.2482 | 240.99 | 0.7198 | 246.80 |
| 0.0426[a] | 228.22 | 0.2872 | 241.74 | 0.7679 | 247.34 |
| 0.0453 | 228.69 | 0.3297 | 242.44 | 0.8108 | 247.96 |
| 0.0567 | 230.18 | 0.3788 | 243.05 | 0.8598 | 248.63 |
| 0.0721 | 232.46 | 0.4354 | 243.56 | 0.8997 | 249.62 |
| 0.1003 | 235.35 | 0.4961 | 244.52 | 0.9299 | 250.19 |
| 0.1287 | 237.59 | 0.5302 | 244.93 | 0.9646 | 251.20 |
| 0.1521 | 238.42 | 0.5799 | 245.45 | 1.0000 | 252.15 |

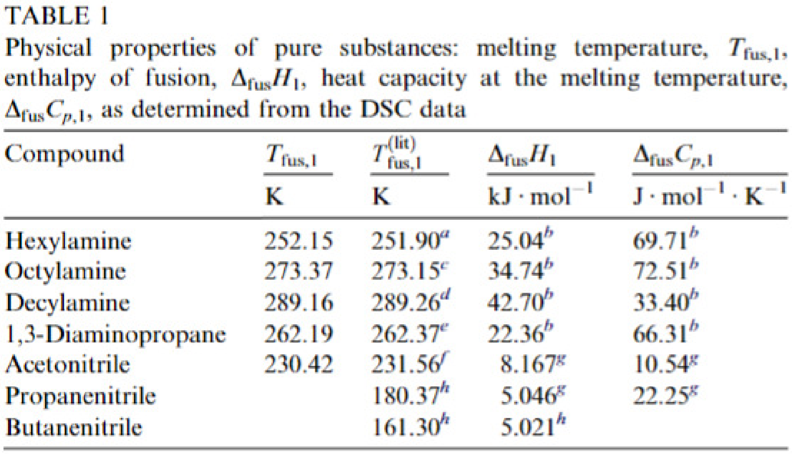


TABLE 1

Physical properties of pure substances: melting temperature, $T_{\mathrm{fus},1}$, enthalpy of fusion, $\Delta_{\mathrm{fus}}H_1$, heat capacity at the melting temperature, $\Delta_{\mathrm{fus}}C_{p,1}$, as determined from the DSC data

| Compound | $\frac{T_{\mathrm{fus},1}}{\mathrm{K}}$ | $\frac{T^{(\mathrm{lit})}_{\mathrm{fus},1}}{\mathrm{K}}$ | $\frac{\Delta_{\mathrm{fus}}H_1}{\mathrm{kJ \cdot mol^{-1}}}$ | $\frac{\Delta_{\mathrm{fus}}C_{p,1}}{\mathrm{J \cdot mol^{-1} \cdot K^{-1}}}$ |
|---|---|---|---|---|
| Hexylamine | 252.15 | 251.90[a] | 25.04[b] | 69.71[b] |
| Octylamine | 273.37 | 273.15[c] | 34.74[b] | 72.51[b] |
| Decylamine | 289.16 | 289.26[d] | 42.70[b] | 33.40[b] |
| 1,3-Diaminopropane | 262.19 | 262.37[e] | 22.36[b] | 66.31[b] |
| Acetonitrile | 230.42 | 231.56[f] | 8.167[g] | 10.54[g] |
| Propanenitrile | | 180.37[h] | 5.046[g] | 22.25[g] |
| Butanenitrile | | 161.30[h] | 5.021[h] | |

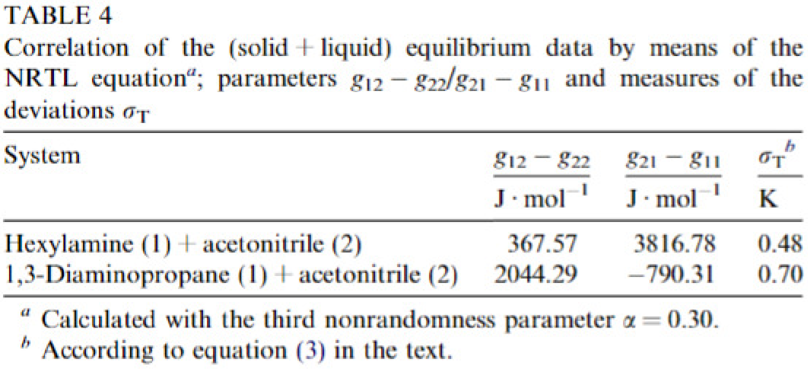


TABLE 4

Correlation of the (solid + liquid) equilibrium data by means of the NRTL equation[a]; parameters $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations $\sigma_T$

| System | $\frac{g_{12} - g_{22}}{\mathrm{J \cdot mol^{-1}}}$ | $\frac{g_{21} - g_{11}}{\mathrm{J \cdot mol^{-1}}}$ | $\frac{\sigma_T{}^{b}}{\mathrm{K}}$ |
|---|---|---|---|
| Hexylamine (1) + acetonitrile (2) | 367.57 | 3816.78 | 0.48 |
| 1,3-Diaminopropane (1) + acetonitrile (2) | 2044.29 | −790.31 | 0.70 |

[a] Calculated with the third nonrandomness parameter $\alpha = 0.30$.

[b] According to equation (3) in the text.

octylamine + acetonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) or (liquid + liquid) phase equilibria of (amine + nitrile) binary mixtures, J. Chem. Thermodynamics 39 (2007) 247–253

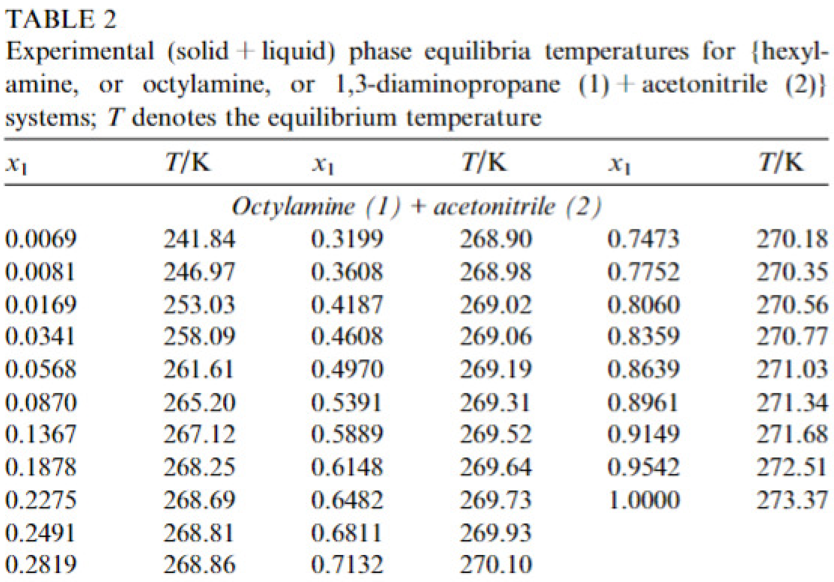


TABLE 2

Experimental (solid + liquid) phase equilibria temperatures for {hexylamine, or octylamine, or 1,3-diaminopropane (1) + acetonitrile (2)} systems; $T$ denotes the equilibrium temperature

| $x_1$ | $T$/K | $x_1$ | $T$/K | $x_1$ | $T$/K |
|---|---|---|---|---|---|
| | | *Octylamine (1) + acetonitrile (2)* | | | |
| 0.0069 | 241.84 | 0.3199 | 268.90 | 0.7473 | 270.18 |
| 0.0081 | 246.97 | 0.3608 | 268.98 | 0.7752 | 270.35 |
| 0.0169 | 253.03 | 0.4187 | 269.02 | 0.8060 | 270.56 |
| 0.0341 | 258.09 | 0.4608 | 269.06 | 0.8359 | 270.77 |
| 0.0568 | 261.61 | 0.4970 | 269.19 | 0.8639 | 271.03 |
| 0.0870 | 265.20 | 0.5391 | 269.31 | 0.8961 | 271.34 |
| 0.1367 | 267.12 | 0.5889 | 269.52 | 0.9149 | 271.68 |
| 0.1878 | 268.25 | 0.6148 | 269.64 | 0.9542 | 272.51 |
| 0.2275 | 268.69 | 0.6482 | 269.73 | 1.0000 | 273.37 |
| 0.2491 | 268.81 | 0.6811 | 269.93 | | |
| 0.2819 | 268.86 | 0.7132 | 270.10 | | |

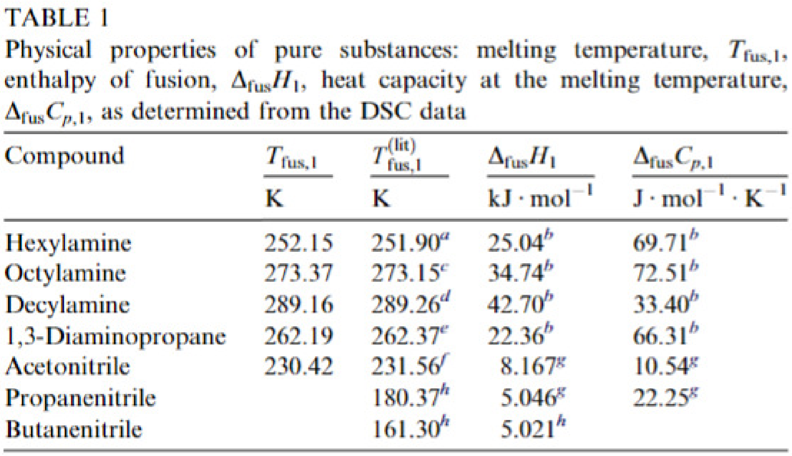


TABLE 1

Physical properties of pure substances: melting temperature, $T_{\mathrm{fus},1}$, enthalpy of fusion, $\Delta_{\mathrm{fus}}H_1$, heat capacity at the melting temperature, $\Delta_{\mathrm{fus}}C_{p,1}$, as determined from the DSC data

| Compound | $T_{\mathrm{fus},1}$ / K | $T_{\mathrm{fus},1}^{(\mathrm{lit})}$ / K | $\Delta_{\mathrm{fus}}H_1$ / $\mathrm{kJ \cdot mol^{-1}}$ | $\Delta_{\mathrm{fus}}C_{p,1}$ / $\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$ |
|---|---|---|---|---|
| Hexylamine | 252.15 | 251.90[a] | 25.04[b] | 69.71[b] |
| Octylamine | 273.37 | 273.15[c] | 34.74[b] | 72.51[b] |
| Decylamine | 289.16 | 289.26[d] | 42.70[b] | 33.40[b] |
| 1,3-Diaminopropane | 262.19 | 262.37[e] | 22.36[b] | 66.31[b] |
| Acetonitrile | 230.42 | 231.56[f] | 8.167[g] | 10.54[g] |
| Propanenitrile | | 180.37[h] | 5.046[g] | 22.25[g] |
| Butanenitrile | | 161.30[h] | 5.021[h] | |

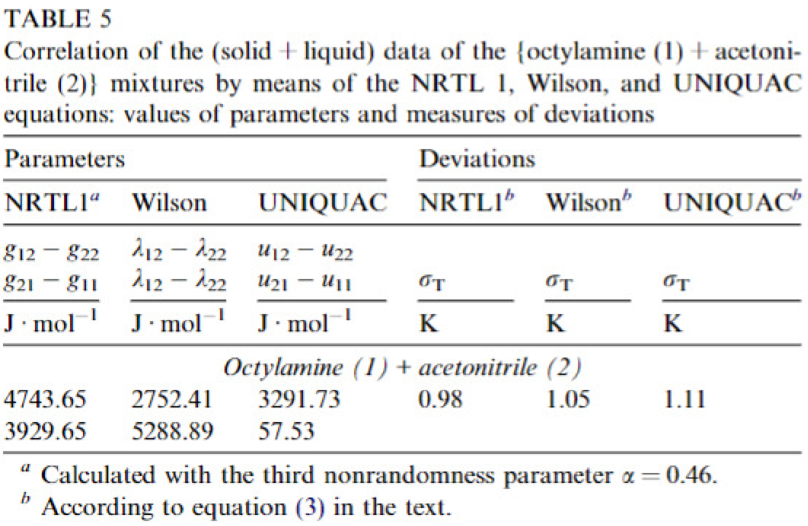


TABLE 5

Correlation of the (solid + liquid) data of the {octylamine (1) + acetonitrile (2)} mixtures by means of the NRTL 1, Wilson, and UNIQUAC equations: values of parameters and measures of deviations

| Parameters | | | Deviations | | |
|---|---|---|---|---|---|
| NRTL1[a] | Wilson | UNIQUAC | NRTL1[b] | Wilson[b] | UNIQUAC[b] |
| $g_{12}-g_{22}$<br>$g_{21}-g_{11}$ | $\lambda_{12}-\lambda_{22}$<br>$\lambda_{12}-\lambda_{22}$ | $u_{12}-u_{22}$<br>$u_{21}-u_{11}$ | $\sigma_T$ | $\sigma_T$ | $\sigma_T$ |
| $\mathrm{J \cdot mol^{-1}}$ | $\mathrm{J \cdot mol^{-1}}$ | $\mathrm{J \cdot mol^{-1}}$ | K | K | K |
| | | *Octylamine (1) + acetonitrile (2)* | | | |
| 4743.65 | 2752.41 | 3291.73 | 0.98 | 1.05 | 1.11 |
| 3929.65 | 5288.89 | 57.53 | | | |

[a] Calculated with the third nonrandomness parameter $\alpha = 0.46$.

[b] According to equation (3) in the text.

ODABRATI JEDAN MODEL

1,3-diaminopropane + acetonitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) or (liquid + liquid) phase equilibria of (amine + nitrile) binary mixtures, J. Chem. Thermodynamics 39 (2007) 247–253

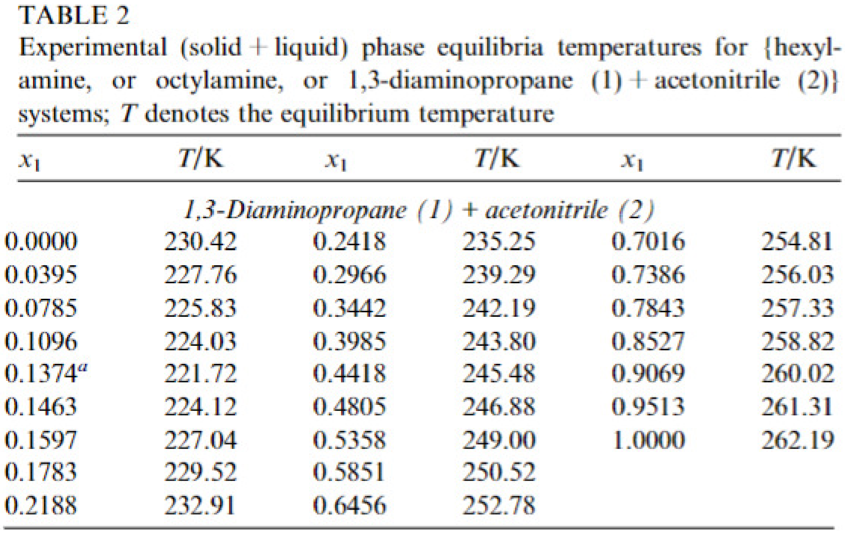


TABLE 2

Experimental (solid + liquid) phase equilibria temperatures for {hexylamine, or octylamine, or 1,3-diaminopropane (1) + acetonitrile (2)} systems; $T$ denotes the equilibrium temperature

| $x_1$ | $T$/K | $x_1$ | $T$/K | $x_1$ | $T$/K |
|---|---|---|---|---|---|
| | | *1,3-Diaminopropane (1) + acetonitrile (2)* | | | |
| 0.0000 | 230.42 | 0.2418 | 235.25 | 0.7016 | 254.81 |
| 0.0395 | 227.76 | 0.2966 | 239.29 | 0.7386 | 256.03 |
| 0.0785 | 225.83 | 0.3442 | 242.19 | 0.7843 | 257.33 |
| 0.1096 | 224.03 | 0.3985 | 243.80 | 0.8527 | 258.82 |
| 0.1374[a] | 221.72 | 0.4418 | 245.48 | 0.9069 | 260.02 |
| 0.1463 | 224.12 | 0.4805 | 246.88 | 0.9513 | 261.31 |
| 0.1597 | 227.04 | 0.5358 | 249.00 | 1.0000 | 262.19 |
| 0.1783 | 229.52 | 0.5851 | 250.52 | | |
| 0.2188 | 232.91 | 0.6456 | 252.78 | | |

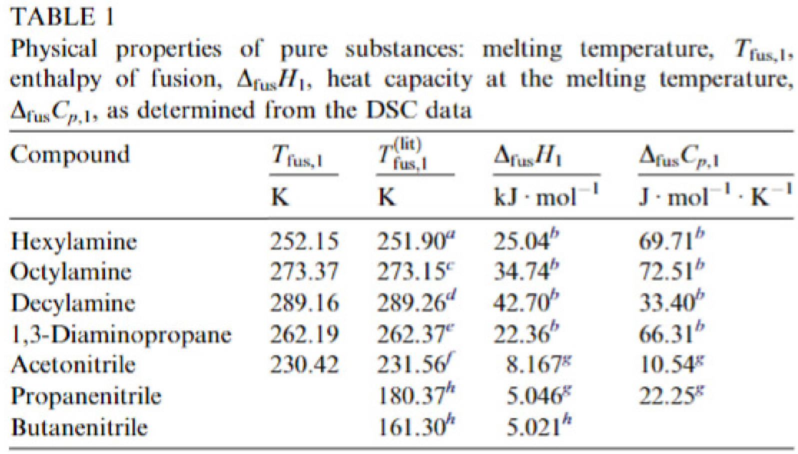


TABLE 1

Physical properties of pure substances: melting temperature, $T_{\mathrm{fus},1}$, enthalpy of fusion, $\Delta_{\mathrm{fus}}H_1$, heat capacity at the melting temperature, $\Delta_{\mathrm{fus}}C_{p,1}$, as determined from the DSC data

| Compound | $T_{\mathrm{fus},1}$ K | $T_{\mathrm{fus},1}^{(\mathrm{lit})}$ K | $\Delta_{\mathrm{fus}}H_1$ kJ · mol$^{-1}$ | $\Delta_{\mathrm{fus}}C_{p,1}$ J · mol$^{-1}$ · K$^{-1}$ |
|---|---|---|---|---|
| Hexylamine | 252.15 | 251.90[a] | 25.04[b] | 69.71[b] |
| Octylamine | 273.37 | 273.15[c] | 34.74[b] | 72.51[b] |
| Decylamine | 289.16 | 289.26[d] | 42.70[b] | 33.40[b] |
| 1,3-Diaminopropane | 262.19 | 262.37[e] | 22.36[b] | 66.31[b] |
| Acetonitrile | 230.42 | 231.56[f] | 8.167[g] | 10.54[g] |
| Propanenitrile | | 180.37[h] | 5.046[g] | 22.25[g] |
| Butanenitrile | | 161.30[h] | 5.021[h] | |

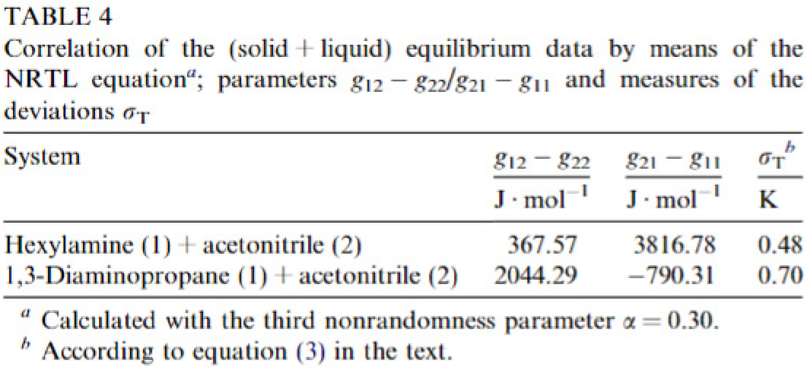


TABLE 4

Correlation of the (solid + liquid) equilibrium data by means of the NRTL equation[a]; parameters $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations $\sigma_T$

| System | $g_{12} - g_{22}$ J · mol$^{-1}$ | $g_{21} - g_{11}$ J · mol$^{-1}$ | $\sigma_T$[b] K |
|---|---|---|---|
| Hexylamine (1) + acetonitrile (2) | 367.57 | 3816.78 | 0.48 |
| 1,3-Diaminopropane (1) + acetonitrile (2) | 2044.29 | −790.31 | 0.70 |

[a] Calculated with the third nonrandomness parameter $\alpha = 0.30$.

[b] According to equation (3) in the text.

octylamine + propanenitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) or (liquid + liquid) phase equilibria of (amine + nitrile) binary mixtures, J. Chem. Thermodynamics 39 (2007) 247–253

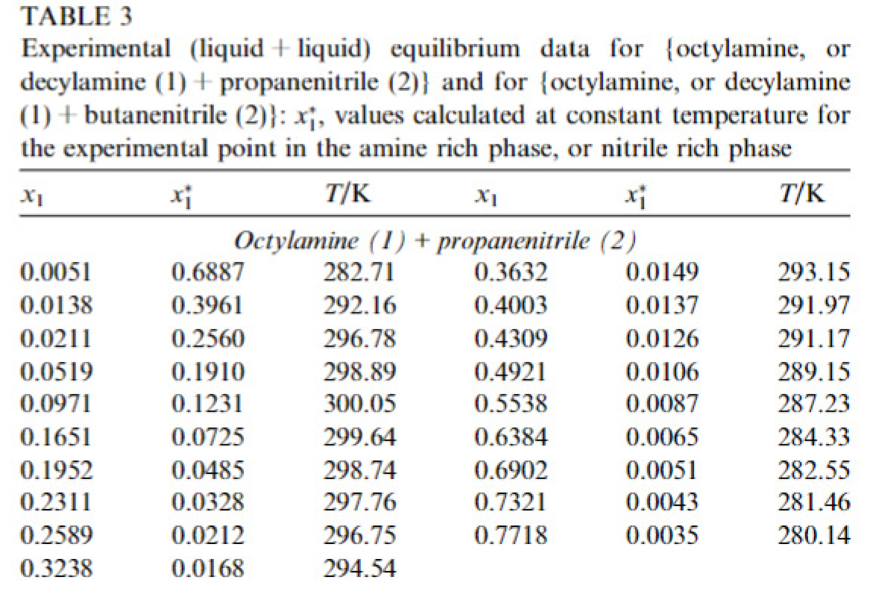


TABLE 3

Experimental (liquid + liquid) equilibrium data for {octylamine, or decylamine (1) + propanenitrile (2)} and for {octylamine, or decylamine (1) + butanenitrile (2)}: $x_1^*$, values calculated at constant temperature for the experimental point in the amine rich phase, or nitrile rich phase

| $x_1$ | $x_1^*$ | $T$/K | $x_1$ | $x_1^*$ | $T$/K |
|---|---|---|---|---|---|
| *Octylamine (1) + propanenitrile (2)* | | | | | |
| 0.0051 | 0.6887 | 282.71 | 0.3632 | 0.0149 | 293.15 |
| 0.0138 | 0.3961 | 292.16 | 0.4003 | 0.0137 | 291.97 |
| 0.0211 | 0.2560 | 296.78 | 0.4309 | 0.0126 | 291.17 |
| 0.0519 | 0.1910 | 298.89 | 0.4921 | 0.0106 | 289.15 |
| 0.0971 | 0.1231 | 300.05 | 0.5538 | 0.0087 | 287.23 |
| 0.1651 | 0.0725 | 299.64 | 0.6384 | 0.0065 | 284.33 |
| 0.1952 | 0.0485 | 298.74 | 0.6902 | 0.0051 | 282.55 |
| 0.2311 | 0.0328 | 297.76 | 0.7321 | 0.0043 | 281.46 |
| 0.2589 | 0.0212 | 296.75 | 0.7718 | 0.0035 | 280.14 |
| 0.3238 | 0.0168 | 294.54 | | | |

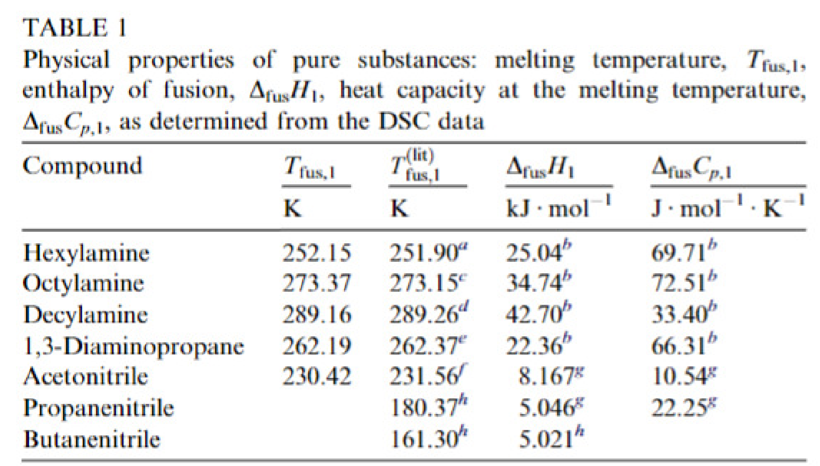


TABLE 1

Physical properties of pure substances: melting temperature, $T_{\mathrm{fus},1}$, enthalpy of fusion, $\Delta_{\mathrm{fus}}H_1$, heat capacity at the melting temperature, $\Delta_{\mathrm{fus}}C_{p,1}$, as determined from the DSC data

| Compound | $T_{\mathrm{fus},1}$ / K | $T_{\mathrm{fus},1}^{(\mathrm{lit})}$ / K | $\Delta_{\mathrm{fus}}H_1$ / $\mathrm{kJ \cdot mol^{-1}}$ | $\Delta_{\mathrm{fus}}C_{p,1}$ / $\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$ |
|---|---|---|---|---|
| Hexylamine | 252.15 | 251.90[a] | 25.04[b] | 69.71[b] |
| Octylamine | 273.37 | 273.15[c] | 34.74[b] | 72.51[b] |
| Decylamine | 289.16 | 289.26[d] | 42.70[b] | 33.40[b] |
| 1,3-Diaminopropane | 262.19 | 262.37[e] | 22.36[b] | 66.31[b] |
| Acetonitrile | 230.42 | 231.56[f] | 8.167[g] | 10.54[g] |
| Propanenitrile | | 180.37[h] | 5.046[g] | 22.25[g] |
| Butanenitrile | | 161.30[h] | 5.021[h] | |

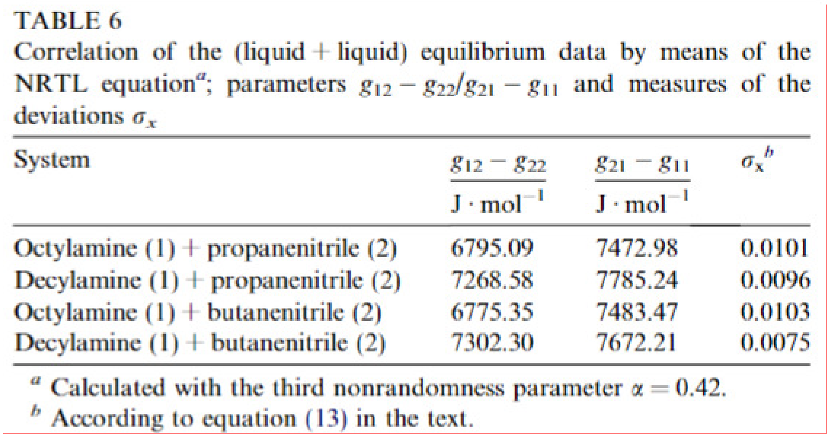


TABLE 6

Correlation of the (liquid + liquid) equilibrium data by means of the NRTL equation[a]; parameters $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations $\sigma_x$

| System | $g_{12} - g_{22}$ / $\mathrm{J \cdot mol^{-1}}$ | $g_{21} - g_{11}$ / $\mathrm{J \cdot mol^{-1}}$ | $\sigma_x$[b] |
|---|---|---|---|
| Octylamine (1) + propanenitrile (2) | 6795.09 | 7472.98 | 0.0101 |
| Decylamine (1) + propanenitrile (2) | 7268.58 | 7785.24 | 0.0096 |
| Octylamine (1) + butanenitrile (2) | 6775.35 | 7483.47 | 0.0103 |
| Decylamine (1) + butanenitrile (2) | 7302.30 | 7672.21 | 0.0075 |

[a] Calculated with the third nonrandomness parameter $\alpha = 0.42$.

[b] According to equation (13) in the text.

decylamine + propanenitrile
Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) or (liquid + liquid) phase equilibria of (amine + nitrile) binary mixtures, J. Chem. Thermodynamics 39 (2007) 247–253

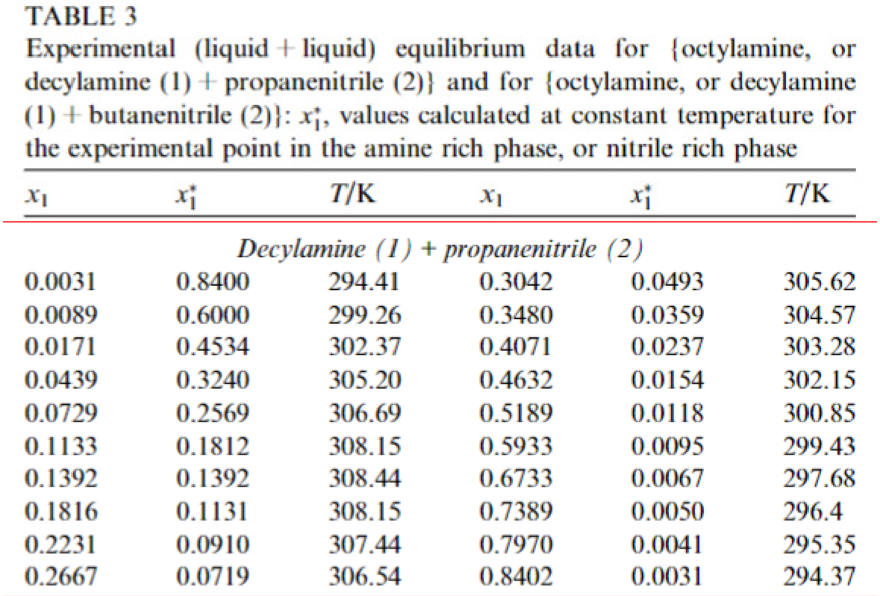


TABLE 3
Experimental (liquid + liquid) equilibrium data for {octylamine, or decylamine (1) + propanenitrile (2)} and for {octylamine, or decylamine (1) + butanenitrile (2)}: $x_1^*$, values calculated at constant temperature for the experimental point in the amine rich phase, or nitrile rich phase

| $x_1$ | $x_1^*$ | $T$/K | $x_1$ | $x_1^*$ | $T$/K |
|---|---|---|---|---|---|
| | | *Decylamine (1) + propanenitrile (2)* | | | |
| 0.0031 | 0.8400 | 294.41 | 0.3042 | 0.0493 | 305.62 |
| 0.0089 | 0.6000 | 299.26 | 0.3480 | 0.0359 | 304.57 |
| 0.0171 | 0.4534 | 302.37 | 0.4071 | 0.0237 | 303.28 |
| 0.0439 | 0.3240 | 305.20 | 0.4632 | 0.0154 | 302.15 |
| 0.0729 | 0.2569 | 306.69 | 0.5189 | 0.0118 | 300.85 |
| 0.1133 | 0.1812 | 308.15 | 0.5933 | 0.0095 | 299.43 |
| 0.1392 | 0.1392 | 308.44 | 0.6733 | 0.0067 | 297.68 |
| 0.1816 | 0.1131 | 308.15 | 0.7389 | 0.0050 | 296.4 |
| 0.2231 | 0.0910 | 307.44 | 0.7970 | 0.0041 | 295.35 |
| 0.2667 | 0.0719 | 306.54 | 0.8402 | 0.0031 | 294.37 |

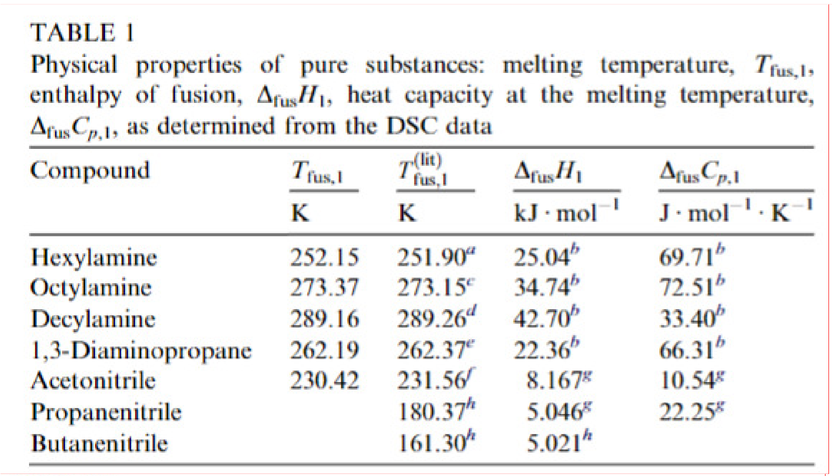


TABLE 1
Physical properties of pure substances: melting temperature, $T_{\text{fus},1}$, enthalpy of fusion, $\Delta_{\text{fus}}H_1$, heat capacity at the melting temperature, $\Delta_{\text{fus}}C_{p,1}$, as determined from the DSC data

| Compound | $T_{\text{fus},1}$<br>K | $T_{\text{fus},1}^{(\text{lit})}$<br>K | $\Delta_{\text{fus}}H_1$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $\Delta_{\text{fus}}C_{p,1}$<br>$\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ |
|---|---|---|---|---|
| Hexylamine | 252.15 | 251.90[a] | 25.04[b] | 69.71[b] |
| Octylamine | 273.37 | 273.15[c] | 34.74[b] | 72.51[b] |
| Decylamine | 289.16 | 289.26[d] | 42.70[b] | 33.40[b] |
| 1,3-Diaminopropane | 262.19 | 262.37[e] | 22.36[b] | 66.31[b] |
| Acetonitrile | 230.42 | 231.56[f] | 8.167[g] | 10.54[g] |
| Propanenitrile | | 180.37[h] | 5.046[g] | 22.25[g] |
| Butanenitrile | | 161.30[h] | 5.021[h] | |

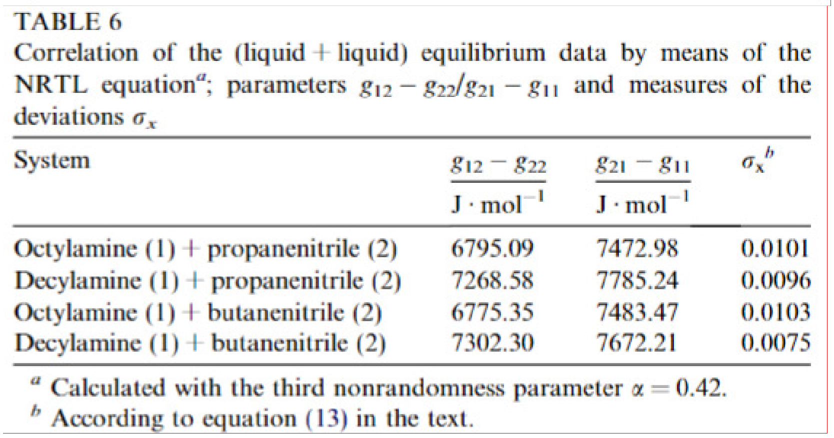


TABLE 6
Correlation of the (liquid + liquid) equilibrium data by means of the NRTL equation[a]; parameters $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations $\sigma_x$

| System | $g_{12} - g_{22}$<br>$\text{J} \cdot \text{mol}^{-1}$ | $g_{21} - g_{11}$<br>$\text{J} \cdot \text{mol}^{-1}$ | $\sigma_x$[b] |
|---|---|---|---|
| Octylamine (1) + propanenitrile (2) | 6795.09 | 7472.98 | 0.0101 |
| Decylamine (1) + propanenitrile (2) | 7268.58 | 7785.24 | 0.0096 |
| Octylamine (1) + butanenitrile (2) | 6775.35 | 7483.47 | 0.0103 |
| Decylamine (1) + butanenitrile (2) | 7302.30 | 7672.21 | 0.0075 |

[a] Calculated with the third nonrandomness parameter $\alpha = 0.42$.
[b] According to equation (13) in the text.

octylamine + butanenitrile

Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) or (liquid + liquid) phase equilibria of (amine + nitrile) binary mixtures, J. Chem. Thermodynamics 39 (2007) 247–253

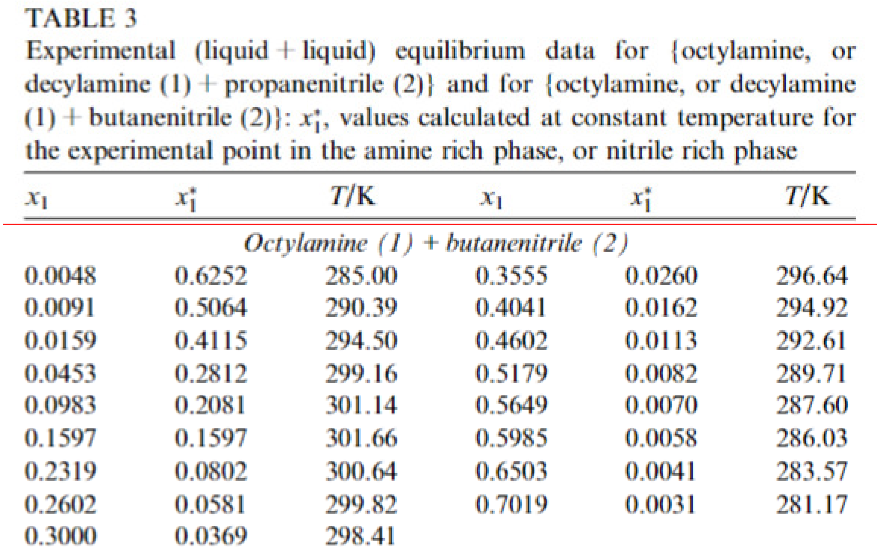


TABLE 3

Experimental (liquid + liquid) equilibrium data for {octylamine, or decylamine (1) + propanenitrile (2)} and for {octylamine, or decylamine (1) + butanenitrile (2)}: $x_1^*$, values calculated at constant temperature for the experimental point in the amine rich phase, or nitrile rich phase

| $x_1$ | $x_1^*$ | $T$/K | $x_1$ | $x_1^*$ | $T$/K |
|---|---|---|---|---|---|
| *Octylamine (1) + butanenitrile (2)* | | | | | |
| 0.0048 | 0.6252 | 285.00 | 0.3555 | 0.0260 | 296.64 |
| 0.0091 | 0.5064 | 290.39 | 0.4041 | 0.0162 | 294.92 |
| 0.0159 | 0.4115 | 294.50 | 0.4602 | 0.0113 | 292.61 |
| 0.0453 | 0.2812 | 299.16 | 0.5179 | 0.0082 | 289.71 |
| 0.0983 | 0.2081 | 301.14 | 0.5649 | 0.0070 | 287.60 |
| 0.1597 | 0.1597 | 301.66 | 0.5985 | 0.0058 | 286.03 |
| 0.2319 | 0.0802 | 300.64 | 0.6503 | 0.0041 | 283.57 |
| 0.2602 | 0.0581 | 299.82 | 0.7019 | 0.0031 | 281.17 |
| 0.3000 | 0.0369 | 298.41 | | | |

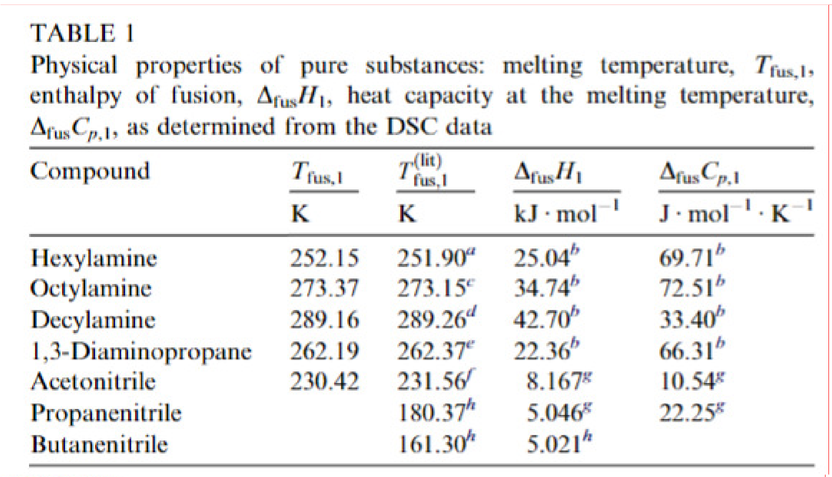


TABLE 1

Physical properties of pure substances: melting temperature, $T_{\mathrm{fus},1}$, enthalpy of fusion, $\Delta_{\mathrm{fus}}H_1$, heat capacity at the melting temperature, $\Delta_{\mathrm{fus}}C_{p,1}$, as determined from the DSC data

| Compound | $T_{\mathrm{fus},1}$ / K | $T_{\mathrm{fus},1}^{(\mathrm{lit})}$ / K | $\Delta_{\mathrm{fus}}H_1$ / $\mathrm{kJ \cdot mol^{-1}}$ | $\Delta_{\mathrm{fus}}C_{p,1}$ / $\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$ |
|---|---|---|---|---|
| Hexylamine | 252.15 | 251.90[a] | 25.04[b] | 69.71[b] |
| Octylamine | 273.37 | 273.15[c] | 34.74[b] | 72.51[b] |
| Decylamine | 289.16 | 289.26[d] | 42.70[b] | 33.40[b] |
| 1,3-Diaminopropane | 262.19 | 262.37[e] | 22.36[b] | 66.31[b] |
| Acetonitrile | 230.42 | 231.56[f] | 8.167[g] | 10.54[g] |
| Propanenitrile | | 180.37[h] | 5.046[g] | 22.25[g] |
| Butanenitrile | | 161.30[h] | 5.021[h] | |

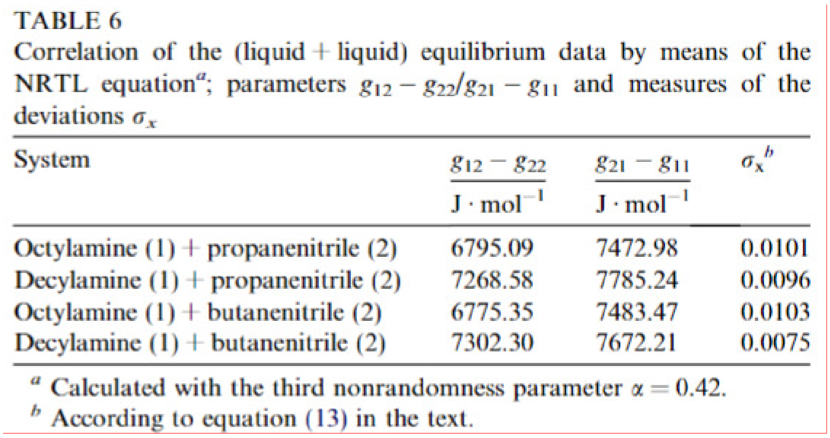


TABLE 6

Correlation of the (liquid + liquid) equilibrium data by means of the NRTL equation[a]; parameters $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations $\sigma_x$

| System | $g_{12} - g_{22}$ / $\mathrm{J \cdot mol^{-1}}$ | $g_{21} - g_{11}$ / $\mathrm{J \cdot mol^{-1}}$ | $\sigma_x$[b] |
|---|---|---|---|
| Octylamine (1) + propanenitrile (2) | 6795.09 | 7472.98 | 0.0101 |
| Decylamine (1) + propanenitrile (2) | 7268.58 | 7785.24 | 0.0096 |
| Octylamine (1) + butanenitrile (2) | 6775.35 | 7483.47 | 0.0103 |
| Decylamine (1) + butanenitrile (2) | 7302.30 | 7672.21 | 0.0075 |

[a] Calculated with the third nonrandomness parameter $\alpha = 0.42$.

[b] According to equation (13) in the text.

decylamine + butanenitrile
Urszula Domanska, Małgorzata Marciniak, Experimental (solid + liquid) or (liquid + liquid) phase equilibria of (amine + nitrile) binary mixtures, J. Chem. Thermodynamics 39 (2007) 247–253

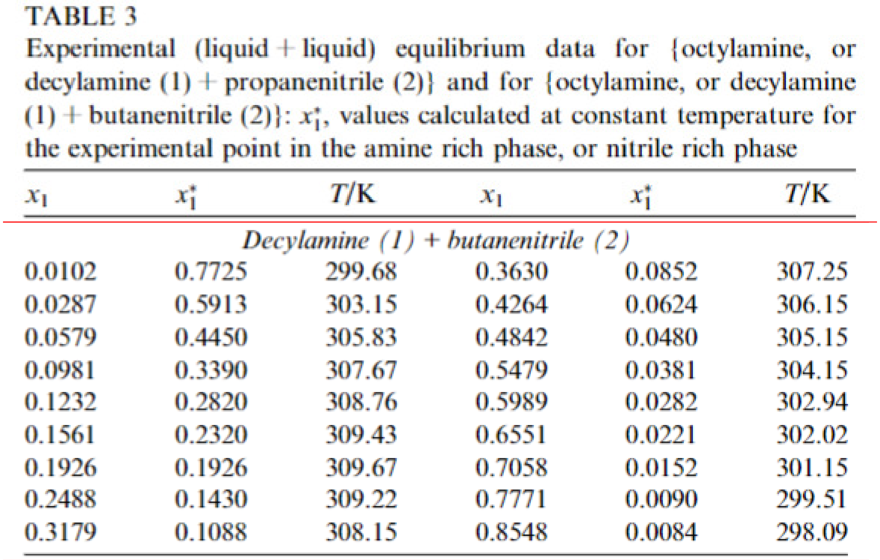


TABLE 3
Experimental (liquid + liquid) equilibrium data for {octylamine, or decylamine (1) + propanenitrile (2)} and for {octylamine, or decylamine (1) + butanenitrile (2)}: $x_1^*$, values calculated at constant temperature for the experimental point in the amine rich phase, or nitrile rich phase

| $x_1$ | $x_1^*$ | $T$/K | $x_1$ | $x_1^*$ | $T$/K |
|---|---|---|---|---|---|
| *Decylamine (1) + butanenitrile (2)* | | | | | |
| 0.0102 | 0.7725 | 299.68 | 0.3630 | 0.0852 | 307.25 |
| 0.0287 | 0.5913 | 303.15 | 0.4264 | 0.0624 | 306.15 |
| 0.0579 | 0.4450 | 305.83 | 0.4842 | 0.0480 | 305.15 |
| 0.0981 | 0.3390 | 307.67 | 0.5479 | 0.0381 | 304.15 |
| 0.1232 | 0.2820 | 308.76 | 0.5989 | 0.0282 | 302.94 |
| 0.1561 | 0.2320 | 309.43 | 0.6551 | 0.0221 | 302.02 |
| 0.1926 | 0.1926 | 309.67 | 0.7058 | 0.0152 | 301.15 |
| 0.2488 | 0.1430 | 309.22 | 0.7771 | 0.0090 | 299.51 |
| 0.3179 | 0.1088 | 308.15 | 0.8548 | 0.0084 | 298.09 |

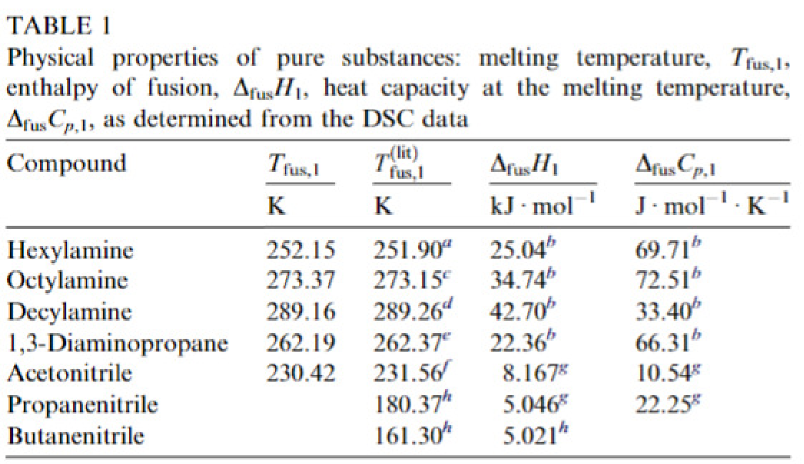


TABLE 1
Physical properties of pure substances: melting temperature, $T_{\mathrm{fus},1}$, enthalpy of fusion, $\Delta_{\mathrm{fus}}H_1$, heat capacity at the melting temperature, $\Delta_{\mathrm{fus}}C_{p,1}$, as determined from the DSC data

| Compound | $T_{\mathrm{fus},1}$ / K | $T_{\mathrm{fus},1}^{(\mathrm{lit})}$ / K | $\Delta_{\mathrm{fus}}H_1$ / $\mathrm{kJ \cdot mol^{-1}}$ | $\Delta_{\mathrm{fus}}C_{p,1}$ / $\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$ |
|---|---|---|---|---|
| Hexylamine | 252.15 | 251.90[a] | 25.04[b] | 69.71[b] |
| Octylamine | 273.37 | 273.15[c] | 34.74[b] | 72.51[b] |
| Decylamine | 289.16 | 289.26[d] | 42.70[b] | 33.40[b] |
| 1,3-Diaminopropane | 262.19 | 262.37[e] | 22.36[b] | 66.31[b] |
| Acetonitrile | 230.42 | 231.56[f] | 8.167[g] | 10.54[g] |
| Propanenitrile | | 180.37[h] | 5.046[g] | 22.25[g] |
| Butanenitrile | | 161.30[h] | 5.021[h] | |

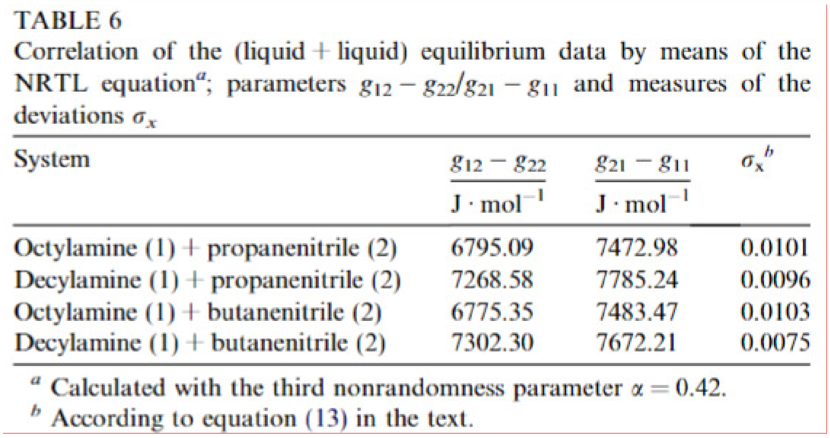


TABLE 6
Correlation of the (liquid + liquid) equilibrium data by means of the NRTL equation[a]; parameters $g_{12} - g_{22}/g_{21} - g_{11}$ and measures of the deviations $\sigma_x$

| System | $g_{12} - g_{22}$ / $\mathrm{J \cdot mol^{-1}}$ | $g_{21} - g_{11}$ / $\mathrm{J \cdot mol^{-1}}$ | $\sigma_x$[b] |
|---|---|---|---|
| Octylamine (1) + propanenitrile (2) | 6795.09 | 7472.98 | 0.0101 |
| Decylamine (1) + propanenitrile (2) | 7268.58 | 7785.24 | 0.0096 |
| Octylamine (1) + butanenitrile (2) | 6775.35 | 7483.47 | 0.0103 |
| Decylamine (1) + butanenitrile (2) | 7302.30 | 7672.21 | 0.0075 |

[a] Calculated with the third nonrandomness parameter $\alpha = 0.42$.
[b] According to equation (13) in the text.

1,4-dioxane + indane

A. Jakob, R. Joh, C. Rose, J. Gmehling, Solid-liquid equilibria in binary mixtures of organic compounds, Fluid Phase Equilibria 113 (1995) 117-126

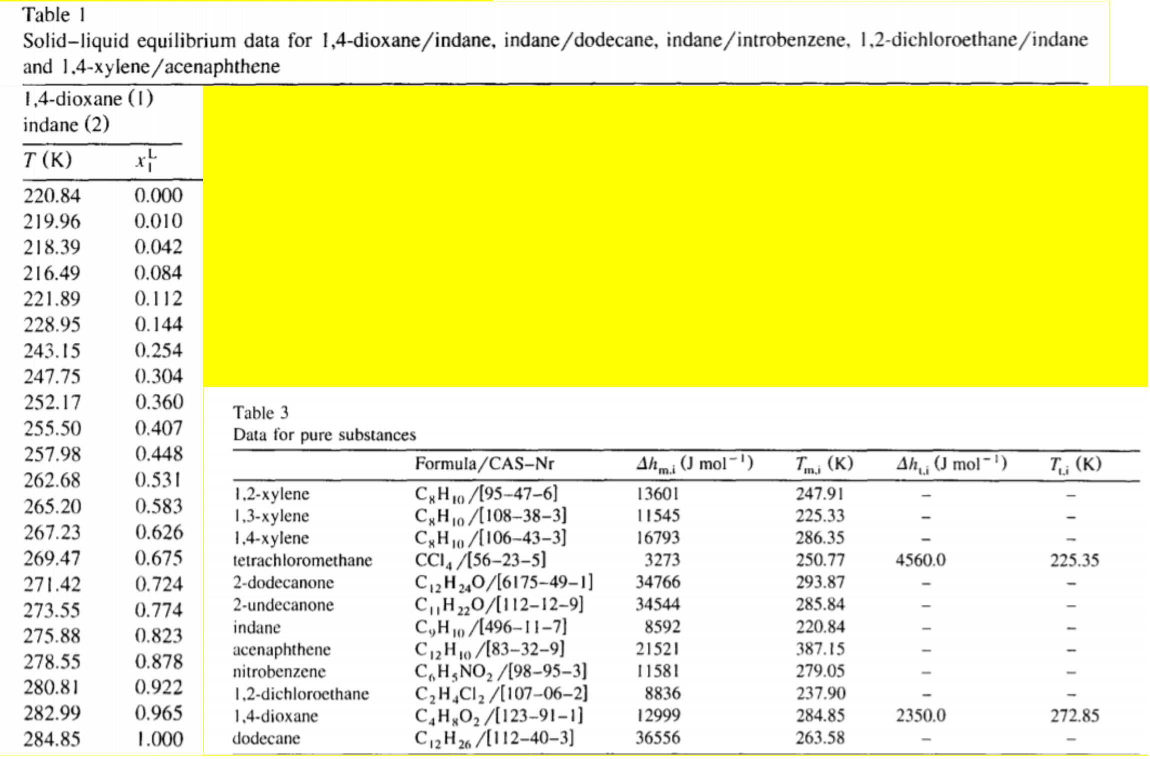


Table 1
Solid–liquid equilibrium data for 1,4-dioxane/indane, indane/dodecane, indane/introbenzene, 1,2-dichloroethane/indane and 1,4-xylene/acenaphthene

| 1,4-dioxane (1)<br>indane (2) | |
|---|---|
| $T$ (K) | $x_1^L$ |
| 220.84 | 0.000 |
| 219.96 | 0.010 |
| 218.39 | 0.042 |
| 216.49 | 0.084 |
| 221.89 | 0.112 |
| 228.95 | 0.144 |
| 243.15 | 0.254 |
| 247.75 | 0.304 |
| 252.17 | 0.360 |
| 255.50 | 0.407 |
| 257.98 | 0.448 |
| 262.68 | 0.531 |
| 265.20 | 0.583 |
| 267.23 | 0.626 |
| 269.47 | 0.675 |
| 271.42 | 0.724 |
| 273.55 | 0.774 |
| 275.88 | 0.823 |
| 278.55 | 0.878 |
| 280.81 | 0.922 |
| 282.99 | 0.965 |
| 284.85 | 1.000 |

[redacted]

Table 3
Data for pure substances

| | Formula/CAS–Nr | $\Delta h_{m,i}$ (J mol$^{-1}$) | $T_{m,i}$ (K) | $\Delta h_{t,i}$ (J mol$^{-1}$) | $T_{t,i}$ (K) |
|---|---|---|---|---|---|
| 1,2-xylene | $C_8H_{10}$/[95–47–6] | 13601 | 247.91 | – | – |
| 1,3-xylene | $C_8H_{10}$/[108–38–3] | 11545 | 225.33 | – | – |
| 1,4-xylene | $C_8H_{10}$/[106–43–3] | 16793 | 286.35 | – | – |
| tetrachloromethane | $CCl_4$/[56–23–5] | 3273 | 250.77 | 4560.0 | 225.35 |
| 2-dodecanone | $C_{12}H_{24}O$/[6175–49–1] | 34766 | 293.87 | – | – |
| 2-undecanone | $C_{11}H_{22}O$/[112–12–9] | 34544 | 285.84 | – | – |
| indane | $C_9H_{10}$/[496–11–7] | 8592 | 220.84 | – | – |
| acenaphthene | $C_{12}H_{10}$/[83–32–9] | 21521 | 387.15 | – | – |
| nitrobenzene | $C_6H_5NO_2$/[98–95–3] | 11581 | 279.05 | – | – |
| 1,2-dichloroethane | $C_2H_4Cl_2$/[107–06–2] | 8836 | 237.90 | – | – |
| 1,4-dioxane | $C_4H_8O_2$/[123–91–1] | 12999 | 284.85 | 2350.0 | 272.85 |
| dodecane | $C_{12}H_{26}$/[112–40–3] | 36556 | 263.58 | – | – |

indane + dodecane

A. Jakob, R. Joh, C. Rose, J. Gmehling, Solid-liquid equilibria in binary mixtures of organic compounds, Fluid Phase Equilibria 113 (1995) 117-126

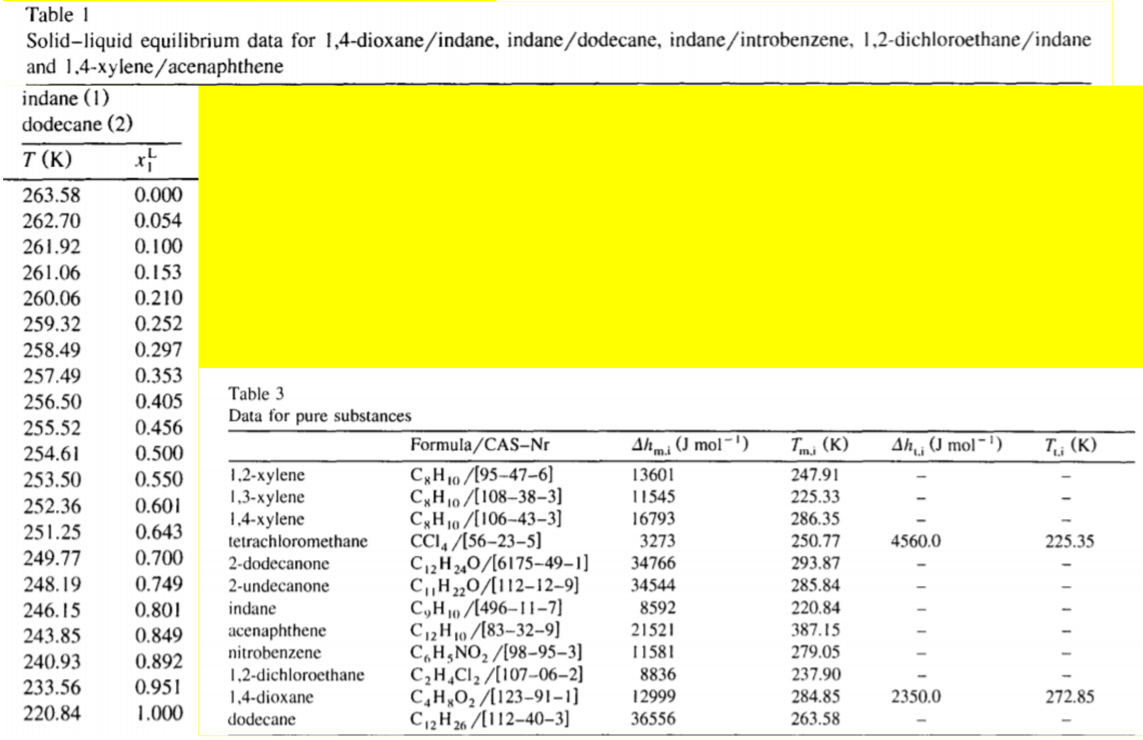


Table 1
Solid–liquid equilibrium data for 1,4-dioxane/indane, indane/dodecane, indane/introbenzene, 1,2-dichloroethane/indane and 1,4-xylene/acenaphthene

| indane (1)<br>dodecane (2)<br>$T$ (K) | $x_1^L$ |
|---|---|
| 263.58 | 0.000 |
| 262.70 | 0.054 |
| 261.92 | 0.100 |
| 261.06 | 0.153 |
| 260.06 | 0.210 |
| 259.32 | 0.252 |
| 258.49 | 0.297 |
| 257.49 | 0.353 |
| 256.50 | 0.405 |
| 255.52 | 0.456 |
| 254.61 | 0.500 |
| 253.50 | 0.550 |
| 252.36 | 0.601 |
| 251.25 | 0.643 |
| 249.77 | 0.700 |
| 248.19 | 0.749 |
| 246.15 | 0.801 |
| 243.85 | 0.849 |
| 240.93 | 0.892 |
| 233.56 | 0.951 |
| 220.84 | 1.000 |

Table 3
Data for pure substances

| | Formula/CAS-Nr | $\Delta h_{m,i}$ (J mol$^{-1}$) | $T_{m,i}$ (K) | $\Delta h_{t,i}$ (J mol$^{-1}$) | $T_{t,i}$ (K) |
|---|---|---|---|---|---|
| 1,2-xylene | $C_8H_{10}$/[95–47–6] | 13601 | 247.91 | – | – |
| 1,3-xylene | $C_8H_{10}$/[108–38–3] | 11545 | 225.33 | – | – |
| 1,4-xylene | $C_8H_{10}$/[106–43–3] | 16793 | 286.35 | – | – |
| tetrachloromethane | $CCl_4$/[56–23–5] | 3273 | 250.77 | 4560.0 | 225.35 |
| 2-dodecanone | $C_{12}H_{24}O$/[6175–49–1] | 34766 | 293.87 | – | – |
| 2-undecanone | $C_{11}H_{22}O$/[112–12–9] | 34544 | 285.84 | – | – |
| indane | $C_9H_{10}$/[496–11–7] | 8592 | 220.84 | – | – |
| acenaphthene | $C_{12}H_{10}$/[83–32–9] | 21521 | 387.15 | – | – |
| nitrobenzene | $C_6H_5NO_2$/[98–95–3] | 11581 | 279.05 | – | – |
| 1,2-dichloroethane | $C_2H_4Cl_2$/[107–06–2] | 8836 | 237.90 | – | – |
| 1,4-dioxane | $C_4H_8O_2$/[123–91–1] | 12999 | 284.85 | 2350.0 | 272.85 |
| dodecane | $C_{12}H_{26}$/[112–40–3] | 36556 | 263.58 | – | – |

indane + nitrobenzene

A. Jakob, R. Joh, C. Rose, J. Gmehling, Solid-liquid equilibria in binary mixtures of organic compounds, Fluid Phase Equilibria 113 (1995) 117-126

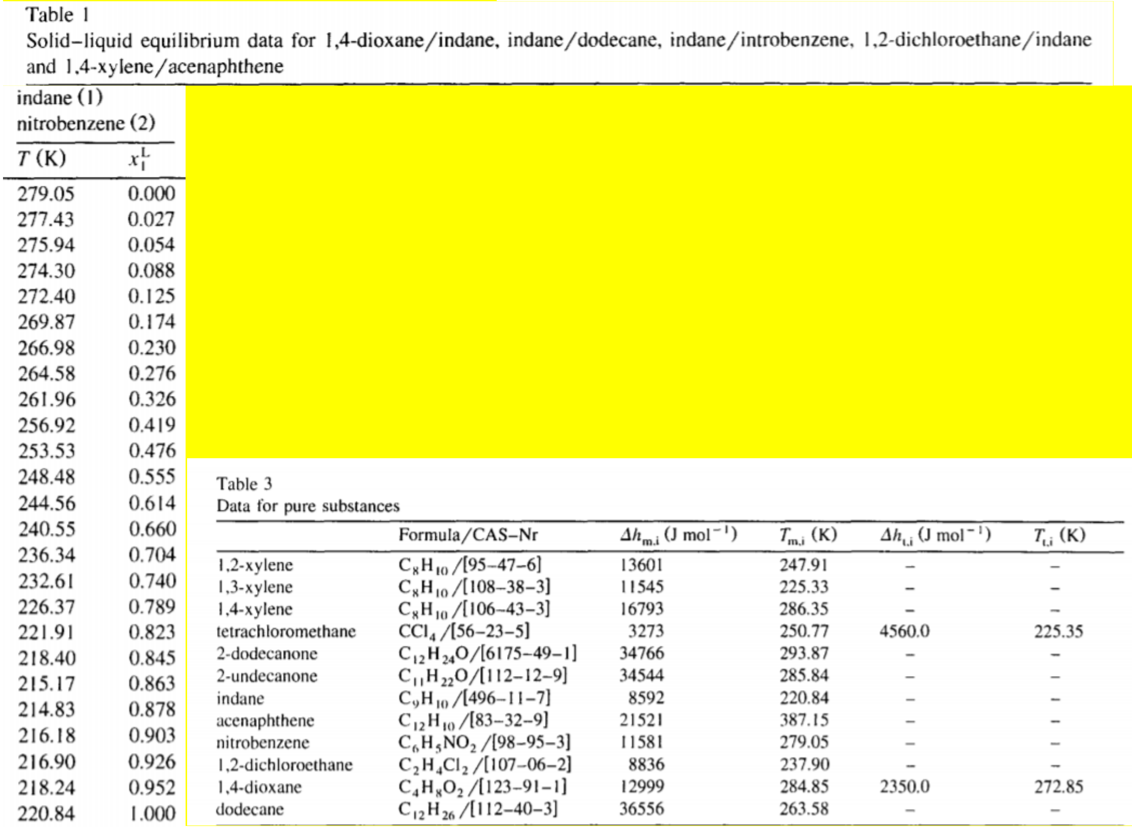


Table 1
Solid–liquid equilibrium data for 1,4-dioxane/indane, indane/dodecane, indane/introbenzene, 1,2-dichloroethane/indane and 1,4-xylene/acenaphthene

| indane (1)<br>nitrobenzene (2) | |
|---|---|
| $T$ (K) | $x_1^L$ |
| 279.05 | 0.000 |
| 277.43 | 0.027 |
| 275.94 | 0.054 |
| 274.30 | 0.088 |
| 272.40 | 0.125 |
| 269.87 | 0.174 |
| 266.98 | 0.230 |
| 264.58 | 0.276 |
| 261.96 | 0.326 |
| 256.92 | 0.419 |
| 253.53 | 0.476 |
| 248.48 | 0.555 |
| 244.56 | 0.614 |
| 240.55 | 0.660 |
| 236.34 | 0.704 |
| 232.61 | 0.740 |
| 226.37 | 0.789 |
| 221.91 | 0.823 |
| 218.40 | 0.845 |
| 215.17 | 0.863 |
| 214.83 | 0.878 |
| 216.18 | 0.903 |
| 216.90 | 0.926 |
| 218.24 | 0.952 |
| 220.84 | 1.000 |

[redacted]

Table 3
Data for pure substances

| | Formula/CAS–Nr | $\Delta h_{m,i}$ (J mol$^{-1}$) | $T_{m,i}$ (K) | $\Delta h_{t,i}$ (J mol$^{-1}$) | $T_{t,i}$ (K) |
|---|---|---|---|---|---|
| 1,2-xylene | $C_8H_{10}$ /[95–47–6] | 13601 | 247.91 | – | – |
| 1,3-xylene | $C_8H_{10}$ /[108–38–3] | 11545 | 225.33 | – | – |
| 1,4-xylene | $C_8H_{10}$ /[106–43–3] | 16793 | 286.35 | – | – |
| tetrachloromethane | $CCl_4$ /[56–23–5] | 3273 | 250.77 | 4560.0 | 225.35 |
| 2-dodecanone | $C_{12}H_{24}O$/[6175–49–1] | 34766 | 293.87 | – | – |
| 2-undecanone | $C_{11}H_{22}O$/[112–12–9] | 34544 | 285.84 | – | – |
| indane | $C_9H_{10}$ /[496–11–7] | 8592 | 220.84 | – | – |
| acenaphthene | $C_{12}H_{10}$ /[83–32–9] | 21521 | 387.15 | – | – |
| nitrobenzene | $C_6H_5NO_2$ /[98–95–3] | 11581 | 279.05 | – | – |
| 1,2-dichloroethane | $C_2H_4Cl_2$ /[107–06–2] | 8836 | 237.90 | – | – |
| 1,4-dioxane | $C_4H_8O_2$ /[123–91–1] | 12999 | 284.85 | 2350.0 | 272.85 |
| dodecane | $C_{12}H_{26}$ /[112–40–3] | 36556 | 263.58 | – | – |

1,2-dichloroethane + indane

A. Jakob, R. Joh, C. Rose, J. Gmehling, Solid-liquid equilibria in binary mixtures of organic compounds, Fluid Phase Equilibria 113 (1995) 117-126

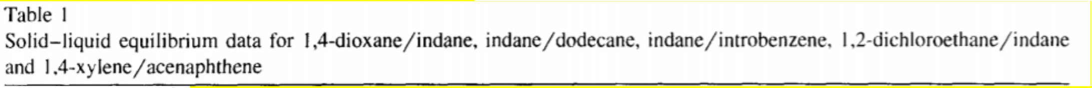
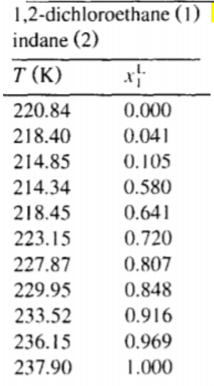


Table 1
Solid–liquid equilibrium data for 1,4-dioxane/indane, indane/dodecane, indane/introbenzene, 1,2-dichloroethane/indane and 1,4-xylene/acenaphthene



1,2-dichloroethane (1)
indane (2)

| $T$ (K) | $x_1^L$ |
|---|---|
| 220.84 | 0.000 |
| 218.40 | 0.041 |
| 214.85 | 0.105 |
| 214.34 | 0.580 |
| 218.45 | 0.641 |
| 223.15 | 0.720 |
| 227.87 | 0.807 |
| 229.95 | 0.848 |
| 233.52 | 0.916 |
| 236.15 | 0.969 |
| 237.90 | 1.000 |

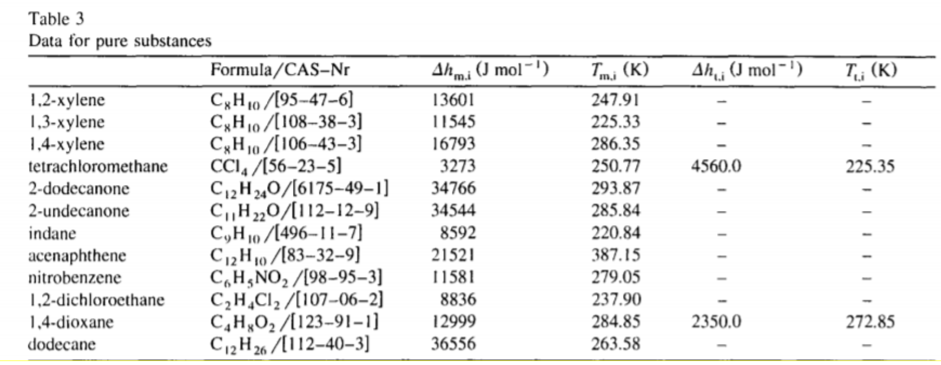


Table 3
Data for pure substances

| | Formula/CAS–Nr | $\Delta h_{m,i}$ (J mol$^{-1}$) | $T_{m,i}$ (K) | $\Delta h_{t,i}$ (J mol$^{-1}$) | $T_{t,i}$ (K) |
|---|---|---|---|---|---|
| 1,2-xylene | $C_8H_{10}$/[95–47–6] | 13601 | 247.91 | – | – |
| 1,3-xylene | $C_8H_{10}$/[108–38–3] | 11545 | 225.33 | – | – |
| 1,4-xylene | $C_8H_{10}$/[106–43–3] | 16793 | 286.35 | – | – |
| tetrachloromethane | $CCl_4$/[56–23–5] | 3273 | 250.77 | 4560.0 | 225.35 |
| 2-dodecanone | $C_{12}H_{24}O$/[6175–49–1] | 34766 | 293.87 | – | – |
| 2-undecanone | $C_{11}H_{22}O$/[112–12–9] | 34544 | 285.84 | – | – |
| indane | $C_9H_{10}$/[496–11–7] | 8592 | 220.84 | – | – |
| acenaphthene | $C_{12}H_{10}$/[83–32–9] | 21521 | 387.15 | – | – |
| nitrobenzene | $C_6H_5NO_2$/[98–95–3] | 11581 | 279.05 | – | – |
| 1,2-dichloroethane | $C_2H_4Cl_2$/[107–06–2] | 8836 | 237.90 | – | – |
| 1,4-dioxane | $C_4H_8O_2$/[123–91–1] | 12999 | 284.85 | 2350.0 | 272.85 |
| dodecane | $C_{12}H_{26}$/[112–40–3] | 36556 | 263.58 | – | – |

1,4-xylene + acenaphthene

A. Jakob, R. Joh, C. Rose, J. Gmehling, Solid-liquid equilibria in binary mixtures of organic compounds, Fluid Phase Equilibria 113 (1995) 117-126

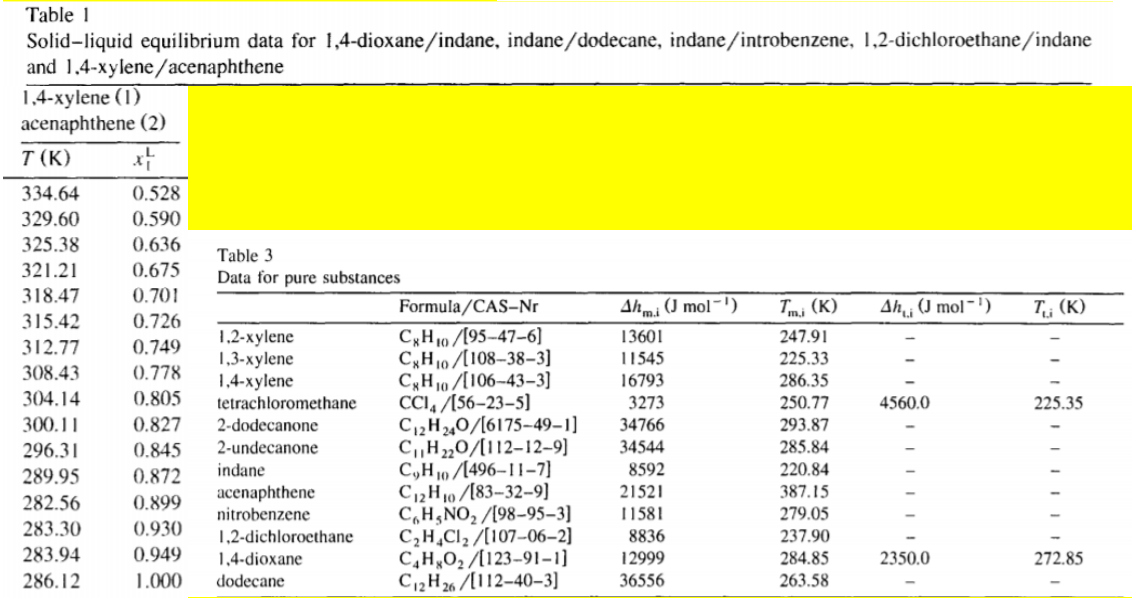


Table 1
Solid–liquid equilibrium data for 1,4-dioxane/indane, indane/dodecane, indane/introbenzene, 1,2-dichloroethane/indane and 1,4-xylene/acenaphthene

| 1,4-xylene (1)<br>acenaphthene (2) | |
|---|---|
| $T$ (K) | $x_1^L$ |
| 334.64 | 0.528 |
| 329.60 | 0.590 |
| 325.38 | 0.636 |
| 321.21 | 0.675 |
| 318.47 | 0.701 |
| 315.42 | 0.726 |
| 312.77 | 0.749 |
| 308.43 | 0.778 |
| 304.14 | 0.805 |
| 300.11 | 0.827 |
| 296.31 | 0.845 |
| 289.95 | 0.872 |
| 282.56 | 0.899 |
| 283.30 | 0.930 |
| 283.94 | 0.949 |
| 286.12 | 1.000 |

Table 3
Data for pure substances

| | Formula/CAS-Nr | $\Delta h_{m,i}$ (J mol$^{-1}$) | $T_{m,i}$ (K) | $\Delta h_{t,i}$ (J mol$^{-1}$) | $T_{t,i}$ (K) |
|---|---|---|---|---|---|
| 1,2-xylene | $C_8H_{10}$/[95–47–6] | 13601 | 247.91 | – | – |
| 1,3-xylene | $C_8H_{10}$/[108–38–3] | 11545 | 225.33 | – | – |
| 1,4-xylene | $C_8H_{10}$/[106–43–3] | 16793 | 286.35 | – | – |
| tetrachloromethane | $CCl_4$/[56–23–5] | 3273 | 250.77 | 4560.0 | 225.35 |
| 2-dodecanone | $C_{12}H_{24}O$/[6175–49–1] | 34766 | 293.87 | – | – |
| 2-undecanone | $C_{11}H_{22}O$/[112–12–9] | 34544 | 285.84 | – | – |
| indane | $C_9H_{10}$/[496–11–7] | 8592 | 220.84 | – | – |
| acenaphthene | $C_{12}H_{10}$/[83–32–9] | 21521 | 387.15 | – | – |
| nitrobenzene | $C_6H_5NO_2$/[98–95–3] | 11581 | 279.05 | – | – |
| 1,2-dichloroethane | $C_2H_4Cl_2$/[107–06–2] | 8836 | 237.90 | – | – |
| 1,4-dioxane | $C_4H_8O_2$/[123–91–1] | 12999 | 284.85 | 2350.0 | 272.85 |
| dodecane | $C_{12}H_{26}$/[112–40–3] | 36556 | 263.58 | – | – |

tetrachloromethane + 2-dodecanone

A. Jakob, R. Joh, C. Rose, J. Gmehling, Solid-liquid equilibria in binary mixtures of organic compounds, Fluid Phase Equilibria 113 (1995) 117-126

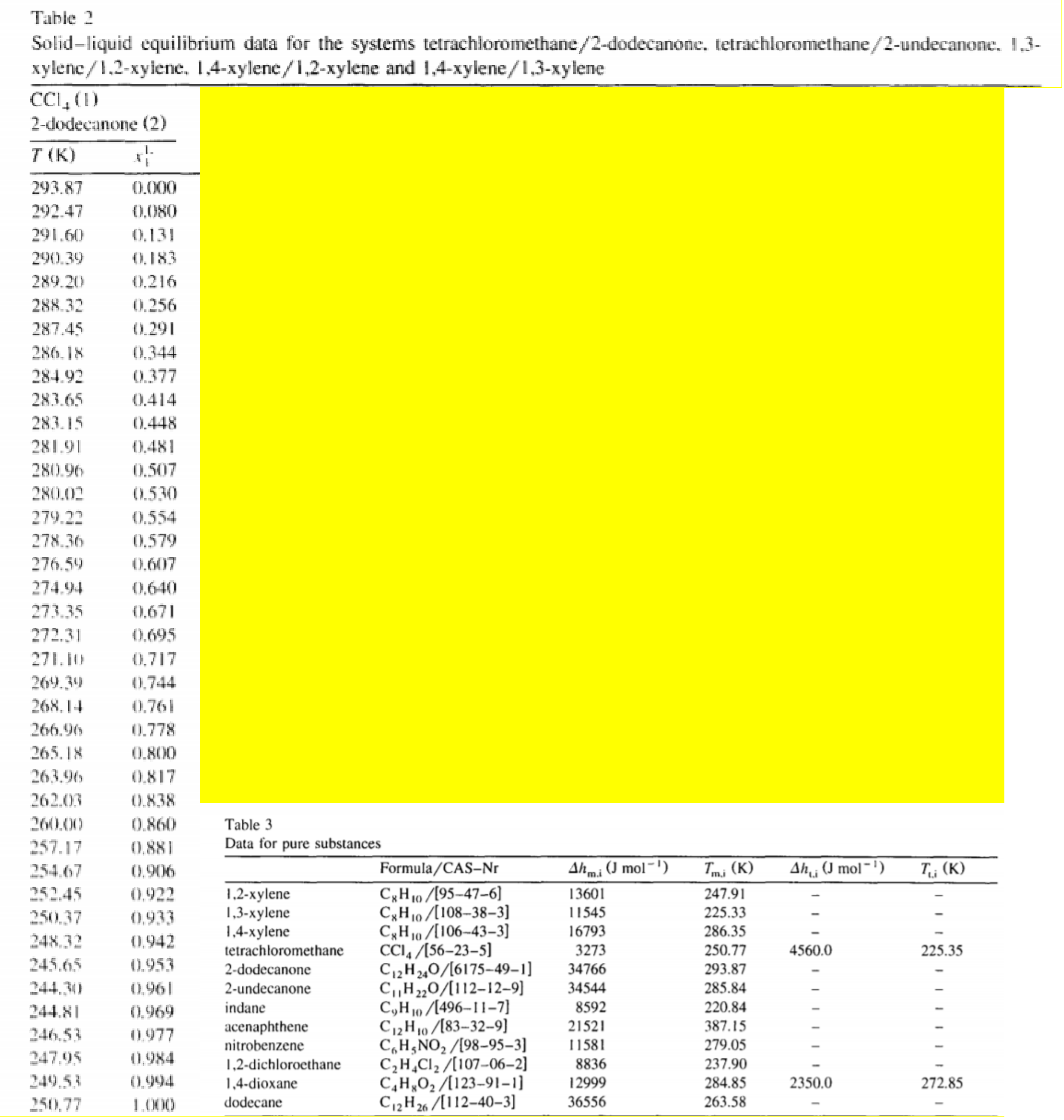


Table 2
Solid–liquid equilibrium data for the systems tetrachloromethane/2-dodecanone, tetrachloromethane/2-undecanone, 1,3-xylene/1,2-xylene, 1,4-xylene/1,2-xylene and 1,4-xylene/1,3-xylene

| $CCl_4$ (1)<br>2-dodecanone (2) | |
|---|---|
| $T$ (K) | $x_1^L$ |
| 293.87 | 0.000 |
| 292.47 | 0.080 |
| 291.60 | 0.131 |
| 290.39 | 0.183 |
| 289.20 | 0.216 |
| 288.32 | 0.256 |
| 287.45 | 0.291 |
| 286.18 | 0.344 |
| 284.92 | 0.377 |
| 283.65 | 0.414 |
| 283.15 | 0.448 |
| 281.91 | 0.481 |
| 280.96 | 0.507 |
| 280.02 | 0.530 |
| 279.22 | 0.554 |
| 278.36 | 0.579 |
| 276.59 | 0.607 |
| 274.94 | 0.640 |
| 273.35 | 0.671 |
| 272.31 | 0.695 |
| 271.10 | 0.717 |
| 269.39 | 0.744 |
| 268.14 | 0.761 |
| 266.96 | 0.778 |
| 265.18 | 0.800 |
| 263.96 | 0.817 |
| 262.03 | 0.838 |
| 260.00 | 0.860 |
| 257.17 | 0.881 |
| 254.67 | 0.906 |
| 252.45 | 0.922 |
| 250.37 | 0.933 |
| 248.32 | 0.942 |
| 245.65 | 0.953 |
| 244.30 | 0.961 |
| 244.81 | 0.969 |
| 246.53 | 0.977 |
| 247.95 | 0.984 |
| 249.53 | 0.994 |
| 250.77 | 1.000 |

Table 3
Data for pure substances

| | Formula/CAS-Nr | $\Delta h_{m,i}$ (J mol$^{-1}$) | $T_{m,i}$ (K) | $\Delta h_{t,i}$ (J mol$^{-1}$) | $T_{t,i}$ (K) |
|---|---|---|---|---|---|
| 1,2-xylene | $C_8H_{10}$/[95–47–6] | 13601 | 247.91 | – | – |
| 1,3-xylene | $C_8H_{10}$/[108–38–3] | 11545 | 225.33 | – | – |
| 1,4-xylene | $C_8H_{10}$/[106–43–3] | 16793 | 286.35 | – | – |
| tetrachloromethane | $CCl_4$/[56–23–5] | 3273 | 250.77 | 4560.0 | 225.35 |
| 2-dodecanone | $C_{12}H_{24}O$/[6175–49–1] | 34766 | 293.87 | – | – |
| 2-undecanone | $C_{11}H_{22}O$/[112–12–9] | 34544 | 285.84 | – | – |
| indane | $C_9H_{10}$/[496–11–7] | 8592 | 220.84 | – | – |
| acenaphthene | $C_{12}H_{10}$/[83–32–9] | 21521 | 387.15 | – | – |
| nitrobenzene | $C_6H_5NO_2$/[98–95–3] | 11581 | 279.05 | – | – |
| 1,2-dichloroethane | $C_2H_4Cl_2$/[107–06–2] | 8836 | 237.90 | – | – |
| 1,4-dioxane | $C_4H_8O_2$/[123–91–1] | 12999 | 284.85 | 2350.0 | 272.85 |
| dodecane | $C_{12}H_{26}$/[112–40–3] | 36556 | 263.58 | – | – |

tetrachloromethane + 2-undecanone

A. Jakob, R. Joh, C. Rose, J. Gmehling, Solid-liquid equilibria in binary mixtures of organic compounds, Fluid Phase Equilibria 113 (1995) 117-126

Table 2
Solid–liquid equilibrium data for the systems tetrachloromethane/2-dodecanone, tetrachloromethane/2-undecanone, 1,3-xylene/1,2-xylene, 1,4-xylene/1,2-xylene and 1,4-xylene/1,3-xylene

| $CCl_4$ (1)<br>2-undecanone (2)<br>$T$ (K) | <br><br>$x_1^L$ |
|---|---|
| 285.84 | 0.000 |
| 285.10 | 0.050 |
| 284.09 | 0.086 |
| 283.47 | 0.115 |
| 283.02 | 0.142 |
| 282.08 | 0.180 |
| 281.07 | 0.224 |
| 280.16 | 0.262 |
| 279.30 | 0.296 |
| 278.36 | 0.329 |
| 277.06 | 0.373 |
| 276.20 | 0.398 |
| 275.65 | 0.414 |
| 275.00 | 0.433 |
| 274.60 | 0.449 |
| 273.92 | 0.469 |
| 272.97 | 0.485 |
| 272.52 | 0.503 |
| 271.72 | 0.514 |
| 271.37 | 0.533 |
| 270.76 | 0.559 |
| 267.81 | 0.610 |
| 266.81 | 0.634 |
| 265.51 | 0.656 |
| 264.59 | 0.674 |
| 264.29 | 0.689 |
| 262.52 | 0.712 |
| 261.25 | 0.733 |
| 260.22 | 0.750 |
| 258.93 | 0.768 |
| 257.40 | 0.787 |
| 255.70 | 0.814 |
| 253.47 | 0.836 |
| 251.49 | 0.856 |
| 249.91 | 0.872 |
| 247.42 | 0.893 |
| 246.89 | 0.901 |
| 246.36 | 0.913 |
| 244.23 | 0.925 |
| 243.31 | 0.945 |
| 244.72 | 0.963 |
| 246.40 | 0.980 |
| 250.77 | 1.000 |

Table 3
Data for pure substances

| | Formula/CAS-Nr | $\Delta h_{m,i}$ (J mol$^{-1}$) | $T_{m,i}$ (K) | $\Delta h_{t,i}$ (J mol$^{-1}$) | $T_{t,i}$ (K) |
|---|---|---|---|---|---|
| 1,2-xylene | $C_8H_{10}$/[95–47–6] | 13601 | 247.91 | – | – |
| 1,3-xylene | $C_8H_{10}$/[108–38–3] | 11545 | 225.33 | – | – |
| 1,4-xylene | $C_8H_{10}$/[106–43–3] | 16793 | 286.35 | – | – |
| tetrachloromethane | $CCl_4$/[56–23–5] | 3273 | 250.77 | 4560.0 | 225.35 |
| 2-dodecanone | $C_{12}H_{24}O$/[6175–49–1] | 34766 | 293.87 | – | – |
| 2-undecanone | $C_{11}H_{22}O$/[112–12–9] | 34544 | 285.84 | – | – |
| indane | $C_9H_{10}$/[496–11–7] | 8592 | 220.84 | – | – |
| acenaphthene | $C_{12}H_{10}$/[83–32–9] | 21521 | 387.15 | – | – |
| nitrobenzene | $C_6H_5NO_2$/[98–95–3] | 11581 | 279.05 | – | – |
| 1,2-dichloroethane | $C_2H_4Cl_2$/[107–06–2] | 8836 | 237.90 | – | – |
| 1,4-dioxane | $C_4H_8O_2$/[123–91–1] | 12999 | 284.85 | 2350.0 | 272.85 |
| dodecane | $C_{12}H_{26}$/[112–40–3] | 36556 | 263.58 | – | – |

1,3-xylene + 1,2-xylene

A. Jakob, R. Joh, C. Rose, J. Gmehling, Solid-liquid equilibria in binary mixtures of organic compounds, Fluid Phase Equilibria 113 (1995) 117-126

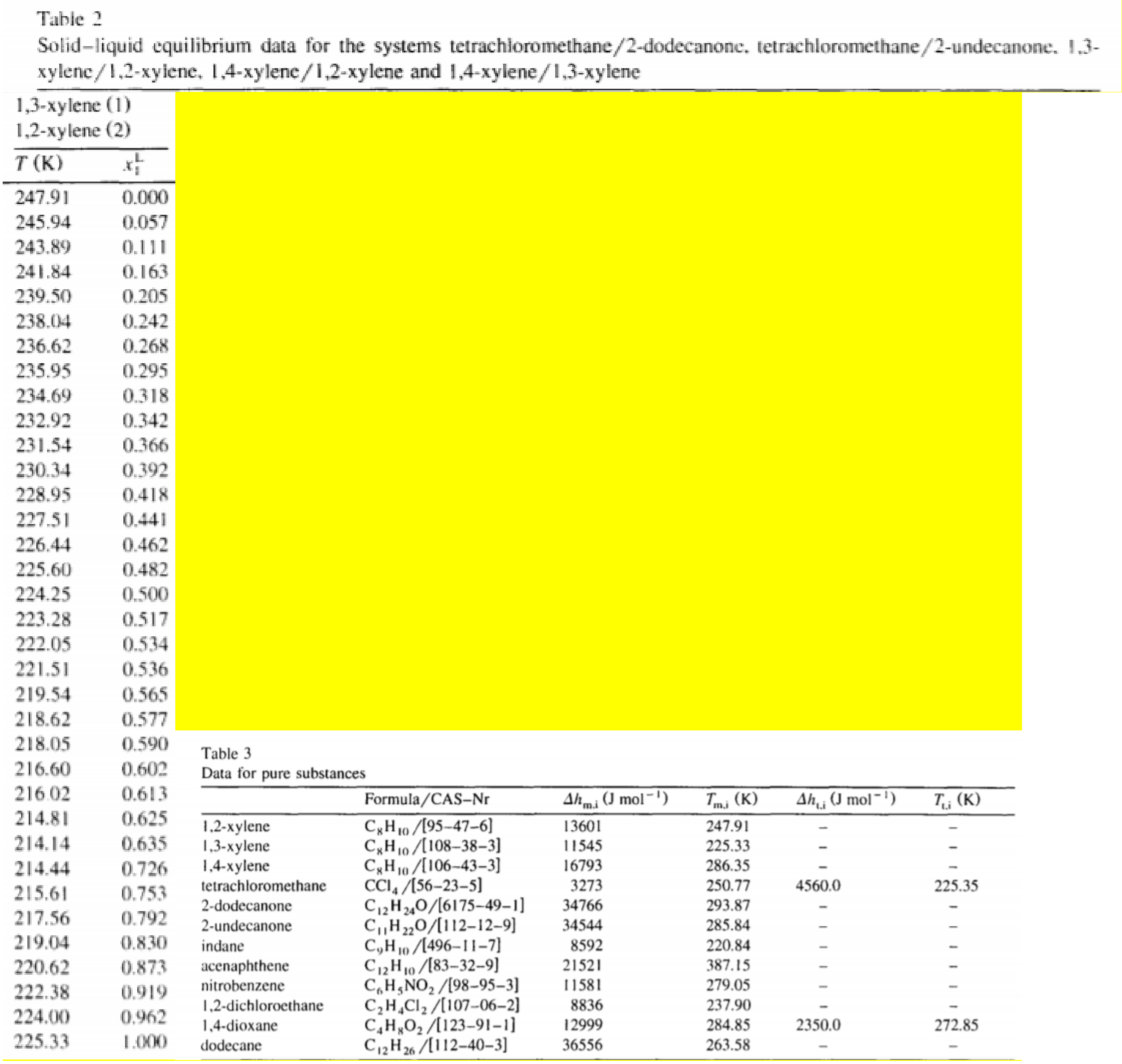


Table 2
Solid–liquid equilibrium data for the systems tetrachloromethane/2-dodecanone, tetrachloromethane/2-undecanone, 1,3-xylene/1,2-xylene, 1,4-xylene/1,2-xylene and 1,4-xylene/1,3-xylene

1,3-xylene (1)
1,2-xylene (2)

| $T$ (K) | $x_1^L$ |
|---|---|
| 247.91 | 0.000 |
| 245.94 | 0.057 |
| 243.89 | 0.111 |
| 241.84 | 0.163 |
| 239.50 | 0.205 |
| 238.04 | 0.242 |
| 236.62 | 0.268 |
| 235.95 | 0.295 |
| 234.69 | 0.318 |
| 232.92 | 0.342 |
| 231.54 | 0.366 |
| 230.34 | 0.392 |
| 228.95 | 0.418 |
| 227.51 | 0.441 |
| 226.44 | 0.462 |
| 225.60 | 0.482 |
| 224.25 | 0.500 |
| 223.28 | 0.517 |
| 222.05 | 0.534 |
| 221.51 | 0.536 |
| 219.54 | 0.565 |
| 218.62 | 0.577 |
| 218.05 | 0.590 |
| 216.60 | 0.602 |
| 216.02 | 0.613 |
| 214.81 | 0.625 |
| 214.14 | 0.635 |
| 214.44 | 0.726 |
| 215.61 | 0.753 |
| 217.56 | 0.792 |
| 219.04 | 0.830 |
| 220.62 | 0.873 |
| 222.38 | 0.919 |
| 224.00 | 0.962 |
| 225.33 | 1.000 |

Table 3
Data for pure substances

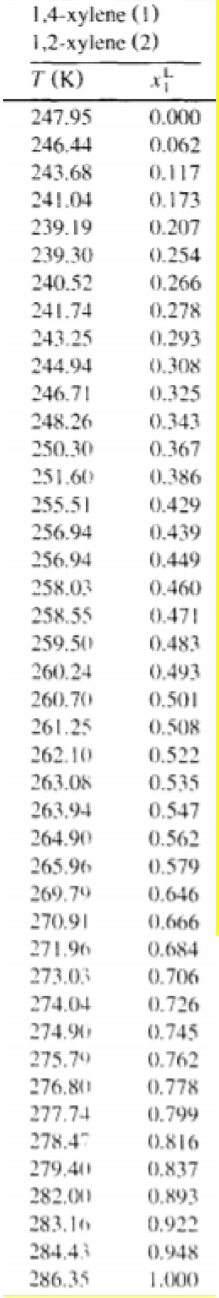
| | Formula/CAS–Nr | $\Delta h_{m,i}$ (J mol$^{-1}$) | $T_{m,i}$ (K) | $\Delta h_{t,i}$ (J mol$^{-1}$) | $T_{t,i}$ (K) |
|---|---|---|---|---|---|
| 1,2-xylene | $C_8H_{10}$/[95–47–6] | 13601 | 247.91 | – | – |
| 1,3-xylene | $C_8H_{10}$/[108–38–3] | 11545 | 225.33 | – | – |
| 1,4-xylene | $C_8H_{10}$/[106–43–3] | 16793 | 286.35 | – | – |
| tetrachloromethane | $CCl_4$/[56–23–5] | 3273 | 250.77 | 4560.0 | 225.35 |
| 2-dodecanone | $C_{12}H_{24}O$/[6175–49–1] | 34766 | 293.87 | – | – |
| 2-undecanone | $C_{11}H_{22}O$/[112–12–9] | 34544 | 285.84 | – | – |
| indane | $C_9H_{10}$/[496–11–7] | 8592 | 220.84 | – | – |
| acenaphthene | $C_{12}H_{10}$/[83–32–9] | 21521 | 387.15 | – | – |
| nitrobenzene | $C_6H_5NO_2$/[98–95–3] | 11581 | 279.05 | – | – |
| 1,2-dichloroethane | $C_2H_4Cl_2$/[107–06–2] | 8836 | 237.90 | – | – |
| 1,4-dioxane | $C_4H_8O_2$/[123–91–1] | 12999 | 284.85 | 2350.0 | 272.85 |
| dodecane | $C_{12}H_{26}$/[112–40–3] | 36556 | 263.58 | – | – |

1,4-xylene + 1,2-xylene

A. Jakob, R. Joh, C. Rose, J. Gmehling, Solid-liquid equilibria in binary mixtures of organic compounds, Fluid Phase Equilibria 113 (1995) 117-126

Table 2

Solid–liquid equilibrium data for the systems tetrachloromethane/2-dodecanone, tetrachloromethane/2-undecanone, 1,3-xylene/1,2-xylene, 1,4-xylene/1,2-xylene and 1,4-xylene/1,3-xylene



| 1,4-xylene (1)<br>1,2-xylene (2) | |
|---|---|
| $T$ (K) | $x_1^L$ |
| 247.95 | 0.000 |
| 246.44 | 0.062 |
| 243.68 | 0.117 |
| 241.04 | 0.173 |
| 239.19 | 0.207 |
| 239.30 | 0.254 |
| 240.52 | 0.266 |
| 241.74 | 0.278 |
| 243.25 | 0.293 |
| 244.94 | 0.308 |
| 246.71 | 0.325 |
| 248.26 | 0.343 |
| 250.30 | 0.367 |
| 251.60 | 0.386 |
| 255.51 | 0.429 |
| 256.94 | 0.439 |
| 256.94 | 0.449 |
| 258.03 | 0.460 |
| 258.55 | 0.471 |
| 259.50 | 0.483 |
| 260.24 | 0.493 |
| 260.70 | 0.501 |
| 261.25 | 0.508 |
| 262.10 | 0.522 |
| 263.08 | 0.535 |
| 263.94 | 0.547 |
| 264.90 | 0.562 |
| 265.96 | 0.579 |
| 269.79 | 0.646 |
| 270.91 | 0.666 |
| 271.96 | 0.684 |
| 273.03 | 0.706 |
| 274.04 | 0.726 |
| 274.90 | 0.745 |
| 275.79 | 0.762 |
| 276.80 | 0.778 |
| 277.74 | 0.799 |
| 278.47 | 0.816 |
| 279.40 | 0.837 |
| 282.00 | 0.893 |
| 283.16 | 0.922 |
| 284.43 | 0.948 |
| 286.35 | 1.000 |

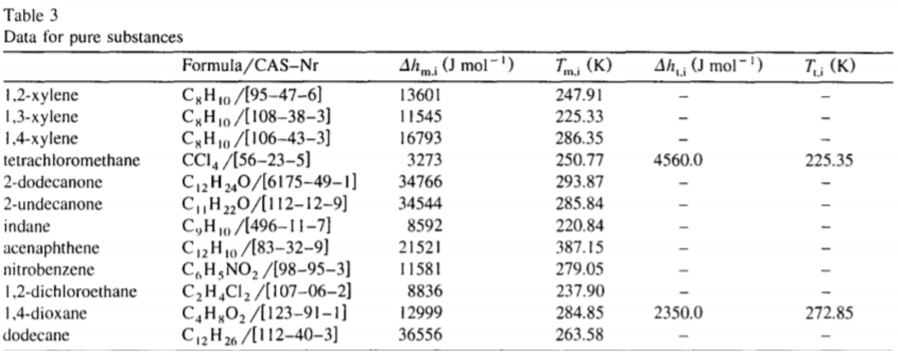


Table 3

Data for pure substances

| | Formula/CAS–Nr | $\Delta h_{m,i}$ (J mol$^{-1}$) | $T_{m,i}$ (K) | $\Delta h_{t,i}$ (J mol$^{-1}$) | $T_{t,i}$ (K) |
|---|---|---|---|---|---|
| 1,2-xylene | $C_8H_{10}$/[95–47–6] | 13601 | 247.91 | – | – |
| 1,3-xylene | $C_8H_{10}$/[108–38–3] | 11545 | 225.33 | – | – |
| 1,4-xylene | $C_8H_{10}$/[106–43–3] | 16793 | 286.35 | – | – |
| tetrachloromethane | $CCl_4$/[56–23–5] | 3273 | 250.77 | 4560.0 | 225.35 |
| 2-dodecanone | $C_{12}H_{24}O$/[6175–49–1] | 34766 | 293.87 | – | – |
| 2-undecanone | $C_{11}H_{22}O$/[112–12–9] | 34544 | 285.84 | – | – |
| indane | $C_9H_{10}$/[496–11–7] | 8592 | 220.84 | – | – |
| acenaphthene | $C_{12}H_{10}$/[83–32–9] | 21521 | 387.15 | – | – |
| nitrobenzene | $C_6H_5NO_2$/[98–95–3] | 11581 | 279.05 | – | – |
| 1,2-dichloroethane | $C_2H_4Cl_2$/[107–06–2] | 8836 | 237.90 | – | – |
| 1,4-dioxane | $C_4H_8O_2$/[123–91–1] | 12999 | 284.85 | 2350.0 | 272.85 |
| dodecane | $C_{12}H_{26}$/[112–40–3] | 36556 | 263.58 | – | – |

1,4-xylene + 1,3-xylene

A. Jakob, R. Joh, C. Rose, J. Gmehling, Solid-liquid equilibria in binary mixtures of organic compounds, Fluid Phase Equilibria 113 (1995) 117-126

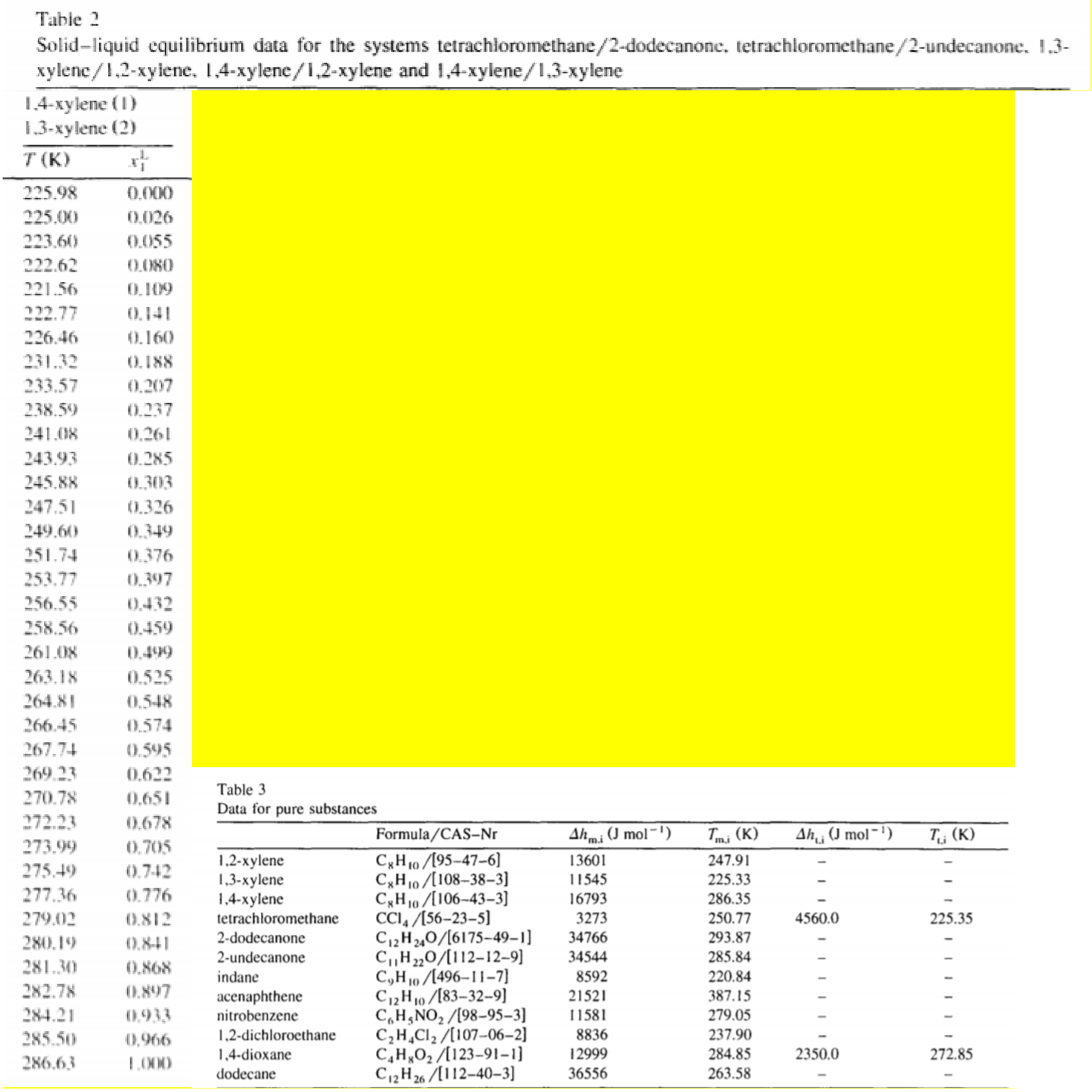


Table 2
Solid–liquid equilibrium data for the systems tetrachloromethane/2-dodecanone, tetrachloromethane/2-undecanone, 1,3-xylene/1,2-xylene, 1,4-xylene/1,2-xylene and 1,4-xylene/1,3-xylene

| 1,4-xylene (1)<br>1,3-xylene (2) | |
|---|---|
| $T$ (K) | $x_1^L$ |
| 225.98 | 0.000 |
| 225.00 | 0.026 |
| 223.60 | 0.055 |
| 222.62 | 0.080 |
| 221.56 | 0.109 |
| 222.77 | 0.141 |
| 226.46 | 0.160 |
| 231.32 | 0.188 |
| 233.57 | 0.207 |
| 238.59 | 0.237 |
| 241.08 | 0.261 |
| 243.93 | 0.285 |
| 245.88 | 0.303 |
| 247.51 | 0.326 |
| 249.60 | 0.349 |
| 251.74 | 0.376 |
| 253.77 | 0.397 |
| 256.55 | 0.432 |
| 258.56 | 0.459 |
| 261.08 | 0.499 |
| 263.18 | 0.525 |
| 264.81 | 0.548 |
| 266.45 | 0.574 |
| 267.74 | 0.595 |
| 269.23 | 0.622 |
| 270.78 | 0.651 |
| 272.23 | 0.678 |
| 273.99 | 0.705 |
| 275.49 | 0.742 |
| 277.36 | 0.776 |
| 279.02 | 0.812 |
| 280.19 | 0.841 |
| 281.30 | 0.868 |
| 282.78 | 0.897 |
| 284.21 | 0.933 |
| 285.50 | 0.966 |
| 286.63 | 1.000 |

Table 3
Data for pure substances

| | Formula/CAS-Nr | $\Delta h_{m,i}$ (J mol$^{-1}$) | $T_{m,i}$ (K) | $\Delta h_{t,i}$ (J mol$^{-1}$) | $T_{t,i}$ (K) |
|---|---|---|---|---|---|
| 1,2-xylene | $C_8H_{10}$/[95–47–6] | 13601 | 247.91 | – | – |
| 1,3-xylene | $C_8H_{10}$/[108–38–3] | 11545 | 225.33 | – | – |
| 1,4-xylene | $C_8H_{10}$/[106–43–3] | 16793 | 286.35 | – | – |
| tetrachloromethane | $CCl_4$/[56–23–5] | 3273 | 250.77 | 4560.0 | 225.35 |
| 2-dodecanone | $C_{12}H_{24}O$/[6175–49–1] | 34766 | 293.87 | – | – |
| 2-undecanone | $C_{11}H_{22}O$/[112–12–9] | 34544 | 285.84 | – | – |
| indane | $C_9H_{10}$/[496–11–7] | 8592 | 220.84 | – | – |
| acenaphthene | $C_{12}H_{10}$/[83–32–9] | 21521 | 387.15 | – | – |
| nitrobenzene | $C_6H_5NO_2$/[98–95–3] | 11581 | 279.05 | – | – |
| 1,2-dichloroethane | $C_2H_4Cl_2$/[107–06–2] | 8836 | 237.90 | – | – |
| 1,4-dioxane | $C_4H_8O_2$/[123–91–1] | 12999 | 284.85 | 2350.0 | 272.85 |
| dodecane | $C_{12}H_{26}$/[112–40–3] | 36556 | 263.58 | – | – |

octadecane + dimethylacetamide

G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

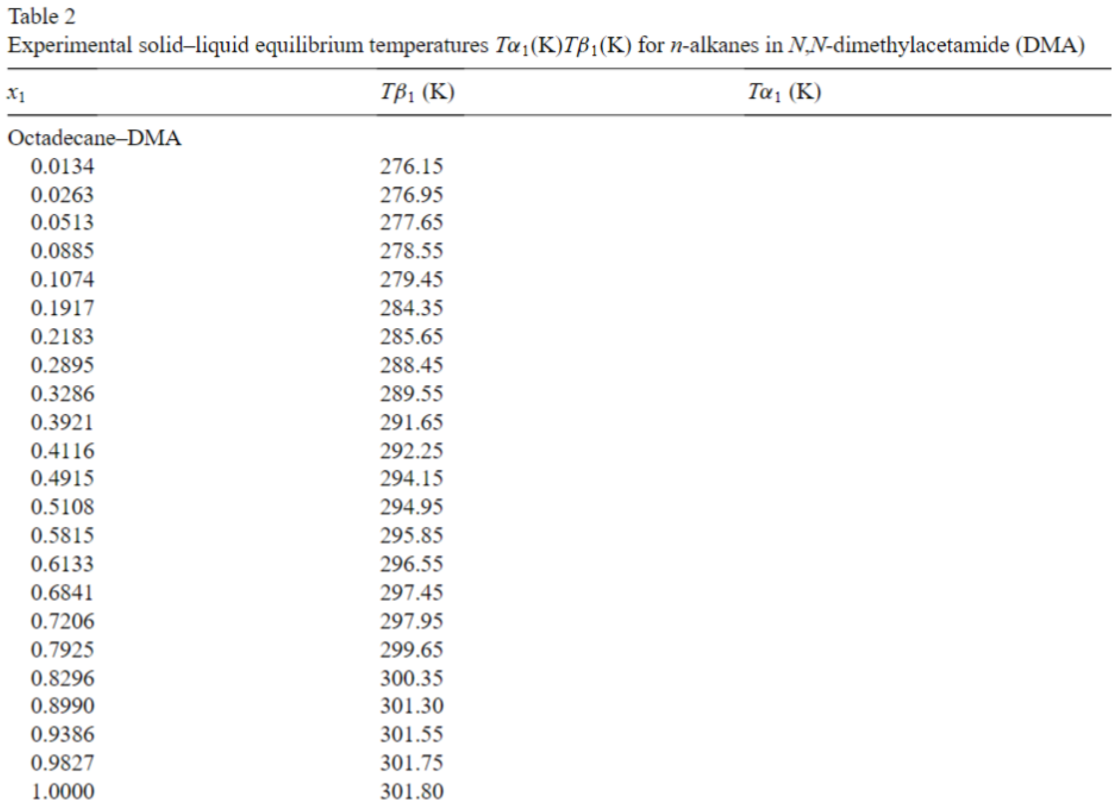


Table 2

Experimental solid–liquid equilibrium temperatures $T\alpha_1$(K)$T\beta_1$(K) for *n*-alkanes in *N*,*N*-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Octadecane–DMA | | |
| 0.0134 | 276.15 | |
| 0.0263 | 276.95 | |
| 0.0513 | 277.65 | |
| 0.0885 | 278.55 | |
| 0.1074 | 279.45 | |
| 0.1917 | 284.35 | |
| 0.2183 | 285.65 | |
| 0.2895 | 288.45 | |
| 0.3286 | 289.55 | |
| 0.3921 | 291.65 | |
| 0.4116 | 292.25 | |
| 0.4915 | 294.15 | |
| 0.5108 | 294.95 | |
| 0.5815 | 295.85 | |
| 0.6133 | 296.55 | |
| 0.6841 | 297.45 | |
| 0.7206 | 297.95 | |
| 0.7925 | 299.65 | |
| 0.8296 | 300.35 | |
| 0.8990 | 301.30 | |
| 0.9386 | 301.55 | |
| 0.9827 | 301.75 | |
| 1.0000 | 301.80 | |

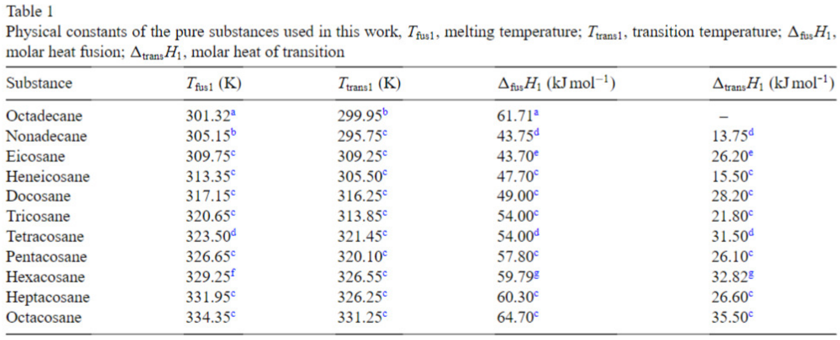


Table 1

Physical constants of the pure substances used in this work, $T_{fus1}$, melting temperature; $T_{trans1}$, transition temperature; $\Delta_{fus}H_1$, molar heat fusion; $\Delta_{trans}H_1$, molar heat of transition

| Substance | $T_{fus1}$ (K) | $T_{trans1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{trans}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32[a] | 299.95[b] | 61.71[a] | – |
| Nonadecane | 305.15[b] | 295.75[c] | 43.75[d] | 13.75[d] |
| Eicosane | 309.75[c] | 309.25[c] | 43.70[e] | 26.20[e] |
| Heneicosane | 313.35[c] | 305.50[c] | 47.70[c] | 15.50[c] |
| Docosane | 317.15[c] | 316.25[c] | 49.00[c] | 28.20[c] |
| Tricosane | 320.65[c] | 313.85[c] | 54.00[c] | 21.80[c] |
| Tetracosane | 323.50[d] | 321.45[c] | 54.00[d] | 31.50[d] |
| Pentacosane | 326.65[c] | 320.10[c] | 57.80[c] | 26.10[c] |
| Hexacosane | 329.25[f] | 326.55[c] | 59.79[g] | 32.82[g] |
| Heptacosane | 331.95[c] | 326.25[c] | 60.30[c] | 26.60[c] |
| Octacosane | 334.35[c] | 331.25[c] | 64.70[c] | 35.50[c] |

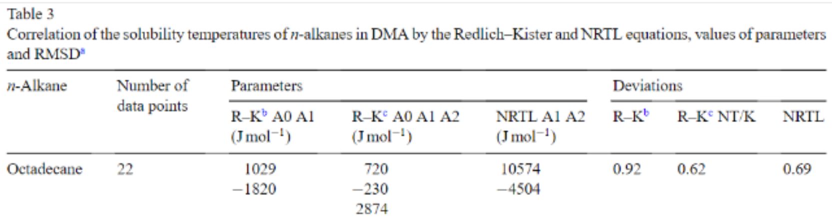


Table 3

Correlation of the solubility temperatures of *n*-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD[a]

| *n*-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K[b] A0 A1 (J mol$^{-1}$) | R–K[c] A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K[b] | R–K[c] NT/K | NRTL |
| Octadecane | 22 | 1029<br>−1820 | 720<br>−230<br>2874 | 10574<br>−4504 | 0.92 | 0.62 | 0.69 |

alpha = 0.2

ODABRATI NRTL

nonadecane + dimethylacetamide

G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

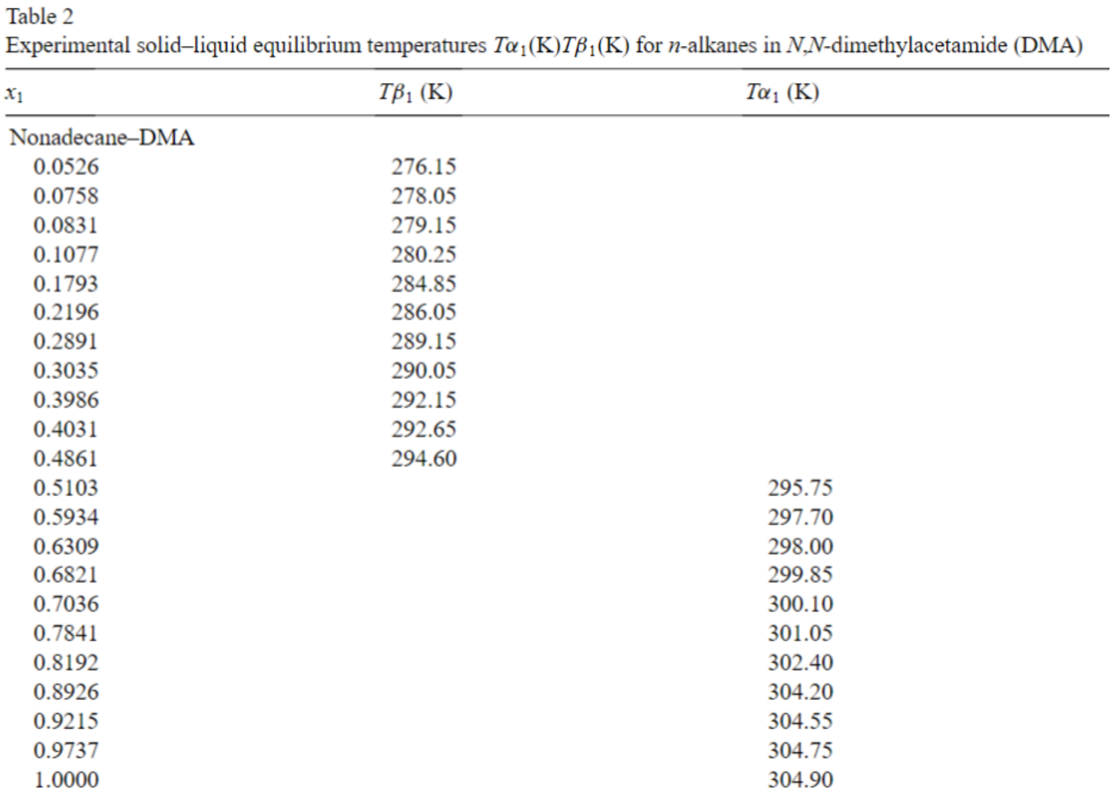


Table 2

Experimental solid–liquid equilibrium temperatures $T\alpha_1$(K)$T\beta_1$(K) for *n*-alkanes in *N*,*N*-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Nonadecane–DMA | | |
| 0.0526 | 276.15 | |
| 0.0758 | 278.05 | |
| 0.0831 | 279.15 | |
| 0.1077 | 280.25 | |
| 0.1793 | 284.85 | |
| 0.2196 | 286.05 | |
| 0.2891 | 289.15 | |
| 0.3035 | 290.05 | |
| 0.3986 | 292.15 | |
| 0.4031 | 292.65 | |
| 0.4861 | 294.60 | |
| 0.5103 | | 295.75 |
| 0.5934 | | 297.70 |
| 0.6309 | | 298.00 |
| 0.6821 | | 299.85 |
| 0.7036 | | 300.10 |
| 0.7841 | | 301.05 |
| 0.8192 | | 302.40 |
| 0.8926 | | 304.20 |
| 0.9215 | | 304.55 |
| 0.9737 | | 304.75 |
| 1.0000 | | 304.90 |

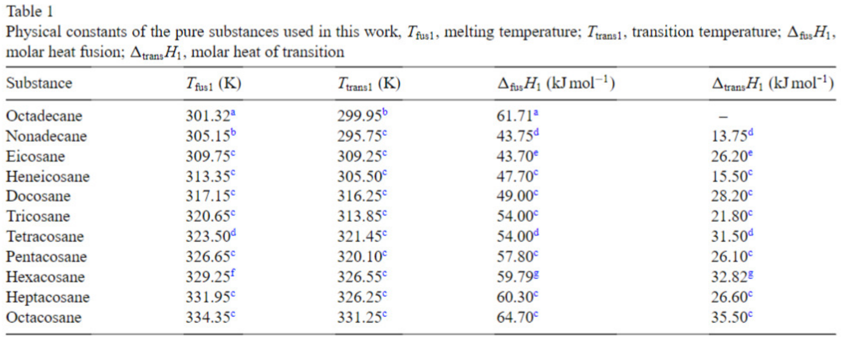


Table 1

Physical constants of the pure substances used in this work, $T_{fus1}$, melting temperature; $T_{trans1}$, transition temperature; $\Delta_{fus}H_1$, molar heat fusion; $\Delta_{trans}H_1$, molar heat of transition

| Substance | $T_{fus1}$ (K) | $T_{trans1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{trans}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32[a] | 299.95[b] | 61.71[a] | – |
| Nonadecane | 305.15[b] | 295.75[c] | 43.75[d] | 13.75[d] |
| Eicosane | 309.75[c] | 309.25[c] | 43.70[e] | 26.20[e] |
| Heneicosane | 313.35[c] | 305.50[c] | 47.70[c] | 15.50[c] |
| Docosane | 317.15[c] | 316.25[c] | 49.00[c] | 28.20[c] |
| Tricosane | 320.65[c] | 313.85[c] | 54.00[c] | 21.80[c] |
| Tetracosane | 323.50[d] | 321.45[c] | 54.00[d] | 31.50[d] |
| Pentacosane | 326.65[c] | 320.10[c] | 57.80[c] | 26.10[c] |
| Hexacosane | 329.25[f] | 326.55[c] | 59.79[g] | 32.82[g] |
| Heptacosane | 331.95[c] | 326.25[c] | 60.30[c] | 26.60[c] |
| Octacosane | 334.35[c] | 331.25[c] | 64.70[c] | 35.50[c] |

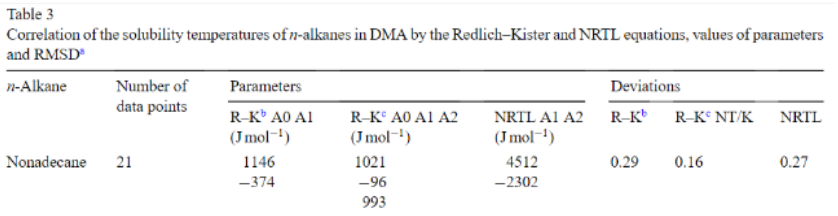


Table 3

Correlation of the solubility temperatures of *n*-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD[a]

| *n*-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K[b] A0 A1 (J mol$^{-1}$) | R–K[c] A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K[b] | R–K[c] NT/K | NRTL |
| Nonadecane | 21 | 1146<br>−374 | 1021<br>−96<br>993 | 4512<br>−2302 | 0.29 | 0.16 | 0.27 |

alpha = 0.2

ODABRATI NRTL

eicosane + dimethylacetamide

G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

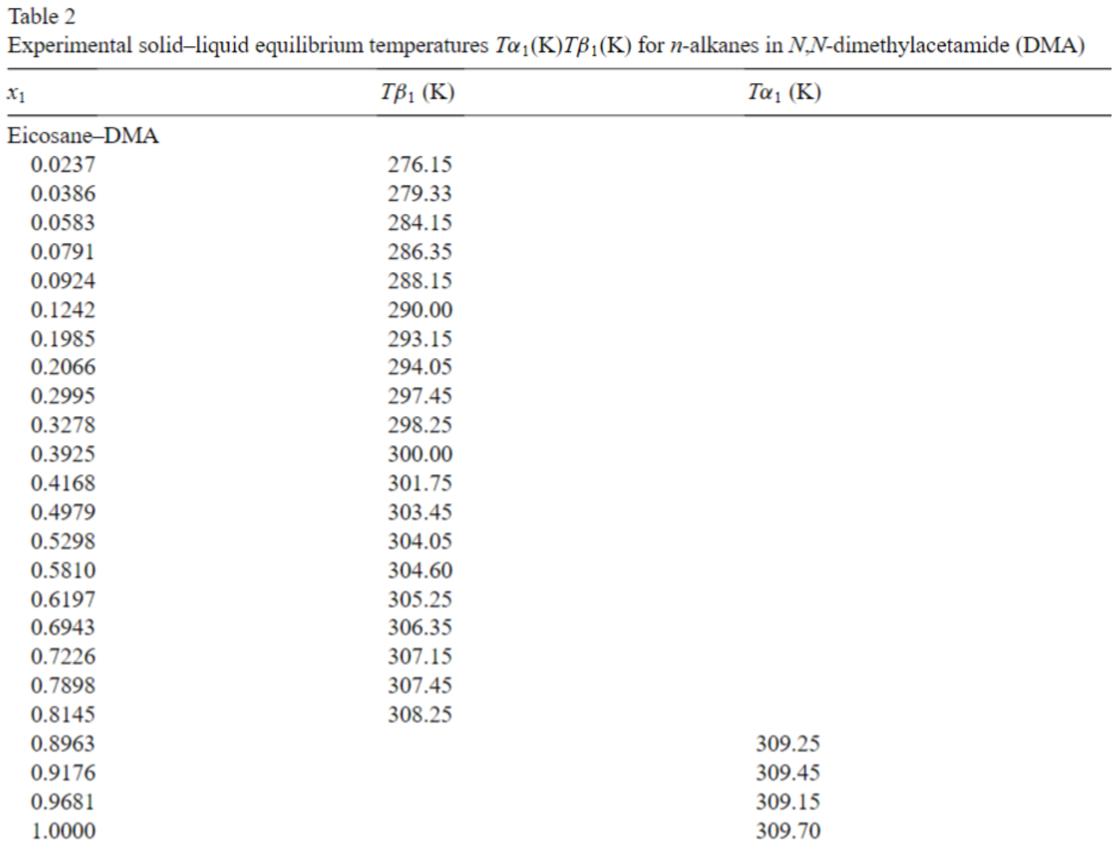


Table 2
Experimental solid–liquid equilibrium temperatures $T\alpha_1$(K)$T\beta_1$(K) for *n*-alkanes in *N*,*N*-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Eicosane–DMA | | |
| 0.0237 | 276.15 | |
| 0.0386 | 279.33 | |
| 0.0583 | 284.15 | |
| 0.0791 | 286.35 | |
| 0.0924 | 288.15 | |
| 0.1242 | 290.00 | |
| 0.1985 | 293.15 | |
| 0.2066 | 294.05 | |
| 0.2995 | 297.45 | |
| 0.3278 | 298.25 | |
| 0.3925 | 300.00 | |
| 0.4168 | 301.75 | |
| 0.4979 | 303.45 | |
| 0.5298 | 304.05 | |
| 0.5810 | 304.60 | |
| 0.6197 | 305.25 | |
| 0.6943 | 306.35 | |
| 0.7226 | 307.15 | |
| 0.7898 | 307.45 | |
| 0.8145 | 308.25 | |
| 0.8963 | | 309.25 |
| 0.9176 | | 309.45 |
| 0.9681 | | 309.15 |
| 1.0000 | | 309.70 |

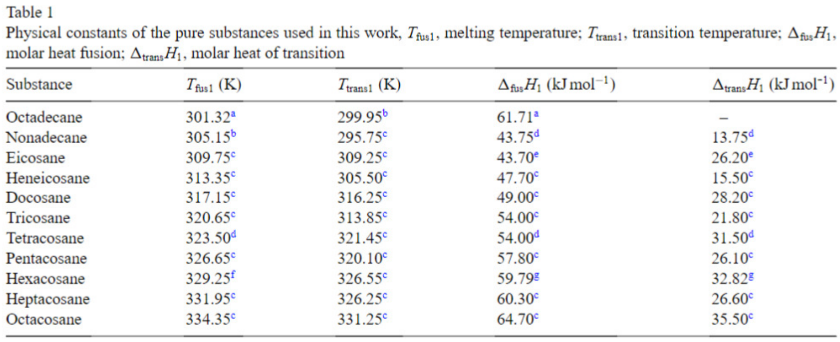


Table 1
Physical constants of the pure substances used in this work, $T_{\mathrm{fus}1}$, melting temperature; $T_{\mathrm{trans}1}$, transition temperature; $\Delta_{\mathrm{fus}}H_1$, molar heat fusion; $\Delta_{\mathrm{trans}}H_1$, molar heat of transition

| Substance | $T_{\mathrm{fus}1}$ (K) | $T_{\mathrm{trans}1}$ (K) | $\Delta_{\mathrm{fus}}H_1$ (kJ mol$^{-1}$) | $\Delta_{\mathrm{trans}}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32[a] | 299.95[b] | 61.71[a] | – |
| Nonadecane | 305.15[b] | 295.75[c] | 43.75[d] | 13.75[d] |
| Eicosane | 309.75[c] | 309.25[c] | 43.70[e] | 26.20[e] |
| Heneicosane | 313.35[c] | 305.50[c] | 47.70[c] | 15.50[c] |
| Docosane | 317.15[c] | 316.25[c] | 49.00[c] | 28.20[c] |
| Tricosane | 320.65[c] | 313.85[c] | 54.00[c] | 21.80[c] |
| Tetracosane | 323.50[d] | 321.45[c] | 54.00[d] | 31.50[d] |
| Pentacosane | 326.65[c] | 320.10[c] | 57.80[c] | 26.10[c] |
| Hexacosane | 329.25[f] | 326.55[c] | 59.79[g] | 32.82[g] |
| Heptacosane | 331.95[c] | 326.25[c] | 60.30[c] | 26.60[c] |
| Octacosane | 334.35[c] | 331.25[c] | 64.70[c] | 35.50[c] |

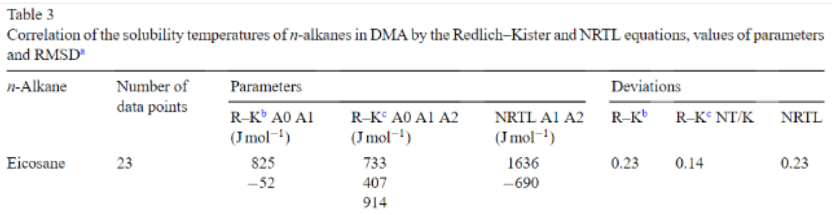


Table 3
Correlation of the solubility temperatures of *n*-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD[a]

| *n*-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K[b] A0 A1 (J mol$^{-1}$) | R–K[c] A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K[b] | R–K[c] NT/K | NRTL |
| Eicosane | 23 | 825<br>−52 | 733<br>407<br>914 | 1636<br>−690 | 0.23 | 0.14 | 0.23 |

alpha = 0.2

ODABRATI NRTL

heneicosane + dimethylacetamide
G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

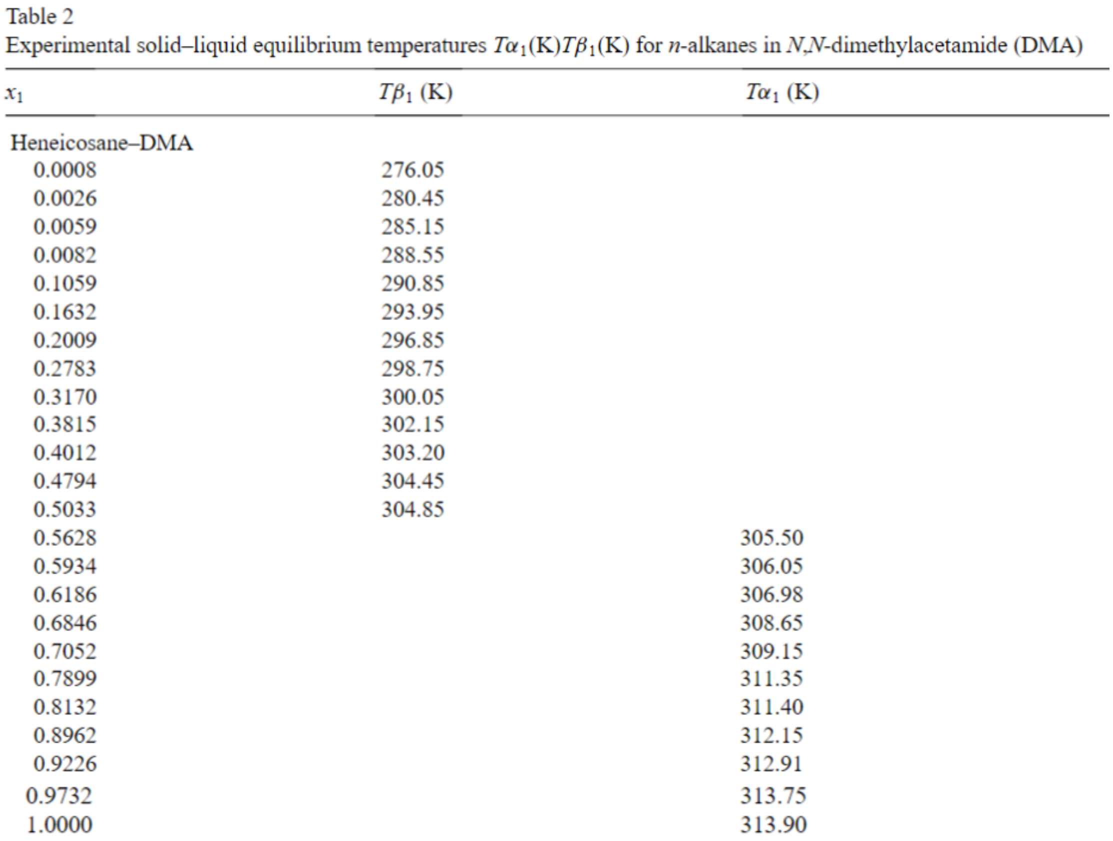


Table 2
Experimental solid–liquid equilibrium temperatures $T\alpha_1(\mathrm{K})T\beta_1(\mathrm{K})$ for *n*-alkanes in *N*,*N*-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Heneicosane–DMA | | |
| 0.0008 | 276.05 | |
| 0.0026 | 280.45 | |
| 0.0059 | 285.15 | |
| 0.0082 | 288.55 | |
| 0.1059 | 290.85 | |
| 0.1632 | 293.95 | |
| 0.2009 | 296.85 | |
| 0.2783 | 298.75 | |
| 0.3170 | 300.05 | |
| 0.3815 | 302.15 | |
| 0.4012 | 303.20 | |
| 0.4794 | 304.45 | |
| 0.5033 | 304.85 | |
| 0.5628 | | 305.50 |
| 0.5934 | | 306.05 |
| 0.6186 | | 306.98 |
| 0.6846 | | 308.65 |
| 0.7052 | | 309.15 |
| 0.7899 | | 311.35 |
| 0.8132 | | 311.40 |
| 0.8962 | | 312.15 |
| 0.9226 | | 312.91 |
| 0.9732 | | 313.75 |
| 1.0000 | | 313.90 |

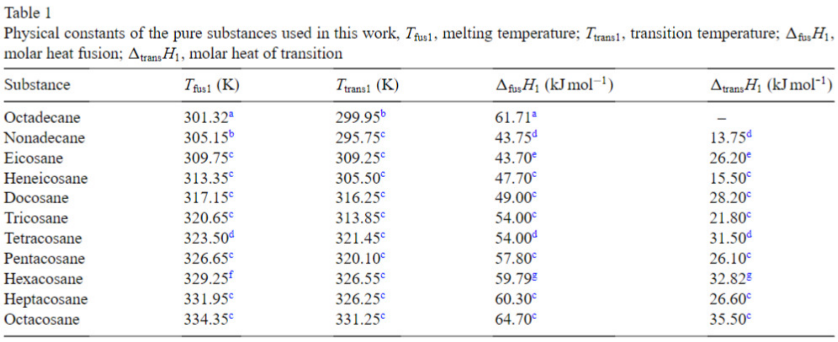


Table 1
Physical constants of the pure substances used in this work, $T_{\mathrm{fus1}}$, melting temperature; $T_{\mathrm{trans1}}$, transition temperature; $\Delta_{\mathrm{fus}}H_1$, molar heat fusion; $\Delta_{\mathrm{trans}}H_1$, molar heat of transition

| Substance | $T_{\mathrm{fus1}}$ (K) | $T_{\mathrm{trans1}}$ (K) | $\Delta_{\mathrm{fus}}H_1$ (kJ mol$^{-1}$) | $\Delta_{\mathrm{trans}}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32[a] | 299.95[b] | 61.71[a] | – |
| Nonadecane | 305.15[b] | 295.75[c] | 43.75[d] | 13.75[d] |
| Eicosane | 309.75[c] | 309.25[c] | 43.70[e] | 26.20[e] |
| Heneicosane | 313.35[c] | 305.50[c] | 47.70[c] | 15.50[c] |
| Docosane | 317.15[c] | 316.25[c] | 49.00[c] | 28.20[c] |
| Tricosane | 320.65[c] | 313.85[c] | 54.00[c] | 21.80[c] |
| Tetracosane | 323.50[d] | 321.45[c] | 54.00[d] | 31.50[d] |
| Pentacosane | 326.65[c] | 320.10[c] | 57.80[c] | 26.10[c] |
| Hexacosane | 329.25[f] | 326.55[c] | 59.79[g] | 32.82[g] |
| Heptacosane | 331.95[c] | 326.25[c] | 60.30[c] | 26.60[c] |
| Octacosane | 334.35[c] | 331.25[c] | 64.70[c] | 35.50[c] |

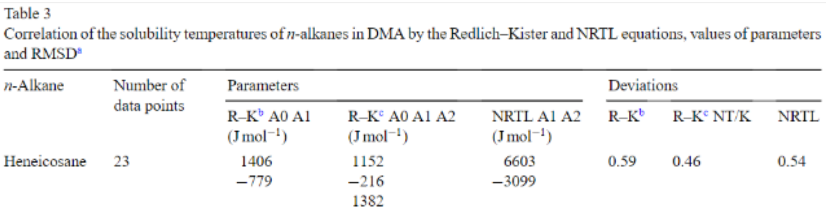


Table 3
Correlation of the solubility temperatures of *n*-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD[a]

| *n*-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K[b] A0 A1 (J mol$^{-1}$) | R–K[c] A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K[b] | R–K[c] NT/K | NRTL |
| Heneicosane | 23 | 1406<br>−779 | 1152<br>−216<br>1382 | 6603<br>−3099 | 0.59 | 0.46 | 0.54 |

alpha = 0.2

ODABRATI NRTL

docosane + dimethylacetamide

G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

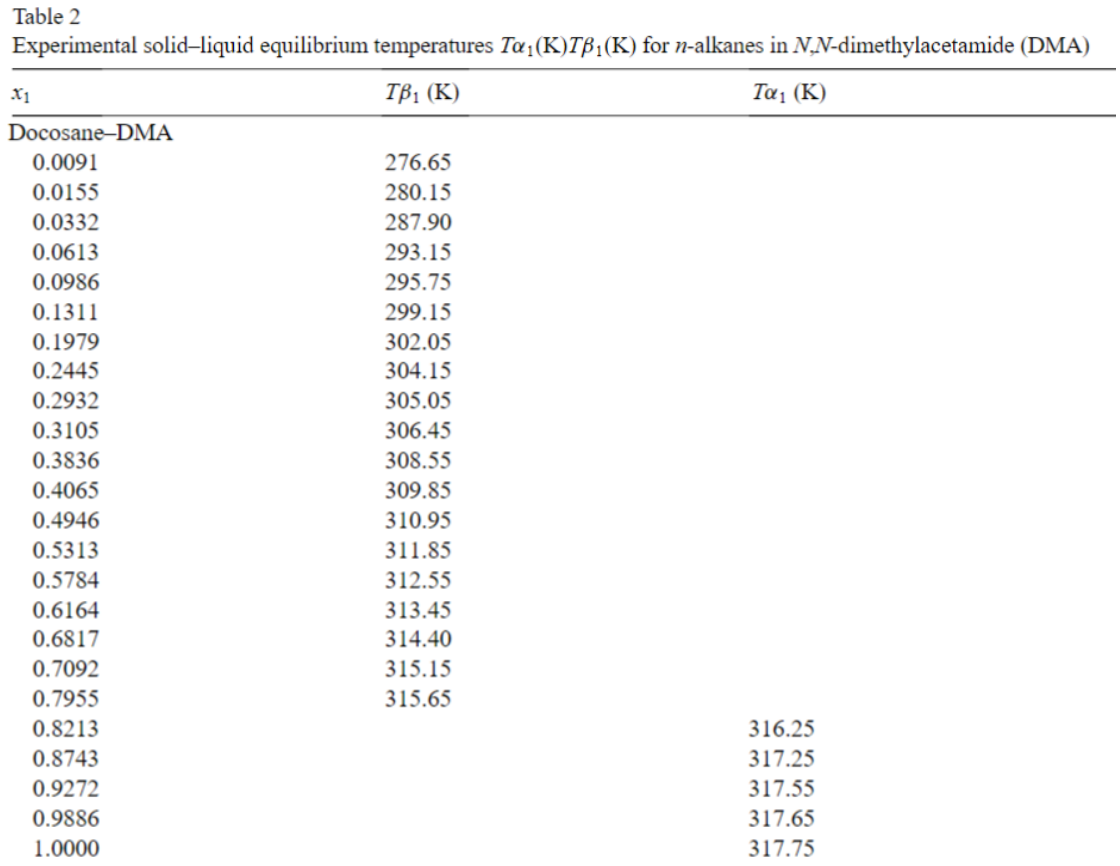


Table 2
Experimental solid–liquid equilibrium temperatures $T\alpha_1$(K)$T\beta_1$(K) for *n*-alkanes in *N*,*N*-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Docosane–DMA | | |
| 0.0091 | 276.65 | |
| 0.0155 | 280.15 | |
| 0.0332 | 287.90 | |
| 0.0613 | 293.15 | |
| 0.0986 | 295.75 | |
| 0.1311 | 299.15 | |
| 0.1979 | 302.05 | |
| 0.2445 | 304.15 | |
| 0.2932 | 305.05 | |
| 0.3105 | 306.45 | |
| 0.3836 | 308.55 | |
| 0.4065 | 309.85 | |
| 0.4946 | 310.95 | |
| 0.5313 | 311.85 | |
| 0.5784 | 312.55 | |
| 0.6164 | 313.45 | |
| 0.6817 | 314.40 | |
| 0.7092 | 315.15 | |
| 0.7955 | 315.65 | |
| 0.8213 | | 316.25 |
| 0.8743 | | 317.25 |
| 0.9272 | | 317.55 |
| 0.9886 | | 317.65 |
| 1.0000 | | 317.75 |

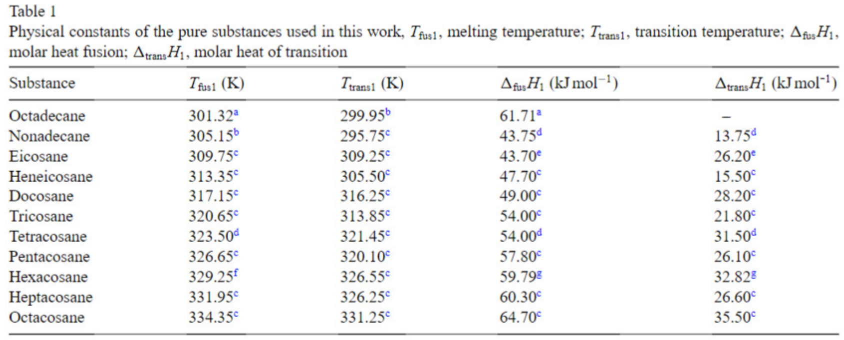


Table 1
Physical constants of the pure substances used in this work, $T_{\text{fus}1}$, melting temperature; $T_{\text{trans}1}$, transition temperature; $\Delta_{\text{fus}}H_1$, molar heat fusion; $\Delta_{\text{trans}}H_1$, molar heat of transition

| Substance | $T_{\text{fus}1}$ (K) | $T_{\text{trans}1}$ (K) | $\Delta_{\text{fus}}H_1$ (kJ mol$^{-1}$) | $\Delta_{\text{trans}}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32[a] | 299.95[b] | 61.71[a] | – |
| Nonadecane | 305.15[b] | 295.75[c] | 43.75[d] | 13.75[d] |
| Eicosane | 309.75[c] | 309.25[c] | 43.70[e] | 26.20[e] |
| Heneicosane | 313.35[c] | 305.50[c] | 47.70[c] | 15.50[c] |
| Docosane | 317.15[c] | 316.25[c] | 49.00[c] | 28.20[c] |
| Tricosane | 320.65[c] | 313.85[c] | 54.00[c] | 21.80[c] |
| Tetracosane | 323.50[d] | 321.45[c] | 54.00[d] | 31.50[d] |
| Pentacosane | 326.65[c] | 320.10[c] | 57.80[c] | 26.10[c] |
| Hexacosane | 329.25[f] | 326.55[c] | 59.79[g] | 32.82[g] |
| Heptacosane | 331.95[c] | 326.25[c] | 60.30[c] | 26.60[c] |
| Octacosane | 334.35[c] | 331.25[c] | 64.70[c] | 35.50[c] |

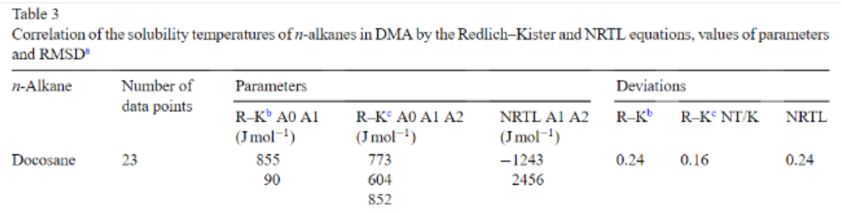


Table 3
Correlation of the solubility temperatures of *n*-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD[a]

| *n*-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K[b] A0 A1 (J mol$^{-1}$) | R–K[c] A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K[b] | R–K[c] NT/K | NRTL |
| Docosane | 23 | 855<br>90 | 773<br>604<br>852 | −1243<br>2456 | 0.24 | 0.16 | 0.24 |

alpha = 0.2

ODABRATI NRTL

tricosane + dimethylacetamide

G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

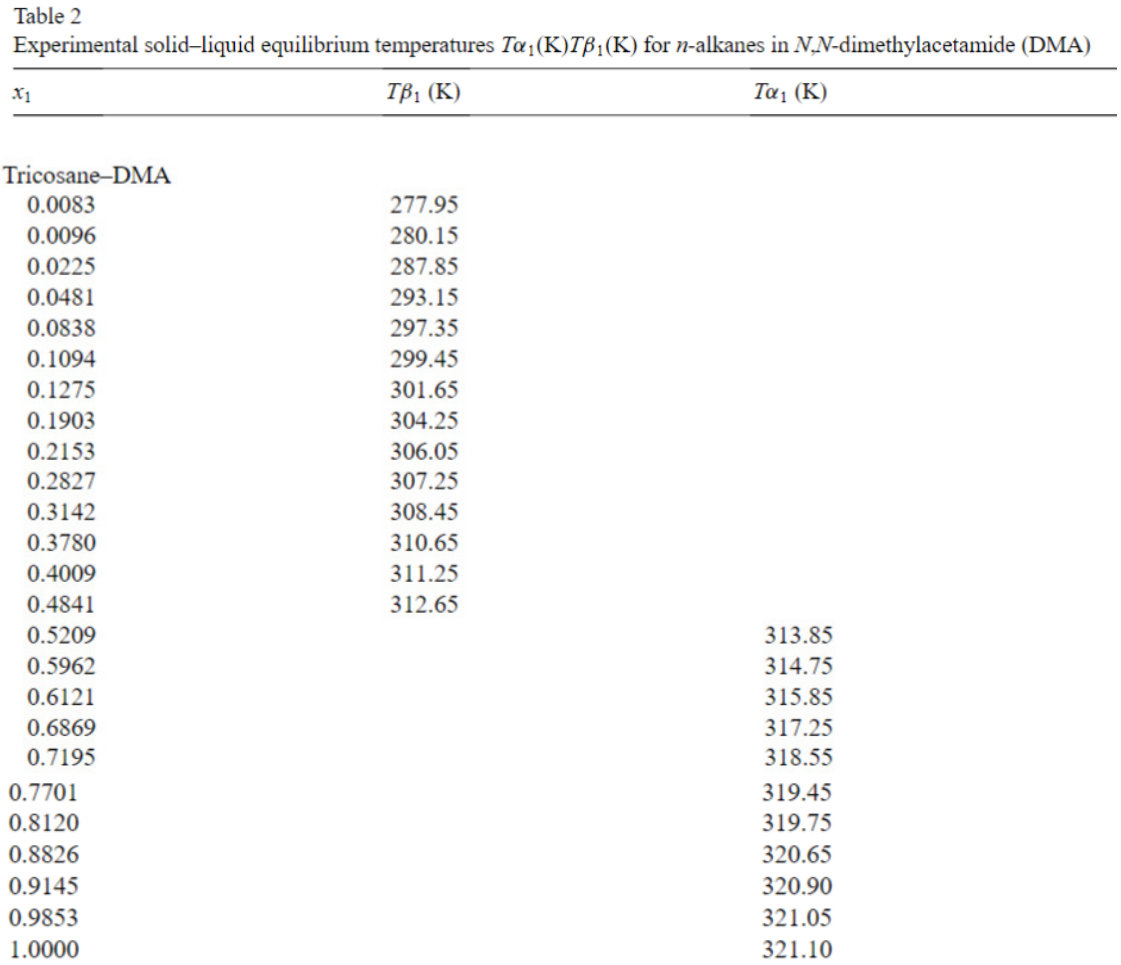


Table 2

Experimental solid–liquid equilibrium temperatures $T\alpha_1$(K)$T\beta_1$(K) for *n*-alkanes in *N*,*N*-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Tricosane–DMA | | |
| 0.0083 | 277.95 | |
| 0.0096 | 280.15 | |
| 0.0225 | 287.85 | |
| 0.0481 | 293.15 | |
| 0.0838 | 297.35 | |
| 0.1094 | 299.45 | |
| 0.1275 | 301.65 | |
| 0.1903 | 304.25 | |
| 0.2153 | 306.05 | |
| 0.2827 | 307.25 | |
| 0.3142 | 308.45 | |
| 0.3780 | 310.65 | |
| 0.4009 | 311.25 | |
| 0.4841 | 312.65 | |
| 0.5209 | | 313.85 |
| 0.5962 | | 314.75 |
| 0.6121 | | 315.85 |
| 0.6869 | | 317.25 |
| 0.7195 | | 318.55 |
| 0.7701 | | 319.45 |
| 0.8120 | | 319.75 |
| 0.8826 | | 320.65 |
| 0.9145 | | 320.90 |
| 0.9853 | | 321.05 |
| 1.0000 | | 321.10 |

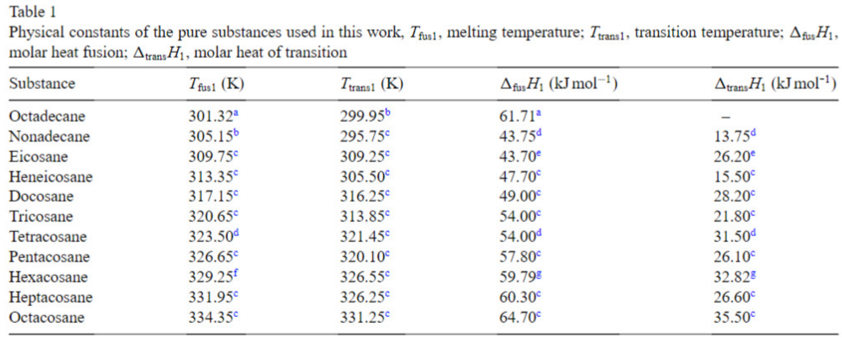


Table 1

Physical constants of the pure substances used in this work, $T_{fus1}$, melting temperature; $T_{trans1}$, transition temperature; $\Delta_{fus}H_1$, molar heat fusion; $\Delta_{trans}H_1$, molar heat of transition

| Substance | $T_{fus1}$ (K) | $T_{trans1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{trans}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32[a] | 299.95[b] | 61.71[a] | – |
| Nonadecane | 305.15[b] | 295.75[c] | 43.75[d] | 13.75[d] |
| Eicosane | 309.75[c] | 309.25[c] | 43.70[e] | 26.20[e] |
| Heneicosane | 313.35[c] | 305.50[c] | 47.70[c] | 15.50[c] |
| Docosane | 317.15[c] | 316.25[c] | 49.00[c] | 28.20[c] |
| Tricosane | 320.65[c] | 313.85[c] | 54.00[c] | 21.80[c] |
| Tetracosane | 323.50[d] | 321.45[c] | 54.00[d] | 31.50[d] |
| Pentacosane | 326.65[c] | 320.10[c] | 57.80[c] | 26.10[c] |
| Hexacosane | 329.25[f] | 326.55[c] | 59.79[g] | 32.82[g] |
| Heptacosane | 331.95[c] | 326.25[c] | 60.30[c] | 26.60[c] |
| Octacosane | 334.35[c] | 331.25[c] | 64.70[c] | 35.50[c] |

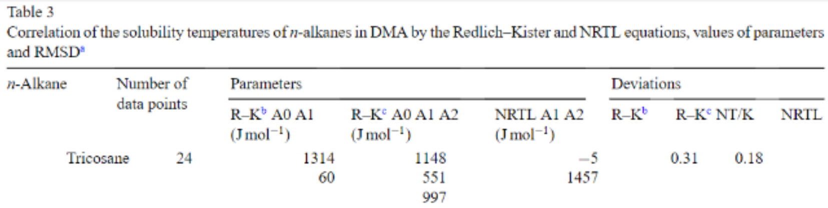


Table 3

Correlation of the solubility temperatures of *n*-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD[a]

| *n*-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K[b] A0 A1 (J mol$^{-1}$) | R–K[c] A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K[b] | R–K[c] NT/K | NRTL |
| Tricosane | 24 | 1314<br>60 | 1148<br>551<br>997 | −5<br>1457 | 0.31 | 0.18 | |

alpha = 0.2

ODABRATI NRTL

tetracosane + dimethylacetamide

G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

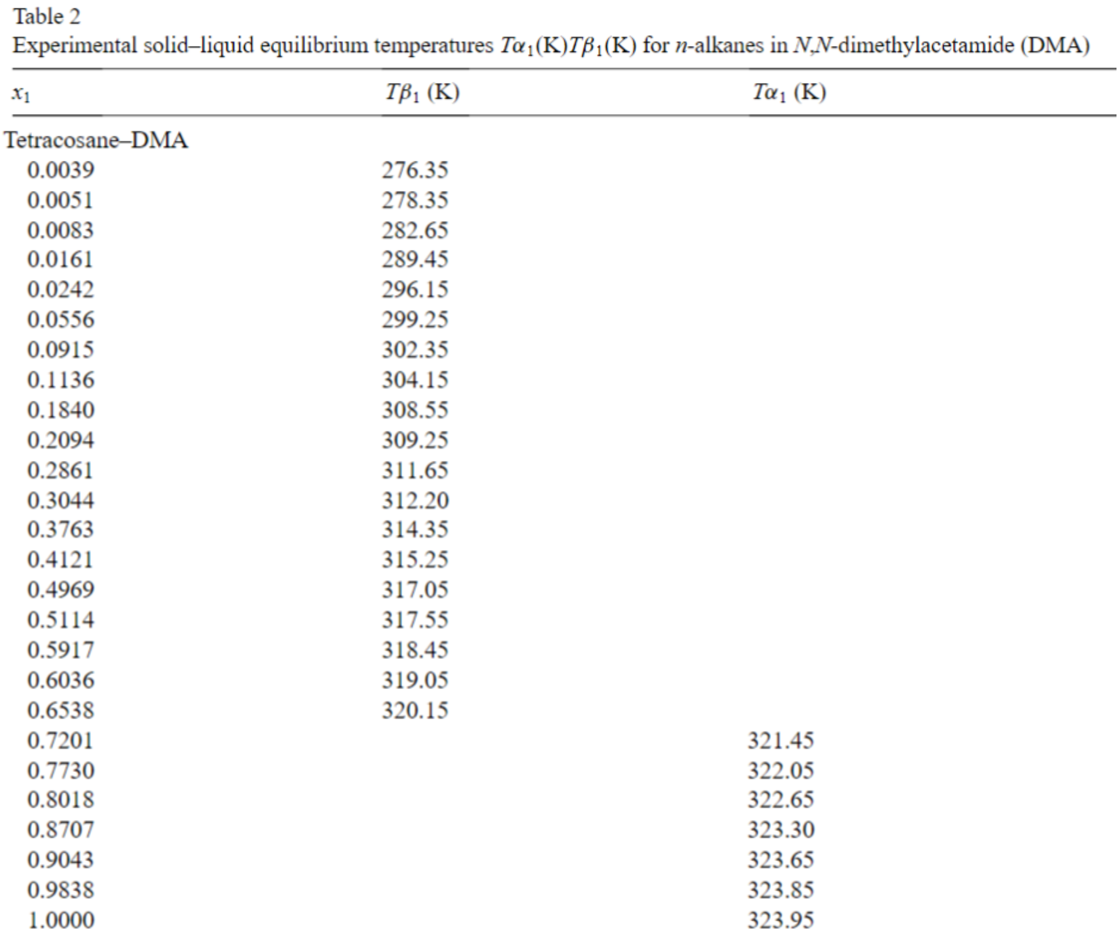


Table 2
Experimental solid–liquid equilibrium temperatures $T\alpha_1$(K)$T\beta_1$(K) for *n*-alkanes in *N*,*N*-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Tetracosane–DMA | | |
| 0.0039 | 276.35 | |
| 0.0051 | 278.35 | |
| 0.0083 | 282.65 | |
| 0.0161 | 289.45 | |
| 0.0242 | 296.15 | |
| 0.0556 | 299.25 | |
| 0.0915 | 302.35 | |
| 0.1136 | 304.15 | |
| 0.1840 | 308.55 | |
| 0.2094 | 309.25 | |
| 0.2861 | 311.65 | |
| 0.3044 | 312.20 | |
| 0.3763 | 314.35 | |
| 0.4121 | 315.25 | |
| 0.4969 | 317.05 | |
| 0.5114 | 317.55 | |
| 0.5917 | 318.45 | |
| 0.6036 | 319.05 | |
| 0.6538 | 320.15 | |
| 0.7201 | | 321.45 |
| 0.7730 | | 322.05 |
| 0.8018 | | 322.65 |
| 0.8707 | | 323.30 |
| 0.9043 | | 323.65 |
| 0.9838 | | 323.85 |
| 1.0000 | | 323.95 |

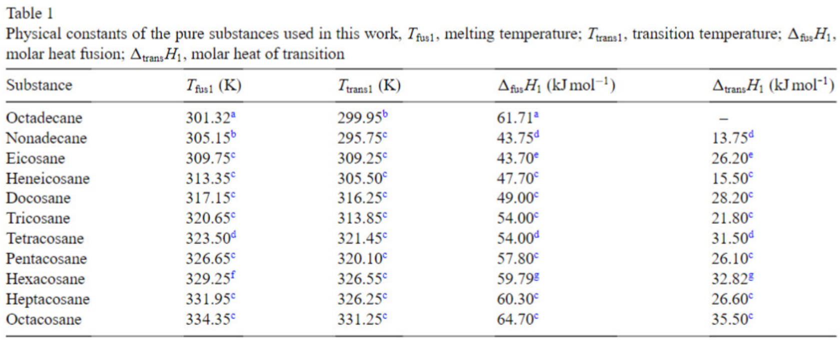


Table 1
Physical constants of the pure substances used in this work, $T_{fus1}$, melting temperature; $T_{trans1}$, transition temperature; $\Delta_{fus}H_1$, molar heat fusion; $\Delta_{trans}H_1$, molar heat of transition

| Substance | $T_{fus1}$ (K) | $T_{trans1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{trans}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32[a] | 299.95[b] | 61.71[a] | – |
| Nonadecane | 305.15[b] | 295.75[c] | 43.75[d] | 13.75[d] |
| Eicosane | 309.75[c] | 309.25[c] | 43.70[e] | 26.20[e] |
| Heneicosane | 313.35[c] | 305.50[c] | 47.70[c] | 15.50[c] |
| Docosane | 317.15[c] | 316.25[c] | 49.00[c] | 28.20[c] |
| Tricosane | 320.65[c] | 313.85[c] | 54.00[c] | 21.80[c] |
| Tetracosane | 323.50[d] | 321.45[c] | 54.00[d] | 31.50[d] |
| Pentacosane | 326.65[c] | 320.10[c] | 57.80[c] | 26.10[c] |
| Hexacosane | 329.25[f] | 326.55[c] | 59.79[g] | 32.82[g] |
| Heptacosane | 331.95[c] | 326.25[c] | 60.30[c] | 26.60[c] |
| Octacosane | 334.35[c] | 331.25[c] | 64.70[c] | 35.50[c] |

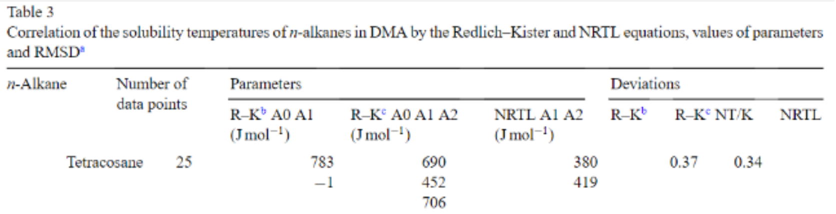


Table 3
Correlation of the solubility temperatures of *n*-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD[a]

| *n*-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K[b] A0 A1 (J mol$^{-1}$) | R–K[c] A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K[b] | R–K[c] NT/K | NRTL |
| Tetracosane | 25 | 783<br>−1 | 690<br>452<br>706 | 380<br>419 | 0.37 | 0.34 | |

alpha = 0.2

ODABRATI NRTL

pentacosane + dimethylacetamide

G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

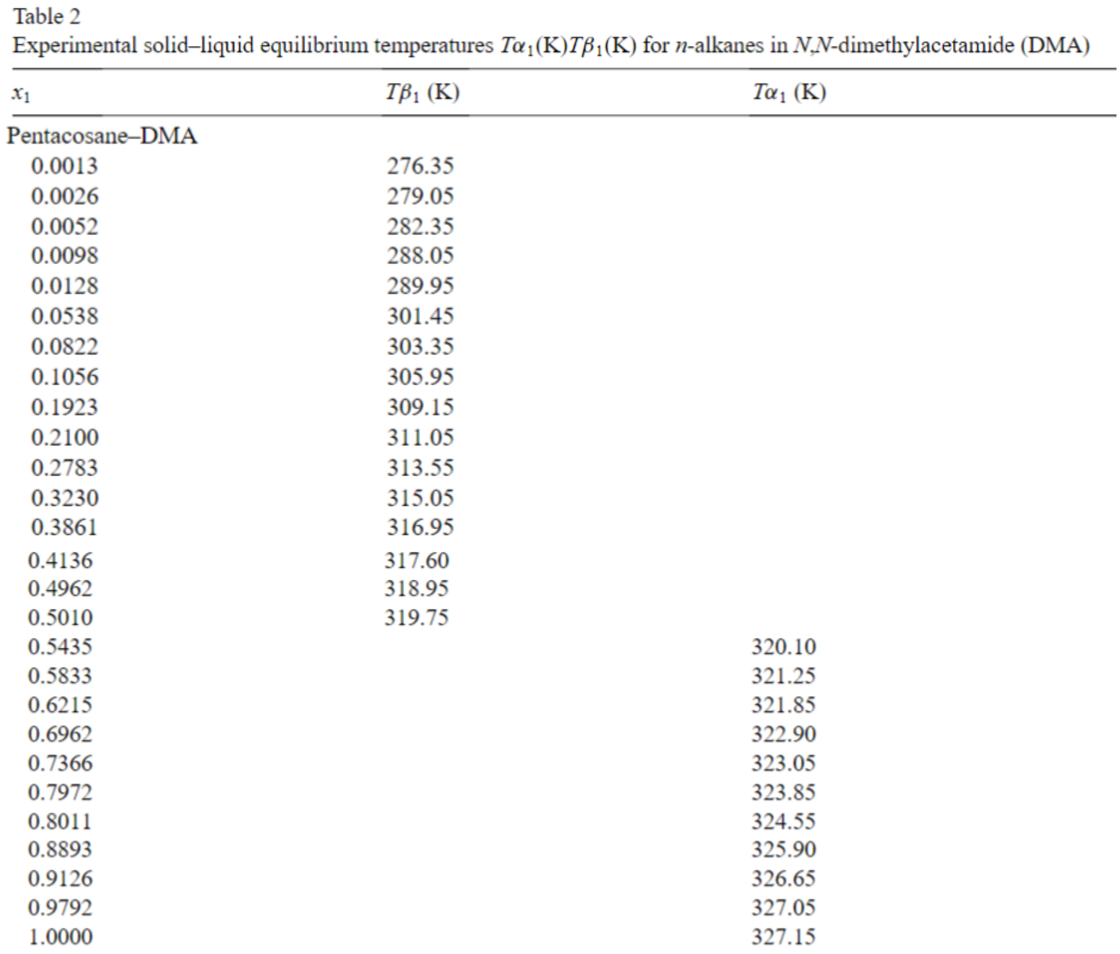


Table 2
Experimental solid–liquid equilibrium temperatures $T\alpha_1$(K)$T\beta_1$(K) for $n$-alkanes in $N$,$N$-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Pentacosane–DMA | | |
| 0.0013 | 276.35 | |
| 0.0026 | 279.05 | |
| 0.0052 | 282.35 | |
| 0.0098 | 288.05 | |
| 0.0128 | 289.95 | |
| 0.0538 | 301.45 | |
| 0.0822 | 303.35 | |
| 0.1056 | 305.95 | |
| 0.1923 | 309.15 | |
| 0.2100 | 311.05 | |
| 0.2783 | 313.55 | |
| 0.3230 | 315.05 | |
| 0.3861 | 316.95 | |
| 0.4136 | 317.60 | |
| 0.4962 | 318.95 | |
| 0.5010 | 319.75 | |
| 0.5435 | | 320.10 |
| 0.5833 | | 321.25 |
| 0.6215 | | 321.85 |
| 0.6962 | | 322.90 |
| 0.7366 | | 323.05 |
| 0.7972 | | 323.85 |
| 0.8011 | | 324.55 |
| 0.8893 | | 325.90 |
| 0.9126 | | 326.65 |
| 0.9792 | | 327.05 |
| 1.0000 | | 327.15 |

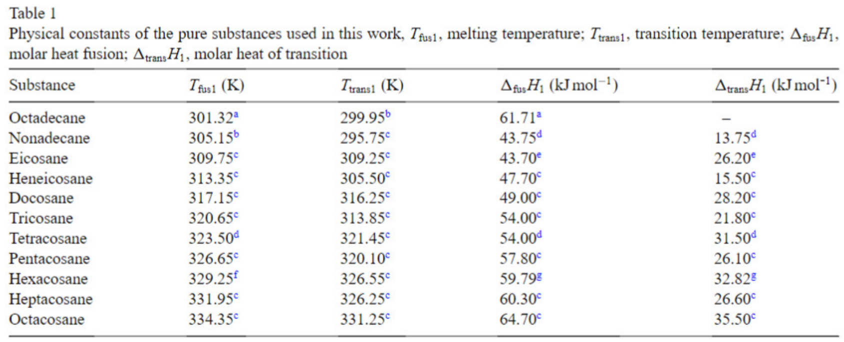


Table 1
Physical constants of the pure substances used in this work, $T_{fus1}$, melting temperature; $T_{trans1}$, transition temperature; $\Delta_{fus}H_1$, molar heat fusion; $\Delta_{trans}H_1$, molar heat of transition

| Substance | $T_{fus1}$ (K) | $T_{trans1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{trans}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32[a] | 299.95[b] | 61.71[a] | – |
| Nonadecane | 305.15[b] | 295.75[c] | 43.75[d] | 13.75[d] |
| Eicosane | 309.75[c] | 309.25[c] | 43.70[e] | 26.20[e] |
| Heneicosane | 313.35[c] | 305.50[c] | 47.70[c] | 15.50[c] |
| Docosane | 317.15[c] | 316.25[c] | 49.00[c] | 28.20[c] |
| Tricosane | 320.65[c] | 313.85[c] | 54.00[c] | 21.80[c] |
| Tetracosane | 323.50[d] | 321.45[c] | 54.00[d] | 31.50[d] |
| Pentacosane | 326.65[c] | 320.10[c] | 57.80[c] | 26.10[c] |
| Hexacosane | 329.25[f] | 326.55[c] | 59.79[g] | 32.82[g] |
| Heptacosane | 331.95[c] | 326.25[c] | 60.30[c] | 26.60[c] |
| Octacosane | 334.35[c] | 331.25[c] | 64.70[c] | 35.50[c] |

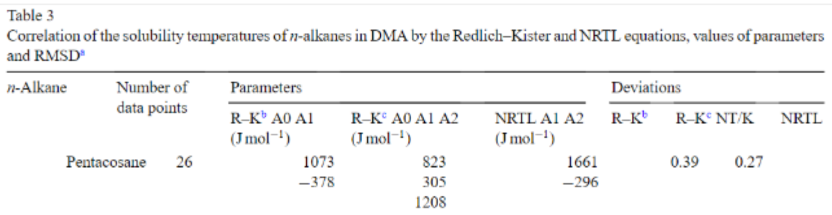


Table 3
Correlation of the solubility temperatures of $n$-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD[a]

| $n$-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K[b] A0 A1 (J mol$^{-1}$) | R–K[c] A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K[b] | R–K[c] NT/K | NRTL |
| Pentacosane | 26 | 1073<br>–378 | 823<br>305<br>1208 | 1661<br>–296 | | 0.39 | 0.27 |

alpha = 0.2

ODABRATI NRTL

hexacosane + dimethylacetamide

G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

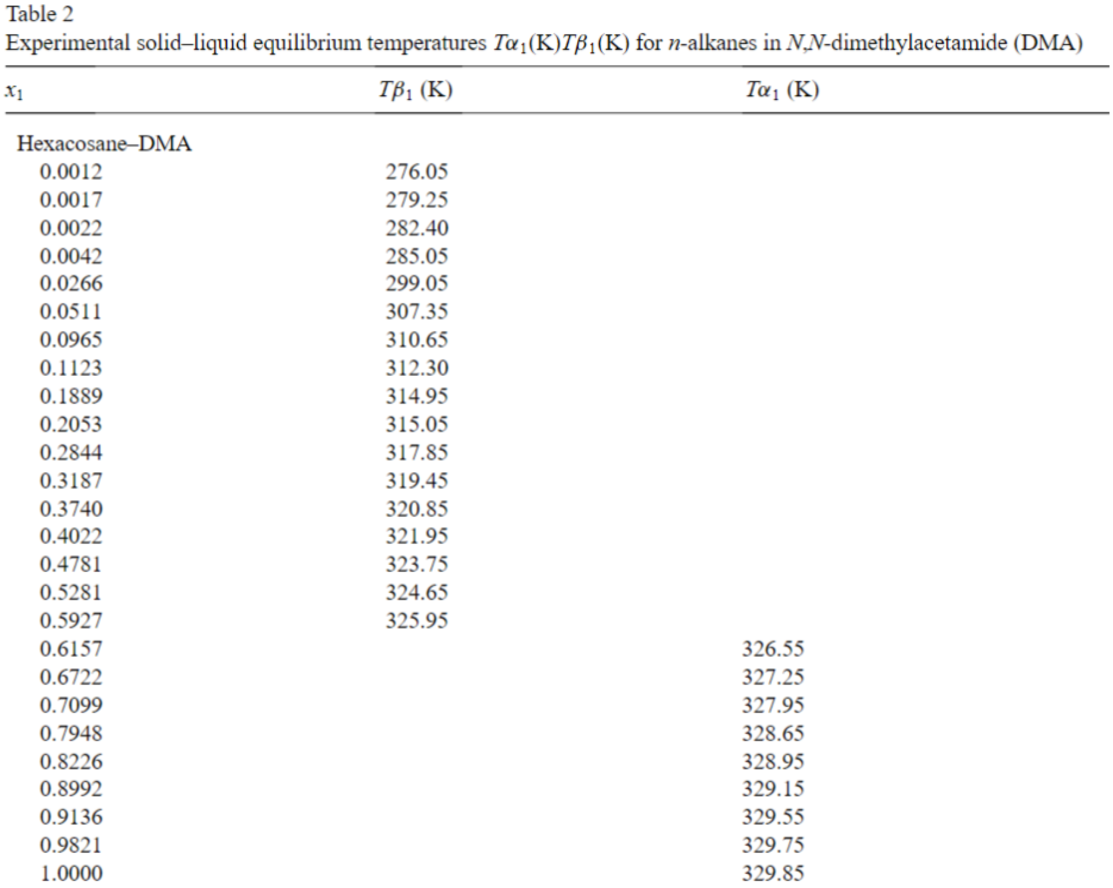


Table 2

Experimental solid–liquid equilibrium temperatures $T\alpha_1$(K)$T\beta_1$(K) for *n*-alkanes in *N*,*N*-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Hexacosane–DMA | | |
| 0.0012 | 276.05 | |
| 0.0017 | 279.25 | |
| 0.0022 | 282.40 | |
| 0.0042 | 285.05 | |
| 0.0266 | 299.05 | |
| 0.0511 | 307.35 | |
| 0.0965 | 310.65 | |
| 0.1123 | 312.30 | |
| 0.1889 | 314.95 | |
| 0.2053 | 315.05 | |
| 0.2844 | 317.85 | |
| 0.3187 | 319.45 | |
| 0.3740 | 320.85 | |
| 0.4022 | 321.95 | |
| 0.4781 | 323.75 | |
| 0.5281 | 324.65 | |
| 0.5927 | 325.95 | |
| 0.6157 | | 326.55 |
| 0.6722 | | 327.25 |
| 0.7099 | | 327.95 |
| 0.7948 | | 328.65 |
| 0.8226 | | 328.95 |
| 0.8992 | | 329.15 |
| 0.9136 | | 329.55 |
| 0.9821 | | 329.75 |
| 1.0000 | | 329.85 |

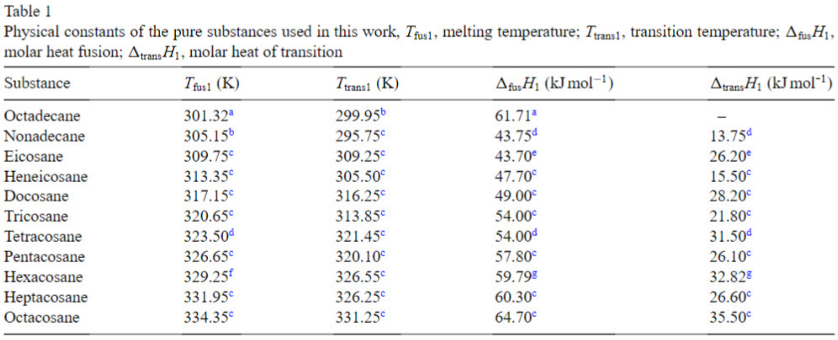


Table 1

Physical constants of the pure substances used in this work, $T_{\mathrm{fus}1}$, melting temperature; $T_{\mathrm{trans}1}$, transition temperature; $\Delta_{\mathrm{fus}}H_1$, molar heat fusion; $\Delta_{\mathrm{trans}}H_1$, molar heat of transition

| Substance | $T_{\mathrm{fus}1}$ (K) | $T_{\mathrm{trans}1}$ (K) | $\Delta_{\mathrm{fus}}H_1$ (kJ mol$^{-1}$) | $\Delta_{\mathrm{trans}}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32$^{a}$ | 299.95$^{b}$ | 61.71$^{a}$ | – |
| Nonadecane | 305.15$^{b}$ | 295.75$^{c}$ | 43.75$^{d}$ | 13.75$^{d}$ |
| Eicosane | 309.75$^{c}$ | 309.25$^{c}$ | 43.70$^{e}$ | 26.20$^{e}$ |
| Heneicosane | 313.35$^{c}$ | 305.50$^{c}$ | 47.70$^{c}$ | 15.50$^{c}$ |
| Docosane | 317.15$^{c}$ | 316.25$^{c}$ | 49.00$^{c}$ | 28.20$^{c}$ |
| Tricosane | 320.65$^{c}$ | 313.85$^{c}$ | 54.00$^{c}$ | 21.80$^{c}$ |
| Tetracosane | 323.50$^{d}$ | 321.45$^{c}$ | 54.00$^{d}$ | 31.50$^{d}$ |
| Pentacosane | 326.65$^{c}$ | 320.10$^{c}$ | 57.80$^{c}$ | 26.10$^{c}$ |
| Hexacosane | 329.25$^{f}$ | 326.55$^{c}$ | 59.79$^{g}$ | 32.82$^{g}$ |
| Heptacosane | 331.95$^{c}$ | 326.25$^{c}$ | 60.30$^{c}$ | 26.60$^{c}$ |
| Octacosane | 334.35$^{c}$ | 331.25$^{c}$ | 64.70$^{c}$ | 35.50$^{c}$ |

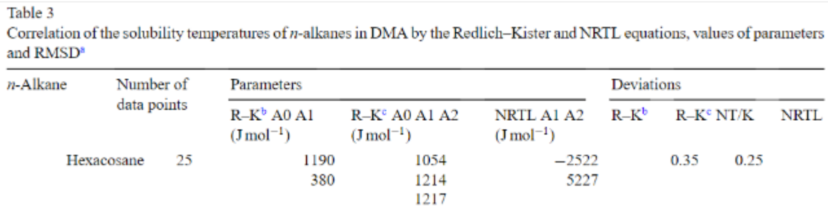


Table 3

Correlation of the solubility temperatures of *n*-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD[a]

| *n*-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K[b] A0 A1 (J mol$^{-1}$) | R–K[c] A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K[b] | R–K[c] NT/K | NRTL |
| Hexacosane | 25 | 1190<br>380 | 1054<br>1214<br>1217 | −2522<br>5227 | 0.35 | 0.25 | |

alpha = 0.2

ODABRATI NRTL

heptacosane + dimethylacetamide

G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

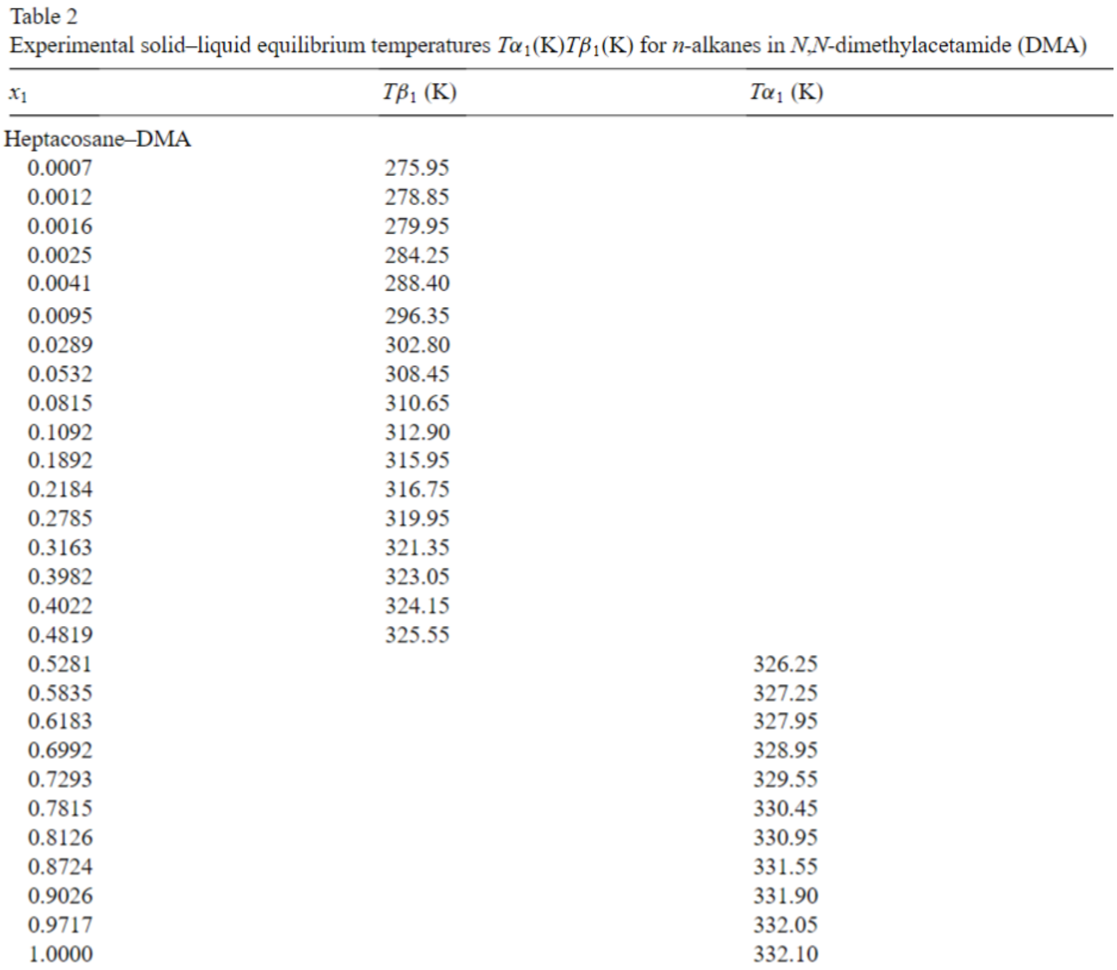


Table 2

Experimental solid–liquid equilibrium temperatures $T\alpha_1$(K)$T\beta_1$(K) for $n$-alkanes in $N$,$N$-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Heptacosane–DMA | | |
| 0.0007 | 275.95 | |
| 0.0012 | 278.85 | |
| 0.0016 | 279.95 | |
| 0.0025 | 284.25 | |
| 0.0041 | 288.40 | |
| 0.0095 | 296.35 | |
| 0.0289 | 302.80 | |
| 0.0532 | 308.45 | |
| 0.0815 | 310.65 | |
| 0.1092 | 312.90 | |
| 0.1892 | 315.95 | |
| 0.2184 | 316.75 | |
| 0.2785 | 319.95 | |
| 0.3163 | 321.35 | |
| 0.3982 | 323.05 | |
| 0.4022 | 324.15 | |
| 0.4819 | 325.55 | |
| 0.5281 | | 326.25 |
| 0.5835 | | 327.25 |
| 0.6183 | | 327.95 |
| 0.6992 | | 328.95 |
| 0.7293 | | 329.55 |
| 0.7815 | | 330.45 |
| 0.8126 | | 330.95 |
| 0.8724 | | 331.55 |
| 0.9026 | | 331.90 |
| 0.9717 | | 332.05 |
| 1.0000 | | 332.10 |

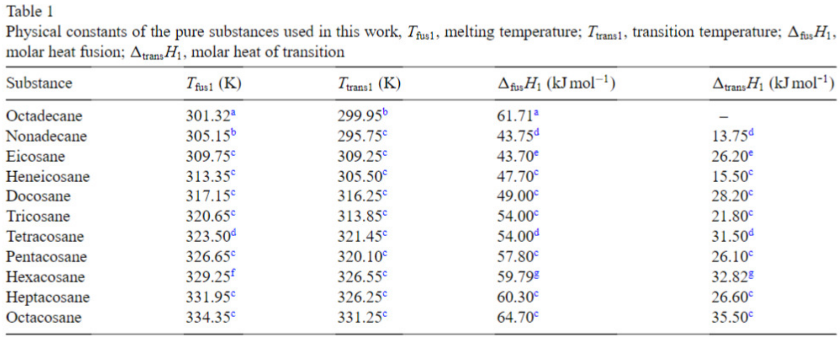


Table 1

Physical constants of the pure substances used in this work, $T_{\mathrm{fus}1}$, melting temperature; $T_{\mathrm{trans}1}$, transition temperature; $\Delta_{\mathrm{fus}}H_1$, molar heat fusion; $\Delta_{\mathrm{trans}}H_1$, molar heat of transition

| Substance | $T_{\mathrm{fus}1}$ (K) | $T_{\mathrm{trans}1}$ (K) | $\Delta_{\mathrm{fus}}H_1$ (kJ mol$^{-1}$) | $\Delta_{\mathrm{trans}}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32[a] | 299.95[b] | 61.71[a] | – |
| Nonadecane | 305.15[b] | 295.75[c] | 43.75[d] | 13.75[d] |
| Eicosane | 309.75[c] | 309.25[c] | 43.70[e] | 26.20[e] |
| Heneicosane | 313.35[c] | 305.50[c] | 47.70[c] | 15.50[c] |
| Docosane | 317.15[c] | 316.25[c] | 49.00[c] | 28.20[c] |
| Tricosane | 320.65[c] | 313.85[c] | 54.00[c] | 21.80[c] |
| Tetracosane | 323.50[d] | 321.45[c] | 54.00[d] | 31.50[d] |
| Pentacosane | 326.65[c] | 320.10[c] | 57.80[c] | 26.10[c] |
| Hexacosane | 329.25[f] | 326.55[c] | 59.79[g] | 32.82[g] |
| Heptacosane | 331.95[c] | 326.25[c] | 60.30[c] | 26.60[c] |
| Octacosane | 334.35[c] | 331.25[c] | 64.70[c] | 35.50[c] |

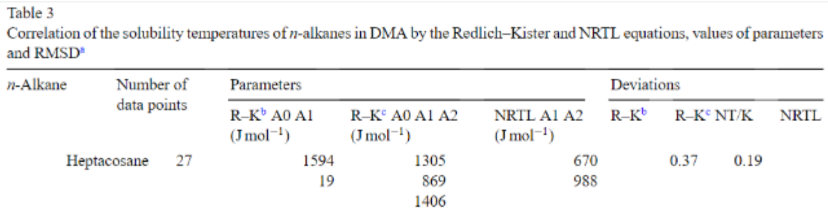


Table 3

Correlation of the solubility temperatures of $n$-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD[a]

| $n$-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K[b] A0 A1 (J mol$^{-1}$) | R–K[c] A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K[b] | R–K[c] NT/K | NRTL |
| Heptacosane | 27 | 1594<br>19 | 1305<br>869<br>1406 | 670<br>988 | | 0.37 | 0.19 |

alpha = 0.2

ODABRATI NRTL

octacosane + dimethylacetamide

G. Chandra Sekhar, P. Venkatesu, T. Hofman, M.V. Prabhakara Rao, Solid–liquid equilibria of long chain-alkanes(C18–C28)inN,N-dimethylacetamide, Fluid Phase Equilibria 201 (2002) 219–231

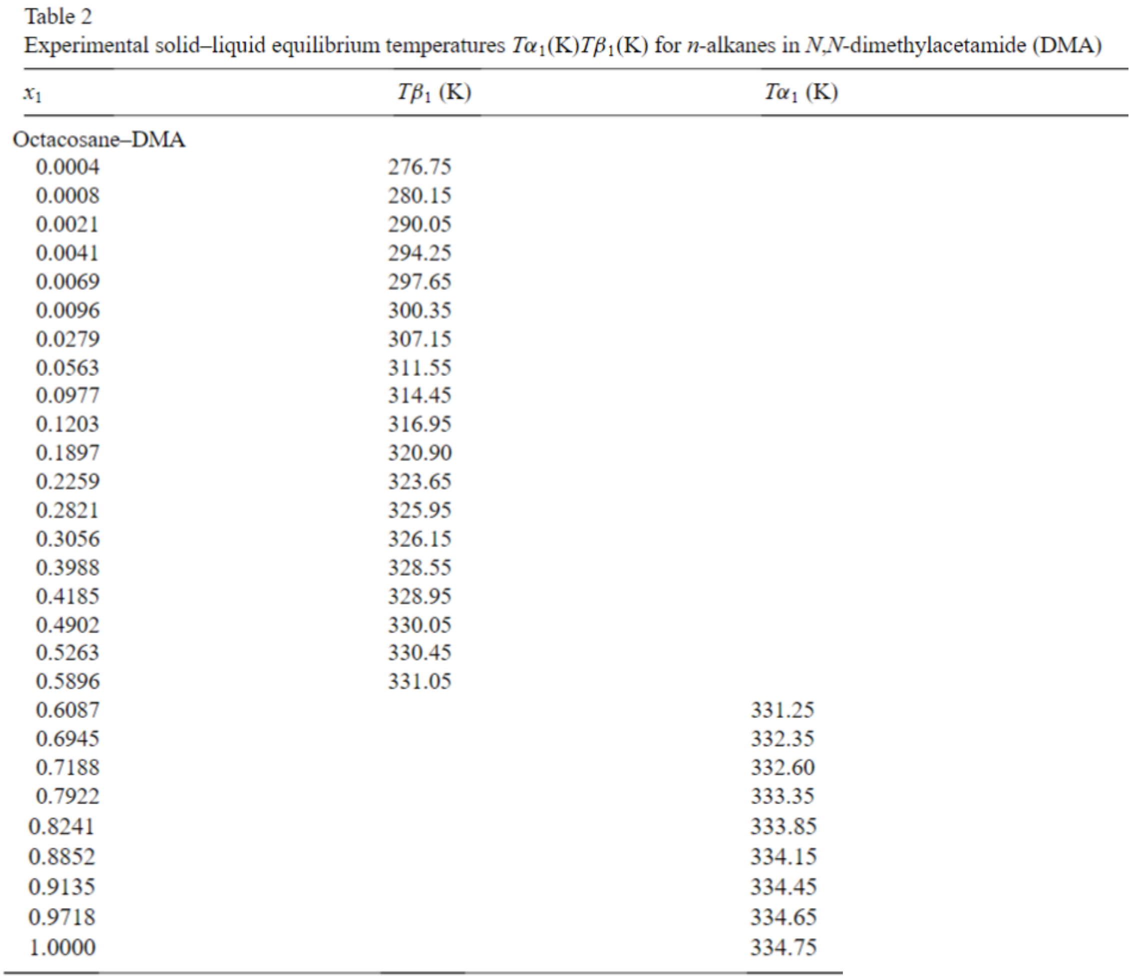


Table 2

Experimental solid–liquid equilibrium temperatures $T\alpha_1$(K)$T\beta_1$(K) for *n*-alkanes in *N*,*N*-dimethylacetamide (DMA)

| $x_1$ | $T\beta_1$ (K) | $T\alpha_1$ (K) |
|---|---|---|
| Octacosane–DMA | | |
| 0.0004 | 276.75 | |
| 0.0008 | 280.15 | |
| 0.0021 | 290.05 | |
| 0.0041 | 294.25 | |
| 0.0069 | 297.65 | |
| 0.0096 | 300.35 | |
| 0.0279 | 307.15 | |
| 0.0563 | 311.55 | |
| 0.0977 | 314.45 | |
| 0.1203 | 316.95 | |
| 0.1897 | 320.90 | |
| 0.2259 | 323.65 | |
| 0.2821 | 325.95 | |
| 0.3056 | 326.15 | |
| 0.3988 | 328.55 | |
| 0.4185 | 328.95 | |
| 0.4902 | 330.05 | |
| 0.5263 | 330.45 | |
| 0.5896 | 331.05 | |
| 0.6087 | | 331.25 |
| 0.6945 | | 332.35 |
| 0.7188 | | 332.60 |
| 0.7922 | | 333.35 |
| 0.8241 | | 333.85 |
| 0.8852 | | 334.15 |
| 0.9135 | | 334.45 |
| 0.9718 | | 334.65 |
| 1.0000 | | 334.75 |

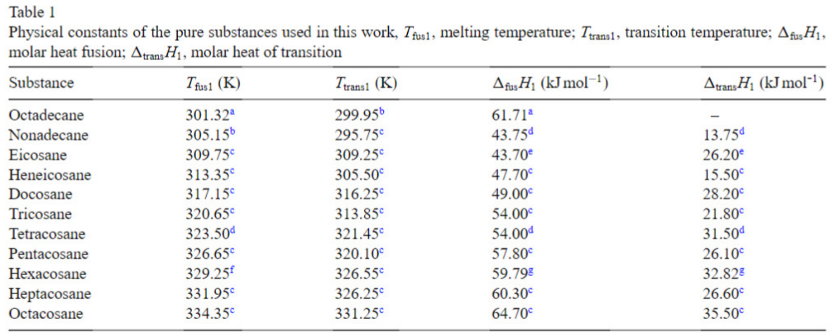


Table 1

Physical constants of the pure substances used in this work, $T_{fus1}$, melting temperature; $T_{trans1}$, transition temperature; $\Delta_{fus}H_1$, molar heat fusion; $\Delta_{trans}H_1$, molar heat of transition

| Substance | $T_{fus1}$ (K) | $T_{trans1}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{trans}H_1$ (kJ mol$^{-1}$) |
|---|---|---|---|---|
| Octadecane | 301.32$^{a}$ | 299.95$^{b}$ | 61.71$^{a}$ | – |
| Nonadecane | 305.15$^{b}$ | 295.75$^{c}$ | 43.75$^{d}$ | 13.75$^{d}$ |
| Eicosane | 309.75$^{c}$ | 309.25$^{c}$ | 43.70$^{e}$ | 26.20$^{e}$ |
| Heneicosane | 313.35$^{c}$ | 305.50$^{c}$ | 47.70$^{c}$ | 15.50$^{c}$ |
| Docosane | 317.15$^{c}$ | 316.25$^{c}$ | 49.00$^{c}$ | 28.20$^{c}$ |
| Tricosane | 320.65$^{c}$ | 313.85$^{c}$ | 54.00$^{c}$ | 21.80$^{c}$ |
| Tetracosane | 323.50$^{d}$ | 321.45$^{c}$ | 54.00$^{d}$ | 31.50$^{d}$ |
| Pentacosane | 326.65$^{c}$ | 320.10$^{c}$ | 57.80$^{c}$ | 26.10$^{c}$ |
| Hexacosane | 329.25$^{f}$ | 326.55$^{c}$ | 59.79$^{g}$ | 32.82$^{g}$ |
| Heptacosane | 331.95$^{c}$ | 326.25$^{c}$ | 60.30$^{c}$ | 26.60$^{c}$ |
| Octacosane | 334.35$^{c}$ | 331.25$^{c}$ | 64.70$^{c}$ | 35.50$^{c}$ |

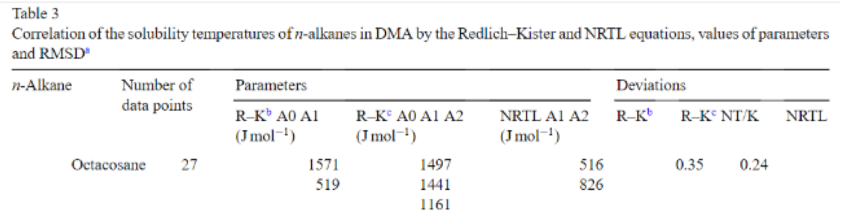


Table 3

Correlation of the solubility temperatures of *n*-alkanes in DMA by the Redlich–Kister and NRTL equations, values of parameters and RMSD$^{a}$

| *n*-Alkane | Number of data points | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|---|
| | | R–K$^{b}$ A0 A1 (J mol$^{-1}$) | R–K$^{c}$ A0 A1 A2 (J mol$^{-1}$) | NRTL A1 A2 (J mol$^{-1}$) | R–K$^{b}$ | R–K$^{c}$ NT/K | NRTL |
| Octacosane | 27 | 1571<br>519 | 1497<br>1441<br>1161 | 516<br>826 | | 0.35 | 0.24 |

alpha = 0.2

ODABRATI NRTL

hexane-1,6-diamine + biphenyl

Kamel Khimeche, Abdallah Dahmani, Measurement and prediction of (solid + liquid) equilibriaof (alkanediamine + biphenyl) mixtures, J. Chem. Thermodynamics 38 (2006) 1192–1198

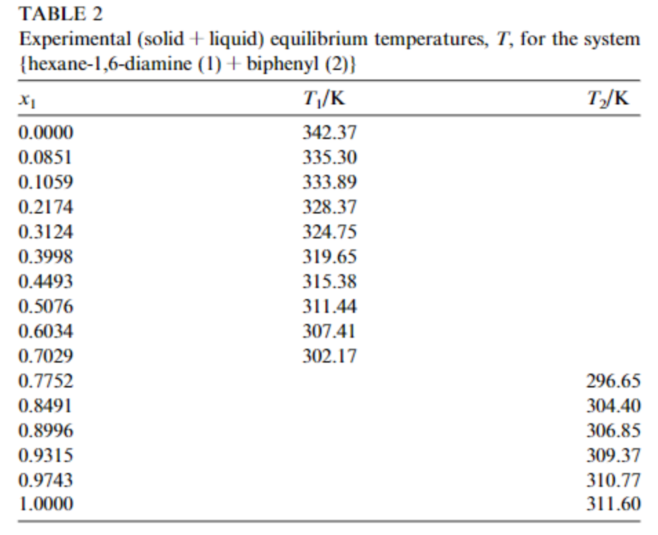


TABLE 2

Experimental (solid + liquid) equilibrium temperatures, $T$, for the system {hexane-1,6-diamine (1) + biphenyl (2)}

| $x_1$ | $T_1$/K | $T_2$/K |
|---|---|---|
| 0.0000 | 342.37 | |
| 0.0851 | 335.30 | |
| 0.1059 | 333.89 | |
| 0.2174 | 328.37 | |
| 0.3124 | 324.75 | |
| 0.3998 | 319.65 | |
| 0.4493 | 315.38 | |
| 0.5076 | 311.44 | |
| 0.6034 | 307.41 | |
| 0.7029 | 302.17 | |
| 0.7752 | | 296.65 |
| 0.8491 | | 304.40 |
| 0.8996 | | 306.85 |
| 0.9315 | | 309.37 |
| 0.9743 | | 310.77 |
| 1.0000 | | 311.60 |

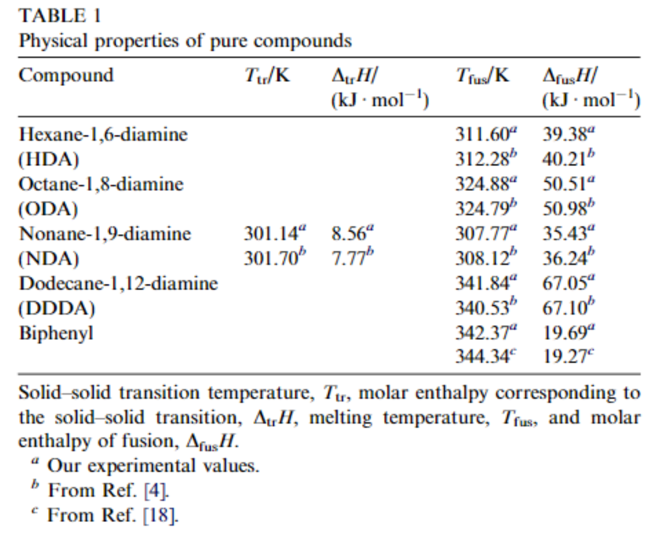


TABLE 1

Physical properties of pure compounds

| Compound | $T_{tr}$/K | $\Delta_{tr}H$/ (kJ · mol$^{-1}$) | $T_{fus}$/K | $\Delta_{fus}H$/ (kJ · mol$^{-1}$) |
|---|---|---|---|---|
| Hexane-1,6-diamine | | | 311.60[a] | 39.38[a] |
| (HDA) | | | 312.28[b] | 40.21[b] |
| Octane-1,8-diamine | | | 324.88[a] | 50.51[a] |
| (ODA) | | | 324.79[b] | 50.98[b] |
| Nonane-1,9-diamine | 301.14[a] | 8.56[a] | 307.77[a] | 35.43[a] |
| (NDA) | 301.70[b] | 7.77[b] | 308.12[b] | 36.24[b] |
| Dodecane-1,12-diamine | | | 341.84[a] | 67.05[a] |
| (DDDA) | | | 340.53[b] | 67.10[b] |
| Biphenyl | | | 342.37[a] | 19.69[a] |
| | | | 344.34[c] | 19.27[c] |

Solid–solid transition temperature, $T_{tr}$, molar enthalpy corresponding to the solid–solid transition, $\Delta_{tr}H$, melting temperature, $T_{fus}$, and molar enthalpy of fusion, $\Delta_{fus}H$.

[a] Our experimental values.

[b] From Ref. [4].

[c] From Ref. [18].

octane-1,6-diamine + biphenyl
Kamel Khimeche, Abdallah Dahmani, Measurement and prediction of (solid + liquid) equilibriaof (alkanediamine + biphenyl) mixtures, J. Chem. Thermodynamics 38 (2006) 1192–1198

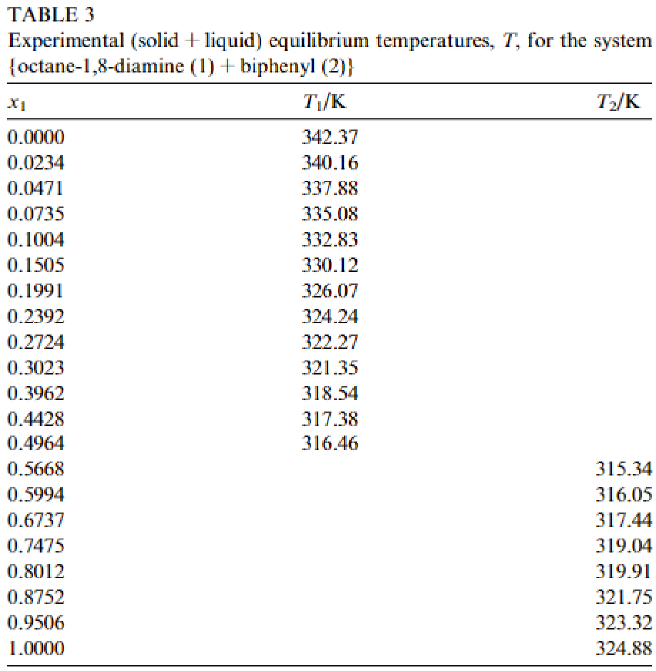


TABLE 3
Experimental (solid + liquid) equilibrium temperatures, $T$, for the system {octane-1,8-diamine (1) + biphenyl (2)}

| $x_1$ | $T_1$/K | $T_2$/K |
|---|---|---|
| 0.0000 | 342.37 | |
| 0.0234 | 340.16 | |
| 0.0471 | 337.88 | |
| 0.0735 | 335.08 | |
| 0.1004 | 332.83 | |
| 0.1505 | 330.12 | |
| 0.1991 | 326.07 | |
| 0.2392 | 324.24 | |
| 0.2724 | 322.27 | |
| 0.3023 | 321.35 | |
| 0.3962 | 318.54 | |
| 0.4428 | 317.38 | |
| 0.4964 | 316.46 | |
| 0.5668 | | 315.34 |
| 0.5994 | | 316.05 |
| 0.6737 | | 317.44 |
| 0.7475 | | 319.04 |
| 0.8012 | | 319.91 |
| 0.8752 | | 321.75 |
| 0.9506 | | 323.32 |
| 1.0000 | | 324.88 |

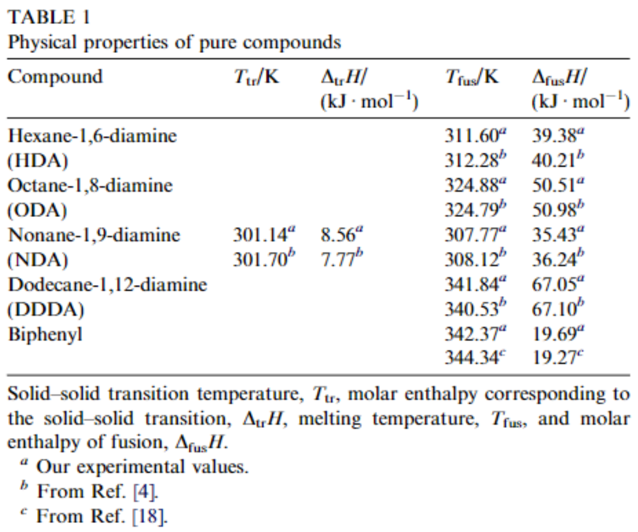


TABLE 1
Physical properties of pure compounds

| Compound | $T_{tr}$/K | $\Delta_{tr}H$/ (kJ · mol$^{-1}$) | $T_{fus}$/K | $\Delta_{fus}H$/ (kJ · mol$^{-1}$) |
|---|---|---|---|---|
| Hexane-1,6-diamine | | | 311.60[a] | 39.38[a] |
| (HDA) | | | 312.28[b] | 40.21[b] |
| Octane-1,8-diamine | | | 324.88[a] | 50.51[a] |
| (ODA) | | | 324.79[b] | 50.98[b] |
| Nonane-1,9-diamine | 301.14[a] | 8.56[a] | 307.77[a] | 35.43[a] |
| (NDA) | 301.70[b] | 7.77[b] | 308.12[b] | 36.24[b] |
| Dodecane-1,12-diamine | | | 341.84[a] | 67.05[a] |
| (DDDA) | | | 340.53[b] | 67.10[b] |
| Biphenyl | | | 342.37[a] | 19.69[a] |
| | | | 344.34[c] | 19.27[c] |

Solid–solid transition temperature, $T_{tr}$, molar enthalpy corresponding to the solid–solid transition, $\Delta_{tr}H$, melting temperature, $T_{fus}$, and molar enthalpy of fusion, $\Delta_{fus}H$.

[a] Our experimental values.
[b] From Ref. [4].
[c] From Ref. [18].

nonane-1,6-diamine + biphenyl
Kamel Khimeche, Abdallah Dahmani, Measurement and prediction of (solid + liquid) equilibriaof (alkanediamine + biphenyl) mixtures, J. Chem. Thermodynamics 38 (2006) 1192–1198

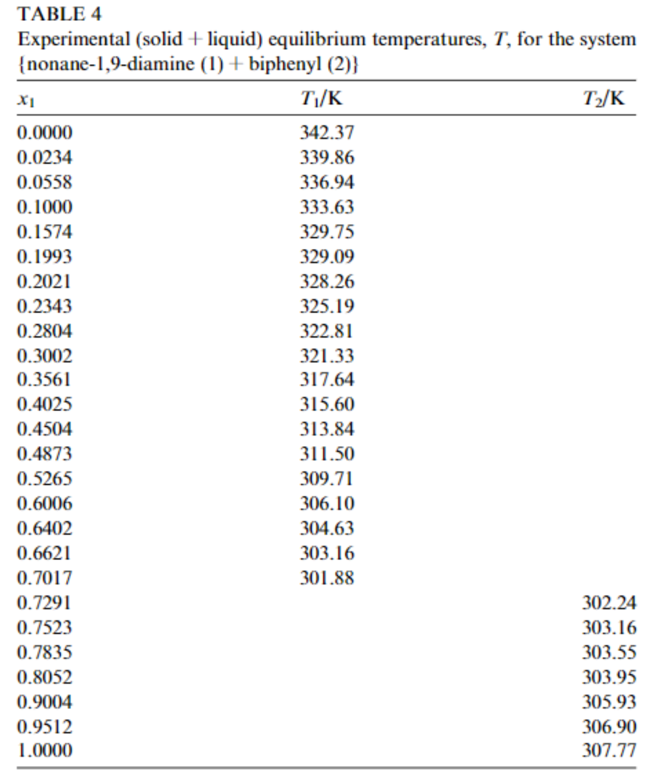


TABLE 4
Experimental (solid + liquid) equilibrium temperatures, $T$, for the system {nonane-1,9-diamine (1) + biphenyl (2)}

| $x_1$ | $T_1$/K | $T_2$/K |
|---|---|---|
| 0.0000 | 342.37 | |
| 0.0234 | 339.86 | |
| 0.0558 | 336.94 | |
| 0.1000 | 333.63 | |
| 0.1574 | 329.75 | |
| 0.1993 | 329.09 | |
| 0.2021 | 328.26 | |
| 0.2343 | 325.19 | |
| 0.2804 | 322.81 | |
| 0.3002 | 321.33 | |
| 0.3561 | 317.64 | |
| 0.4025 | 315.60 | |
| 0.4504 | 313.84 | |
| 0.4873 | 311.50 | |
| 0.5265 | 309.71 | |
| 0.6006 | 306.10 | |
| 0.6402 | 304.63 | |
| 0.6621 | 303.16 | |
| 0.7017 | 301.88 | |
| 0.7291 | | 302.24 |
| 0.7523 | | 303.16 |
| 0.7835 | | 303.55 |
| 0.8052 | | 303.95 |
| 0.9004 | | 305.93 |
| 0.9512 | | 306.90 |
| 1.0000 | | 307.77 |

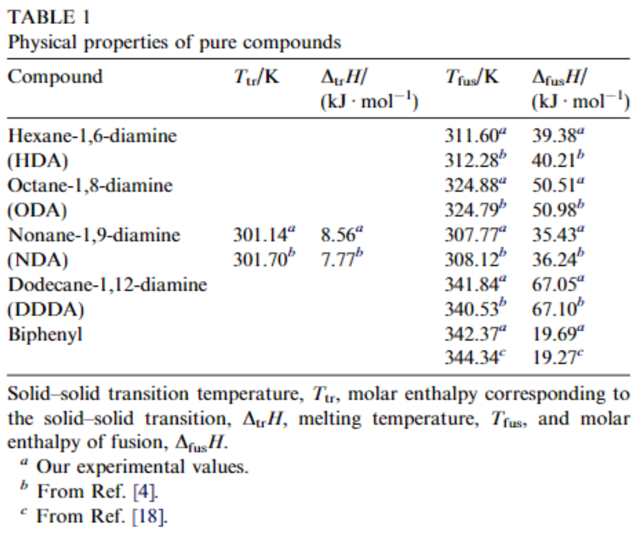


TABLE 1
Physical properties of pure compounds

| Compound | $T_{tr}$/K | $\Delta_{tr}H$/ (kJ · mol$^{-1}$) | $T_{fus}$/K | $\Delta_{fus}H$/ (kJ · mol$^{-1}$) |
|---|---|---|---|---|
| Hexane-1,6-diamine | | | 311.60$^a$ | 39.38$^a$ |
| (HDA) | | | 312.28$^b$ | 40.21$^b$ |
| Octane-1,8-diamine | | | 324.88$^a$ | 50.51$^a$ |
| (ODA) | | | 324.79$^b$ | 50.98$^b$ |
| Nonane-1,9-diamine | 301.14$^a$ | 8.56$^a$ | 307.77$^a$ | 35.43$^a$ |
| (NDA) | 301.70$^b$ | 7.77$^b$ | 308.12$^b$ | 36.24$^b$ |
| Dodecane-1,12-diamine | | | 341.84$^a$ | 67.05$^a$ |
| (DDDA) | | | 340.53$^b$ | 67.10$^b$ |
| Biphenyl | | | 342.37$^a$ | 19.69$^a$ |
| | | | 344.34$^c$ | 19.27$^c$ |

Solid–solid transition temperature, $T_{tr}$, molar enthalpy corresponding to the solid–solid transition, $\Delta_{tr}H$, melting temperature, $T_{fus}$, and molar enthalpy of fusion, $\Delta_{fus}H$.

[a] Our experimental values.

[b] From Ref. [4].

[c] From Ref. [18].

dodecane-1,6-diamine + biphenyl
Kamel Khimeche, Abdallah Dahmani, Measurement and prediction of (solid + liquid) equilibriaof (alkanediamine + biphenyl) mixtures, J. Chem. Thermodynamics 38 (2006) 1192–1198

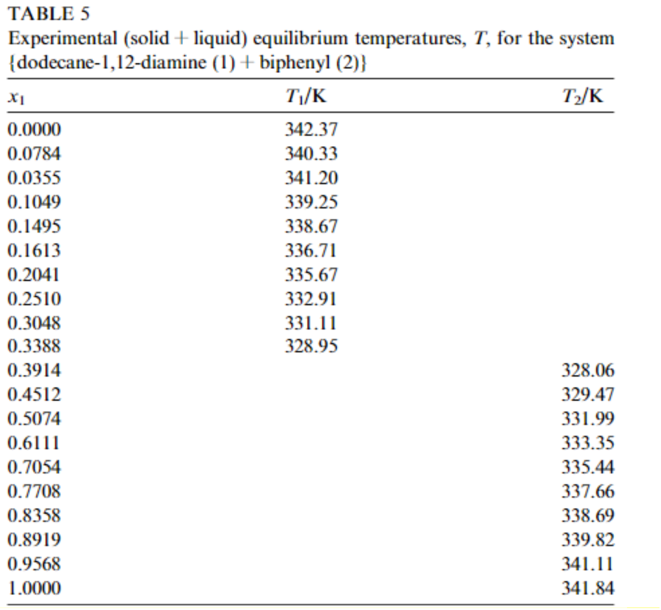


TABLE 5
Experimental (solid + liquid) equilibrium temperatures, $T$, for the system {dodecane-1,12-diamine (1) + biphenyl (2)}

| $x_1$ | $T_1$/K | $T_2$/K |
|---|---|---|
| 0.0000 | 342.37 | |
| 0.0784 | 340.33 | |
| 0.0355 | 341.20 | |
| 0.1049 | 339.25 | |
| 0.1495 | 338.67 | |
| 0.1613 | 336.71 | |
| 0.2041 | 335.67 | |
| 0.2510 | 332.91 | |
| 0.3048 | 331.11 | |
| 0.3388 | 328.95 | |
| 0.3914 | | 328.06 |
| 0.4512 | | 329.47 |
| 0.5074 | | 331.99 |
| 0.6111 | | 333.35 |
| 0.7054 | | 335.44 |
| 0.7708 | | 337.66 |
| 0.8358 | | 338.69 |
| 0.8919 | | 339.82 |
| 0.9568 | | 341.11 |
| 1.0000 | | 341.84 |

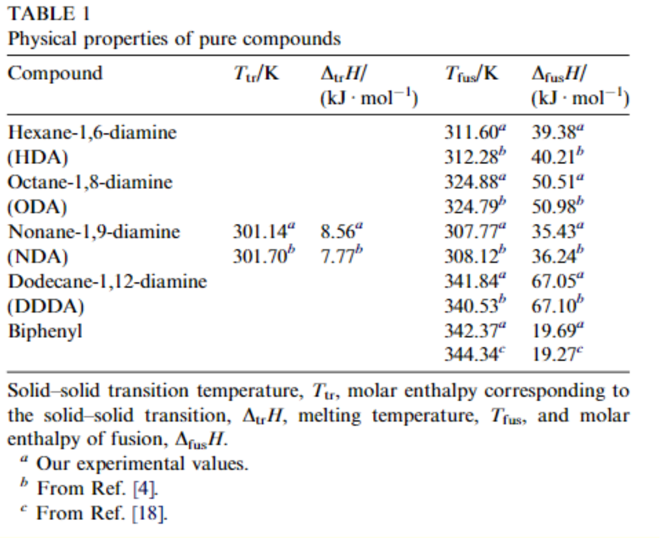


TABLE 1
Physical properties of pure compounds

| Compound | $T_{tr}$/K | $\Delta_{tr}H$/ (kJ · mol$^{-1}$) | $T_{fus}$/K | $\Delta_{fus}H$/ (kJ · mol$^{-1}$) |
|---|---|---|---|---|
| Hexane-1,6-diamine | | | 311.60$^a$ | 39.38$^a$ |
| (HDA) | | | 312.28$^b$ | 40.21$^b$ |
| Octane-1,8-diamine | | | 324.88$^a$ | 50.51$^a$ |
| (ODA) | | | 324.79$^b$ | 50.98$^b$ |
| Nonane-1,9-diamine | 301.14$^a$ | 8.56$^a$ | 307.77$^a$ | 35.43$^a$ |
| (NDA) | 301.70$^b$ | 7.77$^b$ | 308.12$^b$ | 36.24$^b$ |
| Dodecane-1,12-diamine | | | 341.84$^a$ | 67.05$^a$ |
| (DDDA) | | | 340.53$^b$ | 67.10$^b$ |
| Biphenyl | | | 342.37$^a$ | 19.69$^a$ |
| | | | 344.34$^c$ | 19.27$^c$ |

Solid–solid transition temperature, $T_{tr}$, molar enthalpy corresponding to the solid–solid transition, $\Delta_{tr}H$, melting temperature, $T_{fus}$, and molar enthalpy of fusion, $\Delta_{fus}H$.

[a] Our experimental values.

[b] From Ref. [4].

[c] From Ref. [18].

1-butyl-3-methylimidazolium chloride + *tert*-butanol

U. Domanska, E. Bogel-Łukasik, Solid–liquid equilibria for systems containing, 1-butyl-3-methylimidazolium chloride Fluid Phase Equilibria 218 (2004) 123–129.

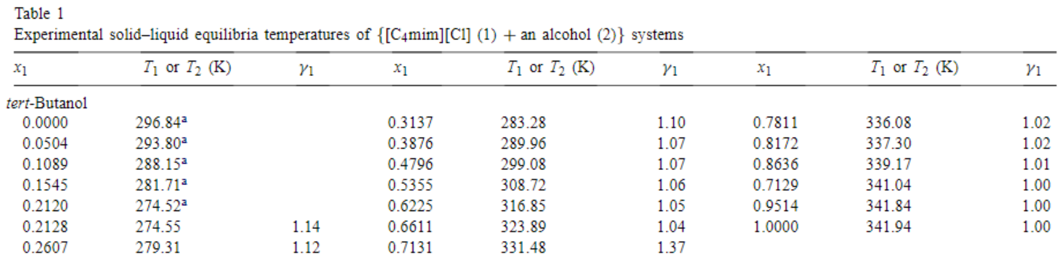


Table 1
Experimental solid–liquid equilibria temperatures of {[C$_4$mim][Cl] (1) + an alcohol (2)} systems

| $x_1$ | $T_1$ or $T_2$ (K) | $\gamma_1$ | $x_1$ | $T_1$ or $T_2$ (K) | $\gamma_1$ | $x_1$ | $T_1$ or $T_2$ (K) | $\gamma_1$ |
|---|---|---|---|---|---|---|---|---|
| *tert*-Butanol | | | | | | | | |
| 0.0000 | 296.84[a] | | 0.3137 | 283.28 | 1.10 | 0.7811 | 336.08 | 1.02 |
| 0.0504 | 293.80[a] | | 0.3876 | 289.96 | 1.07 | 0.8172 | 337.30 | 1.02 |
| 0.1089 | 288.15[a] | | 0.4796 | 299.08 | 1.07 | 0.8636 | 339.17 | 1.01 |
| 0.1545 | 281.71[a] | | 0.5355 | 308.72 | 1.06 | 0.7129 | 341.04 | 1.00 |
| 0.2120 | 274.52[a] | | 0.6225 | 316.85 | 1.05 | 0.9514 | 341.84 | 1.00 |
| 0.2128 | 274.55 | 1.14 | 0.6611 | 323.89 | 1.04 | 1.0000 | 341.94 | 1.00 |
| 0.2607 | 279.31 | 1.12 | 0.7131 | 331.48 | 1.37 | | | |

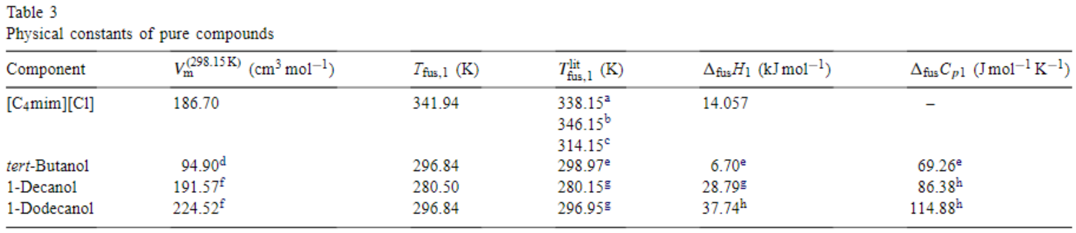


Table 3
Physical constants of pure compounds

| Component | $V_m^{(298.15\,K)}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{lit}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|
| [C$_4$mim][Cl] | 186.70 | 341.94 | 338.15[a]<br>346.15[b]<br>314.15[c] | 14.057 | – |
| *tert*-Butanol | 94.90[d] | 296.84 | 298.97[e] | 6.70[e] | 69.26[e] |
| 1-Decanol | 191.57[f] | 280.50 | 280.15[g] | 28.79[g] | 86.38[h] |
| 1-Dodecanol | 224.52[f] | 296.84 | 296.95[g] | 37.74[h] | 114.88[h] |

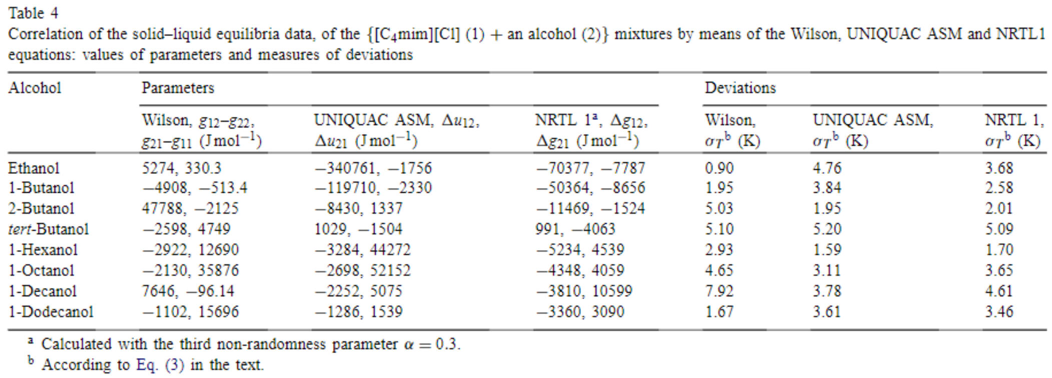


Table 4
Correlation of the solid–liquid equilibria data, of the {[C$_4$mim][Cl] (1) + an alcohol (2)} mixtures by means of the Wilson, UNIQUAC ASM and NRTL1 equations: values of parameters and measures of deviations

| Alcohol | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|
| | Wilson, $g_{12}-g_{22}$, $g_{21}-g_{11}$ (J mol$^{-1}$) | UNIQUAC ASM, $\Delta u_{12}$, $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1[a], $\Delta g_{12}$, $\Delta g_{21}$ (J mol$^{-1}$) | Wilson, $\sigma_T$[b] (K) | UNIQUAC ASM, $\sigma_T$[b] (K) | NRTL 1, $\sigma_T$[b] (K) |
| Ethanol | 5274, 330.3 | −340761, −1756 | −70377, −7787 | 0.90 | 4.76 | 3.68 |
| 1-Butanol | −4908, −513.4 | −119710, −2330 | −50364, −8656 | 1.95 | 3.84 | 2.58 |
| 2-Butanol | 47788, −2125 | −8430, 1337 | −11469, −1524 | 5.03 | 1.95 | 2.01 |
| *tert*-Butanol | −2598, 4749 | 1029, −1504 | 991, −4063 | 5.10 | 5.20 | 5.09 |
| 1-Hexanol | −2922, 12690 | −3284, 44272 | −5234, 4539 | 2.93 | 1.59 | 1.70 |
| 1-Octanol | −2130, 35876 | −2698, 52152 | −4348, 4059 | 4.65 | 3.11 | 3.65 |
| 1-Decanol | 7646, −96.14 | −2252, 5075 | −3810, 10599 | 7.92 | 3.78 | 4.61 |
| 1-Dodecanol | −1102, 15696 | −1286, 1539 | −3360, 3090 | 1.67 | 3.61 | 3.46 |

[a] Calculated with the third non-randomness parameter $\alpha = 0.3$.

[b] According to Eq. (3) in the text.

ODABRATI JEDAN MODEL

1-butyl-3-methylimidazolium chloride + decanol

U. Domanska, E. Bogel-Łukasik, Solid–liquid equilibria for systems containing, 1-butyl-3-methylimidazolium chloride Fluid Phase Equilibria 218 (2004) 123–129.

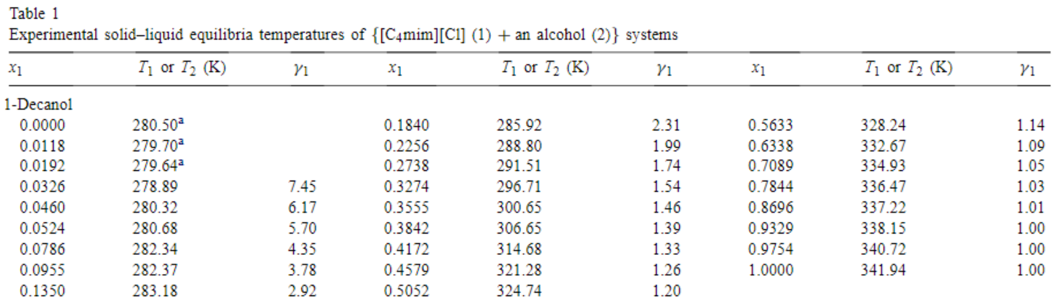


Table 1

Experimental solid–liquid equilibria temperatures of {[C$_4$mim][Cl] (1) + an alcohol (2)} systems

| $x_1$ | $T_1$ or $T_2$ (K) | $\gamma_1$ | $x_1$ | $T_1$ or $T_2$ (K) | $\gamma_1$ | $x_1$ | $T_1$ or $T_2$ (K) | $\gamma_1$ |
|---|---|---|---|---|---|---|---|---|
| 1-Decanol | | | | | | | | |
| 0.0000 | 280.50[a] | | 0.1840 | 285.92 | 2.31 | 0.5633 | 328.24 | 1.14 |
| 0.0118 | 279.70[a] | | 0.2256 | 288.80 | 1.99 | 0.6338 | 332.67 | 1.09 |
| 0.0192 | 279.64[a] | | 0.2738 | 291.51 | 1.74 | 0.7089 | 334.93 | 1.05 |
| 0.0326 | 278.89 | 7.45 | 0.3274 | 296.71 | 1.54 | 0.7844 | 336.47 | 1.03 |
| 0.0460 | 280.32 | 6.17 | 0.3555 | 300.65 | 1.46 | 0.8696 | 337.22 | 1.01 |
| 0.0524 | 280.68 | 5.70 | 0.3842 | 306.65 | 1.39 | 0.9329 | 338.15 | 1.00 |
| 0.0786 | 282.34 | 4.35 | 0.4172 | 314.68 | 1.33 | 0.9754 | 340.72 | 1.00 |
| 0.0955 | 282.37 | 3.78 | 0.4579 | 321.28 | 1.26 | 1.0000 | 341.94 | 1.00 |
| 0.1350 | 283.18 | 2.92 | 0.5052 | 324.74 | 1.20 | | | |

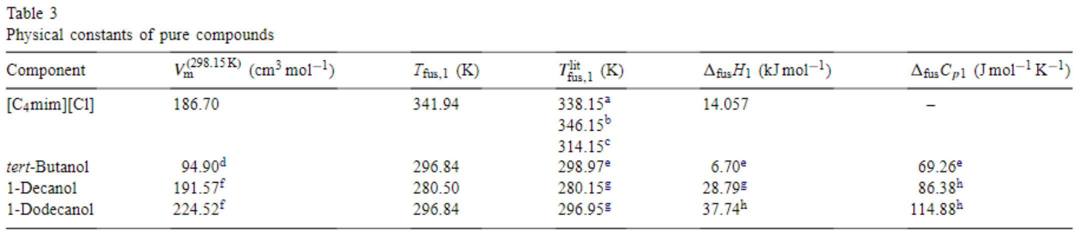


Table 3

Physical constants of pure compounds

| Component | $V_m^{(298.15\,K)}$ (cm$^3$ mol$^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{lit}$ (K) | $\Delta_{fus}H_1$ (kJ mol$^{-1}$) | $\Delta_{fus}C_{p1}$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|---|
| [C$_4$mim][Cl] | 186.70 | 341.94 | 338.15[a]<br>346.15[b]<br>314.15[c] | 14.057 | – |
| *tert*-Butanol | 94.90[d] | 296.84 | 298.97[e] | 6.70[e] | 69.26[e] |
| 1-Decanol | 191.57[f] | 280.50 | 280.15[g] | 28.79[g] | 86.38[h] |
| 1-Dodecanol | 224.52[f] | 296.84 | 296.95[g] | 37.74[h] | 114.88[h] |

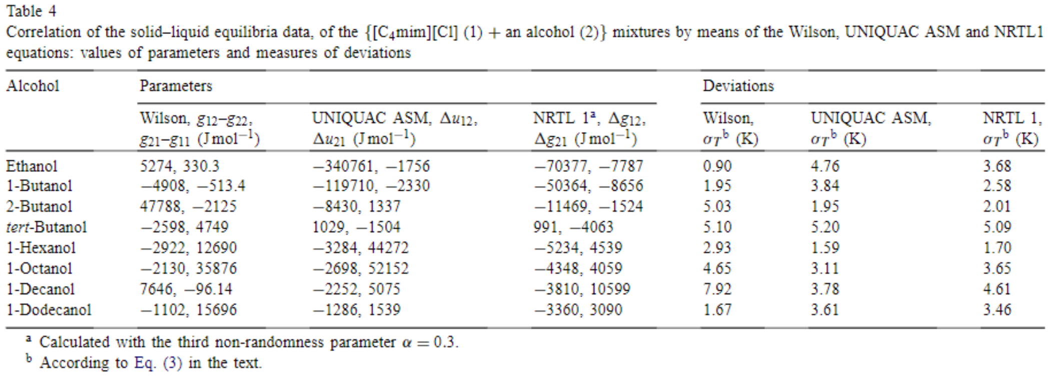


Table 4

Correlation of the solid–liquid equilibria data, of the {[C$_4$mim][Cl] (1) + an alcohol (2)} mixtures by means of the Wilson, UNIQUAC ASM and NRTL1 equations: values of parameters and measures of deviations

| Alcohol | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|
| | Wilson, $g_{12}-g_{22}$, $g_{21}-g_{11}$ (J mol$^{-1}$) | UNIQUAC ASM, $\Delta u_{12}$, $\Delta u_{21}$ (J mol$^{-1}$) | NRTL 1[a], $\Delta g_{12}$, $\Delta g_{21}$ (J mol$^{-1}$) | Wilson, $\sigma_T$[b] (K) | UNIQUAC ASM, $\sigma_T$[b] (K) | NRTL 1, $\sigma_T$[b] (K) |
| Ethanol | 5274, 330.3 | −340761, −1756 | −70377, −7787 | 0.90 | 4.76 | 3.68 |
| 1-Butanol | −4908, −513.4 | −119710, −2330 | −50364, −8656 | 1.95 | 3.84 | 2.58 |
| 2-Butanol | 47788, −2125 | −8430, 1337 | −11469, −1524 | 5.03 | 1.95 | 2.01 |
| *tert*-Butanol | −2598, 4749 | 1029, −1504 | 991, −4063 | 5.10 | 5.20 | 5.09 |
| 1-Hexanol | −2922, 12690 | −3284, 44272 | −5234, 4539 | 2.93 | 1.59 | 1.70 |
| 1-Octanol | −2130, 35876 | −2698, 52152 | −4348, 4059 | 4.65 | 3.11 | 3.65 |
| 1-Decanol | 7646, −96.14 | −2252, 5075 | −3810, 10599 | 7.92 | 3.78 | 4.61 |
| 1-Dodecanol | −1102, 15696 | −1286, 1539 | −3360, 3090 | 1.67 | 3.61 | 3.46 |

[a] Calculated with the third non-randomness parameter $\alpha = 0.3$.

[b] According to Eq. (3) in the text.

ODABRATI JEDAN MODEL

1-butyl-3-methylimidazolium chloride + dodecanol
U. Domanska, E. Bogel-Łukasik, Solid–liquid equilibria for systems containing, 1-butyl-3-methylimidazolium chloride Fluid Phase Equilibria 218 (2004) 123–129.

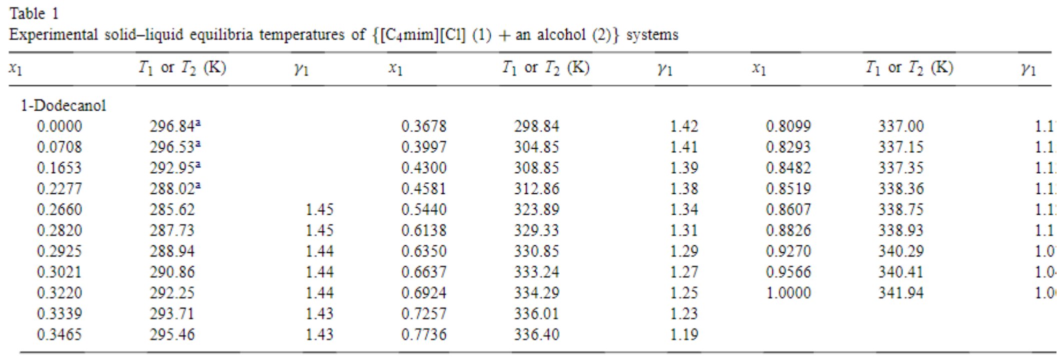


Table 1
Experimental solid–liquid equilibria temperatures of {[$C_4$mim][Cl] (1) + an alcohol (2)} systems

| $x_1$ | $T_1$ or $T_2$ (K) | $\gamma_1$ | $x_1$ | $T_1$ or $T_2$ (K) | $\gamma_1$ | $x_1$ | $T_1$ or $T_2$ (K) | $\gamma_1$ |
|---|---|---|---|---|---|---|---|---|
| 1-Dodecanol | | | | | | | | |
| 0.0000 | 296.84[a] | | 0.3678 | 298.84 | 1.42 | 0.8099 | 337.00 | 1.1 |
| 0.0708 | 296.53[a] | | 0.3997 | 304.85 | 1.41 | 0.8293 | 337.15 | 1.1 |
| 0.1653 | 292.95[a] | | 0.4300 | 308.85 | 1.39 | 0.8482 | 337.35 | 1.1 |
| 0.2277 | 288.02[a] | | 0.4581 | 312.86 | 1.38 | 0.8519 | 338.36 | 1.1 |
| 0.2660 | 285.62 | 1.45 | 0.5440 | 323.89 | 1.34 | 0.8607 | 338.75 | 1.1 |
| 0.2820 | 287.73 | 1.45 | 0.6138 | 329.33 | 1.31 | 0.8826 | 338.93 | 1.1 |
| 0.2925 | 288.94 | 1.44 | 0.6350 | 330.85 | 1.29 | 0.9270 | 340.29 | 1.0 |
| 0.3021 | 290.86 | 1.44 | 0.6637 | 333.24 | 1.27 | 0.9566 | 340.41 | 1.0 |
| 0.3220 | 292.25 | 1.44 | 0.6924 | 334.29 | 1.25 | 1.0000 | 341.94 | 1.0 |
| 0.3339 | 293.71 | 1.43 | 0.7257 | 336.01 | 1.23 | | | |
| 0.3465 | 295.46 | 1.43 | 0.7736 | 336.40 | 1.19 | | | |

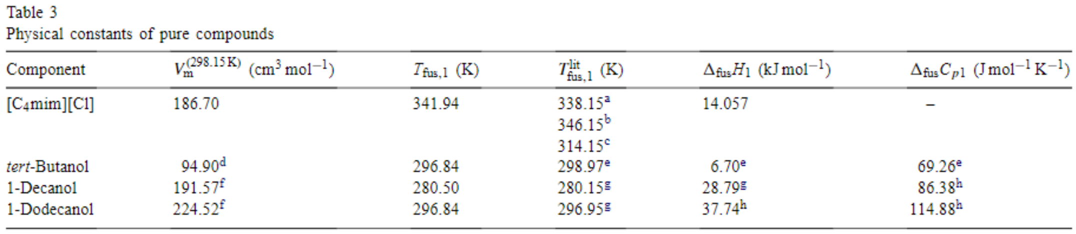


Table 3
Physical constants of pure compounds

| Component | $V_m^{(298.15\,K)}$ ($cm^3\,mol^{-1}$) | $T_{fus,1}$ (K) | $T_{fus,1}^{lit}$ (K) | $\Delta_{fus}H_1$ ($kJ\,mol^{-1}$) | $\Delta_{fus}C_{p1}$ ($J\,mol^{-1}\,K^{-1}$) |
|---|---|---|---|---|---|
| [$C_4$mim][Cl] | 186.70 | 341.94 | 338.15[a]<br>346.15[b]<br>314.15[c] | 14.057 | – |
| *tert*-Butanol | 94.90[d] | 296.84 | 298.97[e] | 6.70[e] | 69.26[e] |
| 1-Decanol | 191.57[f] | 280.50 | 280.15[g] | 28.79[g] | 86.38[h] |
| 1-Dodecanol | 224.52[f] | 296.84 | 296.95[g] | 37.74[h] | 114.88[h] |

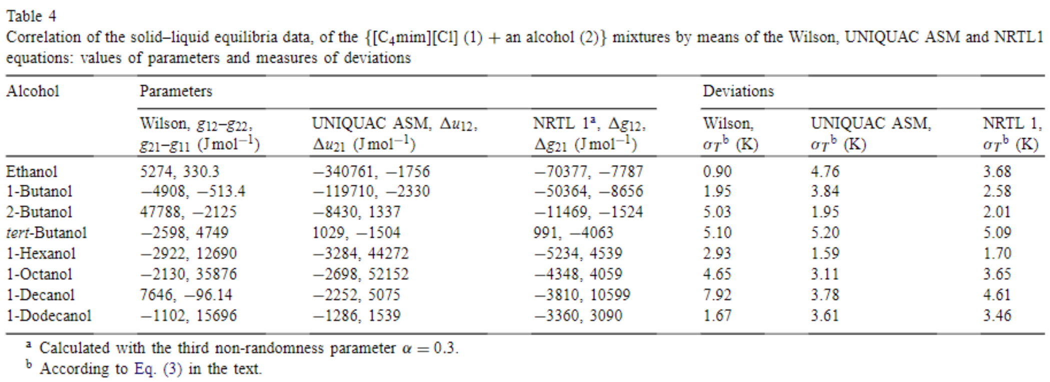


Table 4
Correlation of the solid–liquid equilibria data, of the {[$C_4$mim][Cl] (1) + an alcohol (2)} mixtures by means of the Wilson, UNIQUAC ASM and NRTL1 equations: values of parameters and measures of deviations

| Alcohol | Parameters | | | Deviations | | |
|---|---|---|---|---|---|---|
| | Wilson, $g_{12}-g_{22}$, $g_{21}-g_{11}$ ($J\,mol^{-1}$) | UNIQUAC ASM, $\Delta u_{12}$, $\Delta u_{21}$ ($J\,mol^{-1}$) | NRTL 1[a], $\Delta g_{12}$, $\Delta g_{21}$ ($J\,mol^{-1}$) | Wilson, $\sigma_T$[b] (K) | UNIQUAC ASM, $\sigma_T$[b] (K) | NRTL 1, $\sigma_T$[b] (K) |
| Ethanol | 5274, 330.3 | −340761, −1756 | −70377, −7787 | 0.90 | 4.76 | 3.68 |
| 1-Butanol | −4908, −513.4 | −119710, −2330 | −50364, −8656 | 1.95 | 3.84 | 2.58 |
| 2-Butanol | 47788, −2125 | −8430, 1337 | −11469, −1524 | 5.03 | 1.95 | 2.01 |
| *tert*-Butanol | −2598, 4749 | 1029, −1504 | 991, −4063 | 5.10 | 5.20 | 5.09 |
| 1-Hexanol | −2922, 12690 | −3284, 44272 | −5234, 4539 | 2.93 | 1.59 | 1.70 |
| 1-Octanol | −2130, 35876 | −2698, 52152 | −4348, 4059 | 4.65 | 3.11 | 3.65 |
| 1-Decanol | 7646, −96.14 | −2252, 5075 | −3810, 10599 | 7.92 | 3.78 | 4.61 |
| 1-Dodecanol | −1102, 15696 | −1286, 1539 | −3360, 3090 | 1.67 | 3.61 | 3.46 |

[a] Calculated with the third non-randomness parameter $\alpha = 0.3$.
[b] According to Eq. (3) in the text.

ODABRATI JEDAN MODEL

octan-1-ol + 1,3-diaminopropane

U. Domanska, M. Marciniak, Experimental solid–liquid equilibria for systems containingalkan-1-ol + 1,3-diaminopropaneHeat capacities of alkan-1-ols and amines—Thermodynamic functions ofdissociation and enthalpies of melting of the congruently meltingcompounds for the systems (alkan-1-ol + amine), Fluid Phase Equilibria 235 (2005) 30–41

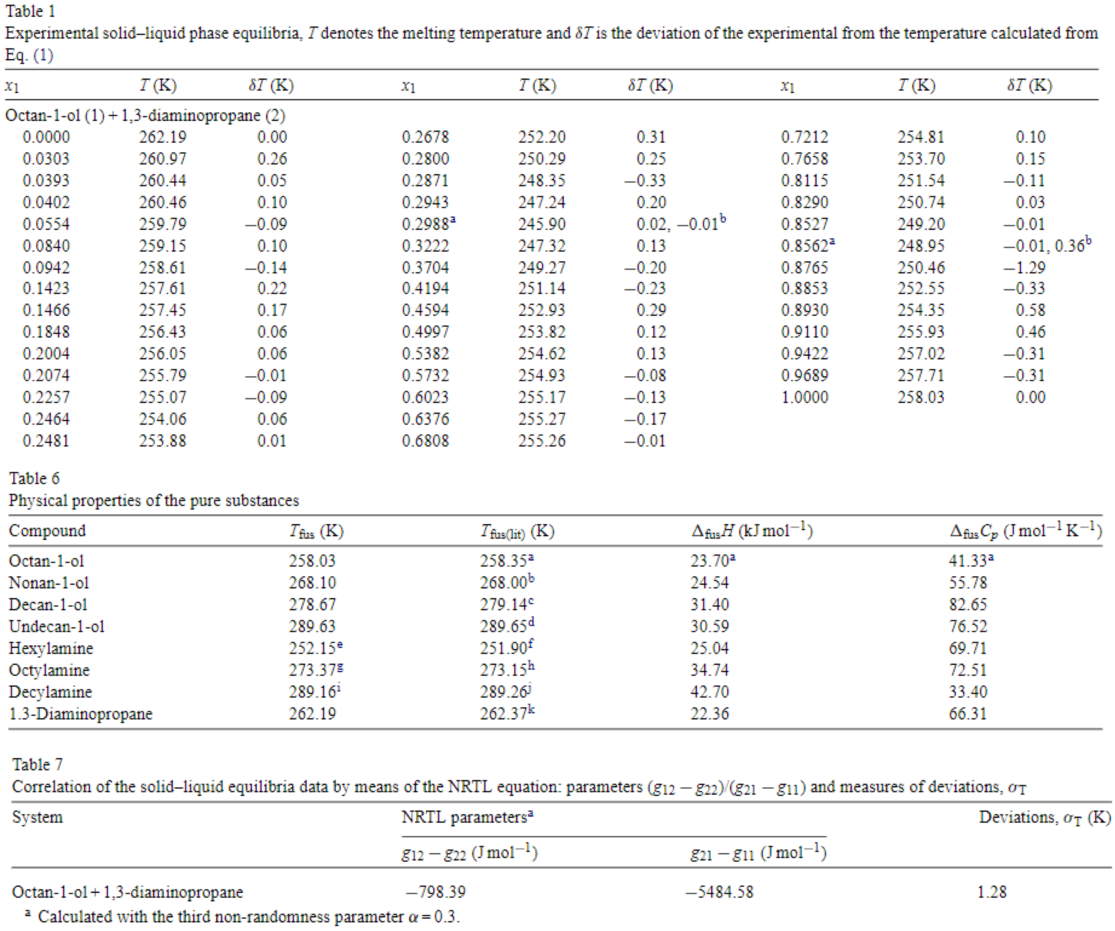


Table 1

Experimental solid–liquid phase equilibria, $T$ denotes the melting temperature and $\delta T$ is the deviation of the experimental from the temperature calculated from Eq. (1)

| $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) |
|---|---|---|---|---|---|---|---|---|
| Octan-1-ol (1) + 1,3-diaminopropane (2) | | | | | | | | |
| 0.0000 | 262.19 | 0.00 | 0.2678 | 252.20 | 0.31 | 0.7212 | 254.81 | 0.10 |
| 0.0303 | 260.97 | 0.26 | 0.2800 | 250.29 | 0.25 | 0.7658 | 253.70 | 0.15 |
| 0.0393 | 260.44 | 0.05 | 0.2871 | 248.35 | −0.33 | 0.8115 | 251.54 | −0.11 |
| 0.0402 | 260.46 | 0.10 | 0.2943 | 247.24 | 0.20 | 0.8290 | 250.74 | 0.03 |
| 0.0554 | 259.79 | −0.09 | 0.2988[a] | 245.90 | 0.02, −0.01[b] | 0.8527 | 249.20 | −0.01 |
| 0.0840 | 259.15 | 0.10 | 0.3222 | 247.32 | 0.13 | 0.8562[a] | 248.95 | −0.01, 0.36[b] |
| 0.0942 | 258.61 | −0.14 | 0.3704 | 249.27 | −0.20 | 0.8765 | 250.46 | −1.29 |
| 0.1423 | 257.61 | 0.22 | 0.4194 | 251.14 | −0.23 | 0.8853 | 252.55 | −0.33 |
| 0.1466 | 257.45 | 0.17 | 0.4594 | 252.93 | 0.29 | 0.8930 | 254.35 | 0.58 |
| 0.1848 | 256.43 | 0.06 | 0.4997 | 253.82 | 0.12 | 0.9110 | 255.93 | 0.46 |
| 0.2004 | 256.05 | 0.06 | 0.5382 | 254.62 | 0.13 | 0.9422 | 257.02 | −0.31 |
| 0.2074 | 255.79 | −0.01 | 0.5732 | 254.93 | −0.08 | 0.9689 | 257.71 | −0.31 |
| 0.2257 | 255.07 | −0.09 | 0.6023 | 255.17 | −0.13 | 1.0000 | 258.03 | 0.00 |
| 0.2464 | 254.06 | 0.06 | 0.6376 | 255.27 | −0.17 | | | |
| 0.2481 | 253.88 | 0.01 | 0.6808 | 255.26 | −0.01 | | | |

Table 6

Physical properties of the pure substances

| Compound | $T_{fus}$ (K) | $T_{fus(lit)}$ (K) | $\Delta_{fus}H$ (kJ mol$^{-1}$) | $\Delta_{fus}C_p$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35[a] | 23.70[a] | 41.33[a] |
| Nonan-1-ol | 268.10 | 268.00[b] | 24.54 | 55.78 |
| Decan-1-ol | 278.67 | 279.14[c] | 31.40 | 82.65 |
| Undecan-1-ol | 289.63 | 289.65[d] | 30.59 | 76.52 |
| Hexylamine | 252.15[e] | 251.90[f] | 25.04 | 69.71 |
| Octylamine | 273.37[g] | 273.15[h] | 34.74 | 72.51 |
| Decylamine | 289.16[i] | 289.26[j] | 42.70 | 33.40 |
| 1.3-Diaminopropane | 262.19 | 262.37[k] | 22.36 | 66.31 |

Table 7

Correlation of the solid–liquid equilibria data by means of the NRTL equation: parameters $(g_{12} - g_{22})/(g_{21} - g_{11})$ and measures of deviations, $\sigma_T$

| System | NRTL parameters[a] | | Deviations, $\sigma_T$ (K) |
|---|---|---|---|
| | $g_{12} - g_{22}$ (J mol$^{-1}$) | $g_{21} - g_{11}$ (J mol$^{-1}$) | |
| Octan-1-ol + 1,3-diaminopropane | −798.39 | −5484.58 | 1.28 |

[a] Calculated with the third non-randomness parameter $\alpha = 0.3$.

nonan-1-ol + 1,3-diaminopropane

U. Domanska, M. Marciniak, Experimental solid–liquid equilibria for systems containingalkan-1-ol + 1,3-diaminopropaneHeat capacities of alkan-1-ols and amines—Thermodynamic functions ofdissociation and enthalpies of melting of the congruently meltingcompounds for the systems (alkan-1-ol + amine), Fluid Phase Equilibria 235 (2005) 30–41

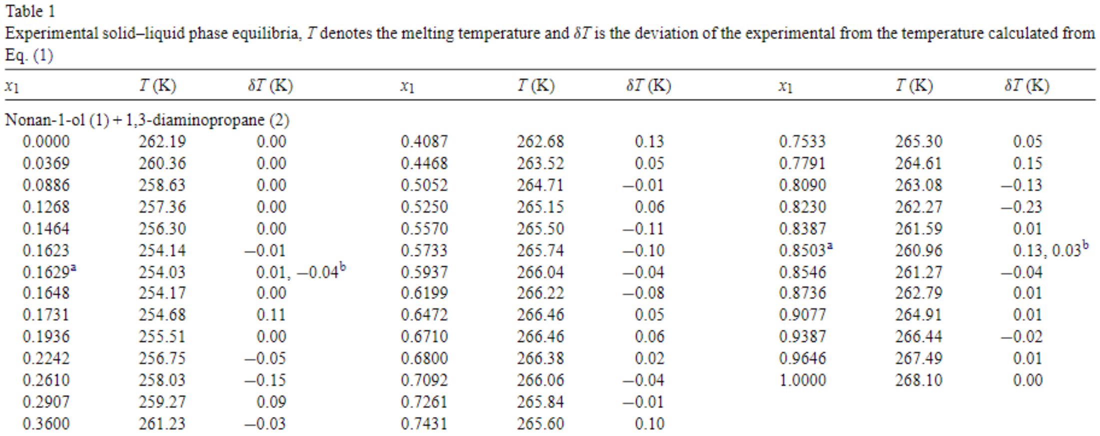


Table 1

Experimental solid–liquid phase equilibria, $T$ denotes the melting temperature and $\delta T$ is the deviation of the experimental from the temperature calculated from Eq. (1)

| $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) |
|---|---|---|---|---|---|---|---|---|
| Nonan-1-ol (1) + 1,3-diaminopropane (2) | | | | | | | | |
| 0.0000 | 262.19 | 0.00 | 0.4087 | 262.68 | 0.13 | 0.7533 | 265.30 | 0.05 |
| 0.0369 | 260.36 | 0.00 | 0.4468 | 263.52 | 0.05 | 0.7791 | 264.61 | 0.15 |
| 0.0886 | 258.63 | 0.00 | 0.5052 | 264.71 | −0.01 | 0.8090 | 263.08 | −0.13 |
| 0.1268 | 257.36 | 0.00 | 0.5250 | 265.15 | 0.06 | 0.8230 | 262.27 | −0.23 |
| 0.1464 | 256.30 | 0.00 | 0.5570 | 265.50 | −0.11 | 0.8387 | 261.59 | 0.01 |
| 0.1623 | 254.14 | −0.01 | 0.5733 | 265.74 | −0.10 | 0.8503[a] | 260.96 | 0.13, 0.03[b] |
| 0.1629[a] | 254.03 | 0.01, −0.04[b] | 0.5937 | 266.04 | −0.04 | 0.8546 | 261.27 | −0.04 |
| 0.1648 | 254.17 | 0.00 | 0.6199 | 266.22 | −0.08 | 0.8736 | 262.79 | 0.01 |
| 0.1731 | 254.68 | 0.11 | 0.6472 | 266.46 | 0.05 | 0.9077 | 264.91 | 0.01 |
| 0.1936 | 255.51 | 0.00 | 0.6710 | 266.46 | 0.06 | 0.9387 | 266.44 | −0.02 |
| 0.2242 | 256.75 | −0.05 | 0.6800 | 266.38 | 0.02 | 0.9646 | 267.49 | 0.01 |
| 0.2610 | 258.03 | −0.15 | 0.7092 | 266.06 | −0.04 | 1.0000 | 268.10 | 0.00 |
| 0.2907 | 259.27 | 0.09 | 0.7261 | 265.84 | −0.01 | | | |
| 0.3600 | 261.23 | −0.03 | 0.7431 | 265.60 | 0.10 | | | |

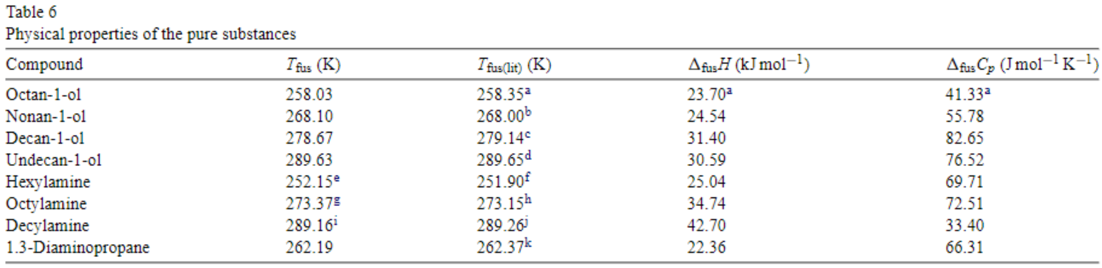


Table 6

Physical properties of the pure substances

| Compound | $T_{fus}$ (K) | $T_{fus(lit)}$ (K) | $\Delta_{fus}H$ (kJ mol$^{-1}$) | $\Delta_{fus}C_p$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35[a] | 23.70[a] | 41.33[a] |
| Nonan-1-ol | 268.10 | 268.00[b] | 24.54 | 55.78 |
| Decan-1-ol | 278.67 | 279.14[c] | 31.40 | 82.65 |
| Undecan-1-ol | 289.63 | 289.65[d] | 30.59 | 76.52 |
| Hexylamine | 252.15[e] | 251.90[f] | 25.04 | 69.71 |
| Octylamine | 273.37[g] | 273.15[h] | 34.74 | 72.51 |
| Decylamine | 289.16[i] | 289.26[j] | 42.70 | 33.40 |
| 1.3-Diaminopropane | 262.19 | 262.37[k] | 22.36 | 66.31 |

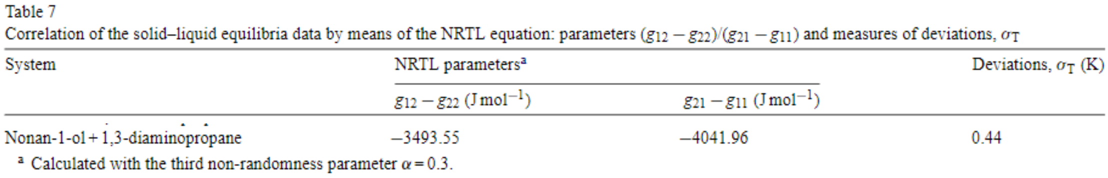


Table 7

Correlation of the solid–liquid equilibria data by means of the NRTL equation: parameters $(g_{12}-g_{22})/(g_{21}-g_{11})$ and measures of deviations, $\sigma_T$

| System | NRTL parameters[a] | | Deviations, $\sigma_T$ (K) |
|---|---|---|---|
| | $g_{12}-g_{22}$ (J mol$^{-1}$) | $g_{21}-g_{11}$ (J mol$^{-1}$) | |
| Nonan-1-ol + 1,3-diaminopropane | −3493.55 | −4041.96 | 0.44 |

[a] Calculated with the third non-randomness parameter $\alpha = 0.3$.

decan-1-ol + 1,3-diaminopropane

U. Domanska, M. Marciniak, Experimental solid–liquid equilibria for systems containingalkan-1-ol + 1,3-diaminopropaneHeat capacities of alkan-1-ols and amines—Thermodynamic functions ofdissociation and enthalpies of melting of the congruently meltingcompounds for the systems (alkan-1-ol + amine), Fluid Phase Equilibria 235 (2005) 30–41

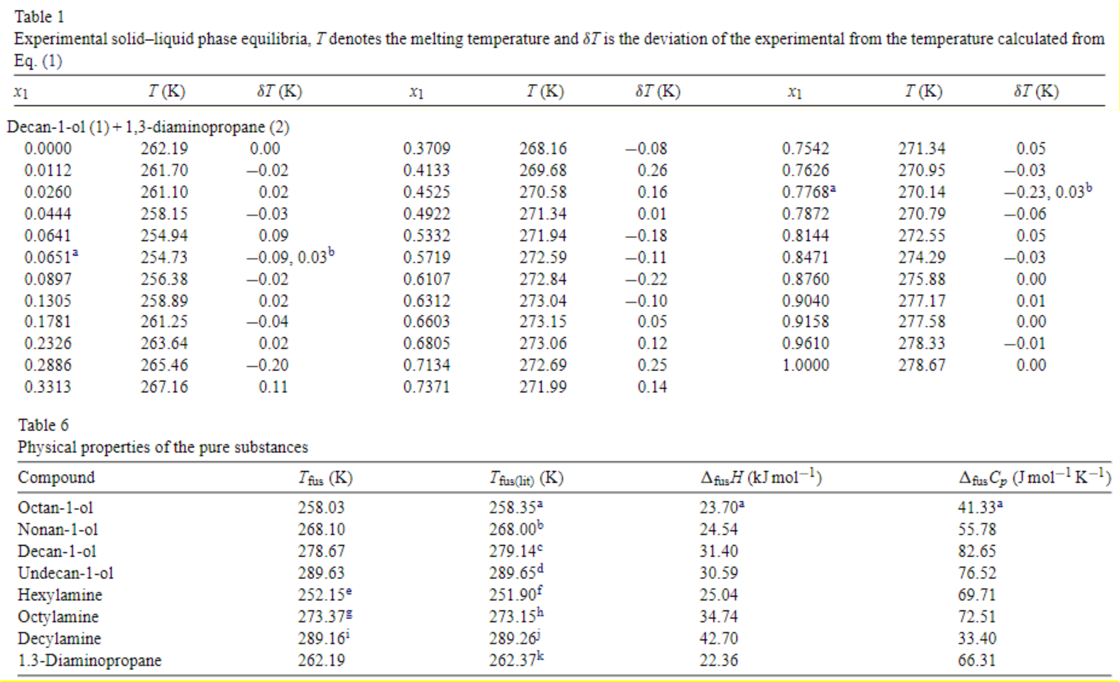


Table 1

Experimental solid–liquid phase equilibria, $T$ denotes the melting temperature and $\delta T$ is the deviation of the experimental from the temperature calculated from Eq. (1)

| $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) |
|---|---|---|---|---|---|---|---|---|
| Decan-1-ol (1) + 1,3-diaminopropane (2) | | | | | | | | |
| 0.0000 | 262.19 | 0.00 | 0.3709 | 268.16 | −0.08 | 0.7542 | 271.34 | 0.05 |
| 0.0112 | 261.70 | −0.02 | 0.4133 | 269.68 | 0.26 | 0.7626 | 270.95 | −0.03 |
| 0.0260 | 261.10 | 0.02 | 0.4525 | 270.58 | 0.16 | 0.7768[a] | 270.14 | −0.23, 0.03[b] |
| 0.0444 | 258.15 | −0.03 | 0.4922 | 271.34 | 0.01 | 0.7872 | 270.79 | −0.06 |
| 0.0641 | 254.94 | 0.09 | 0.5332 | 271.94 | −0.18 | 0.8144 | 272.55 | 0.05 |
| 0.0651[a] | 254.73 | −0.09, 0.03[b] | 0.5719 | 272.59 | −0.11 | 0.8471 | 274.29 | −0.03 |
| 0.0897 | 256.38 | −0.02 | 0.6107 | 272.84 | −0.22 | 0.8760 | 275.88 | 0.00 |
| 0.1305 | 258.89 | 0.02 | 0.6312 | 273.04 | −0.10 | 0.9040 | 277.17 | 0.01 |
| 0.1781 | 261.25 | −0.04 | 0.6603 | 273.15 | 0.05 | 0.9158 | 277.58 | 0.00 |
| 0.2326 | 263.64 | 0.02 | 0.6805 | 273.06 | 0.12 | 0.9610 | 278.33 | −0.01 |
| 0.2886 | 265.46 | −0.20 | 0.7134 | 272.69 | 0.25 | 1.0000 | 278.67 | 0.00 |
| 0.3313 | 267.16 | 0.11 | 0.7371 | 271.99 | 0.14 | | | |

Table 6

Physical properties of the pure substances

| Compound | $T_{fus}$ (K) | $T_{fus(lit)}$ (K) | $\Delta_{fus}H$ (kJ mol$^{-1}$) | $\Delta_{fus}C_p$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35[a] | 23.70[a] | 41.33[a] |
| Nonan-1-ol | 268.10 | 268.00[b] | 24.54 | 55.78 |
| Decan-1-ol | 278.67 | 279.14[c] | 31.40 | 82.65 |
| Undecan-1-ol | 289.63 | 289.65[d] | 30.59 | 76.52 |
| Hexylamine | 252.15[e] | 251.90[f] | 25.04 | 69.71 |
| Octylamine | 273.37[g] | 273.15[h] | 34.74 | 72.51 |
| Decylamine | 289.16[i] | 289.26[j] | 42.70 | 33.40 |
| 1.3-Diaminopropane | 262.19 | 262.37[k] | 22.36 | 66.31 |

undecan-1-ol + 1,3-diaminopropane

U. Domanska, M. Marciniak, Experimental solid–liquid equilibria for systems containingalkan-1-ol + 1,3-diaminopropaneHeat capacities of alkan-1-ols and amines—Thermodynamic functions ofdissociation and enthalpies of melting of the congruently meltingcompounds for the systems (alkan-1-ol + amine), Fluid Phase Equilibria 235 (2005) 30–41

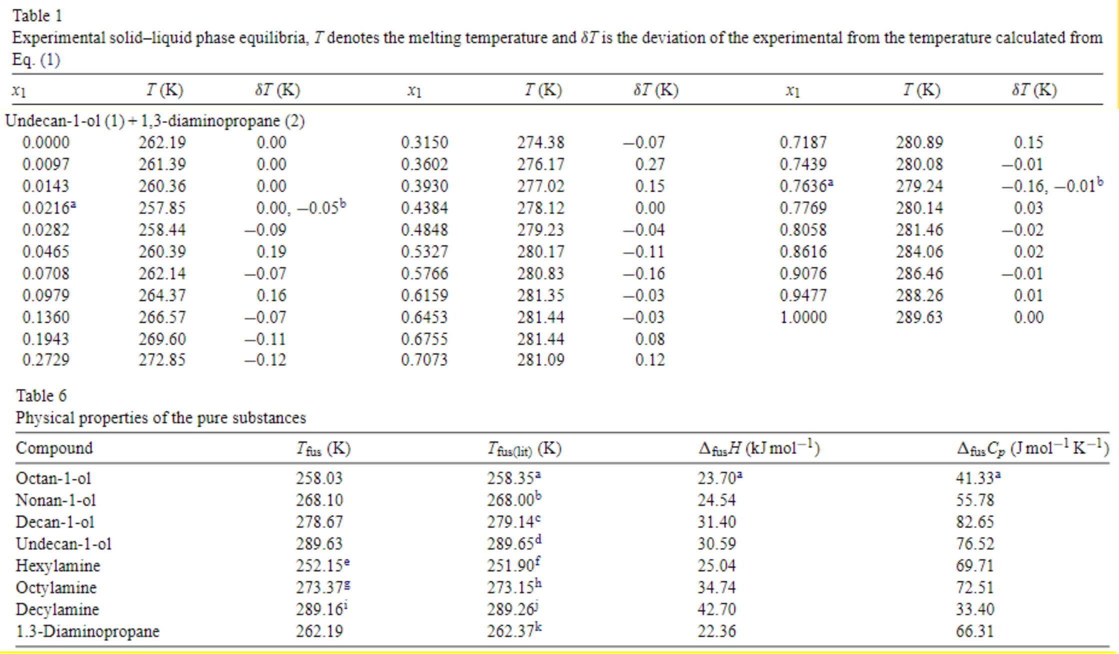


Table 1

Experimental solid–liquid phase equilibria, $T$ denotes the melting temperature and $\delta T$ is the deviation of the experimental from the temperature calculated from Eq. (1)

| $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) |
|---|---|---|---|---|---|---|---|---|
| Undecan-1-ol (1) + 1,3-diaminopropane (2) | | | | | | | | |
| 0.0000 | 262.19 | 0.00 | 0.3150 | 274.38 | −0.07 | 0.7187 | 280.89 | 0.15 |
| 0.0097 | 261.39 | 0.00 | 0.3602 | 276.17 | 0.27 | 0.7439 | 280.08 | −0.01 |
| 0.0143 | 260.36 | 0.00 | 0.3930 | 277.02 | 0.15 | 0.7636[a] | 279.24 | −0.16, −0.01[b] |
| 0.0216[a] | 257.85 | 0.00, −0.05[b] | 0.4384 | 278.12 | 0.00 | 0.7769 | 280.14 | 0.03 |
| 0.0282 | 258.44 | −0.09 | 0.4848 | 279.23 | −0.04 | 0.8058 | 281.46 | −0.02 |
| 0.0465 | 260.39 | 0.19 | 0.5327 | 280.17 | −0.11 | 0.8616 | 284.06 | 0.02 |
| 0.0708 | 262.14 | −0.07 | 0.5766 | 280.83 | −0.16 | 0.9076 | 286.46 | −0.01 |
| 0.0979 | 264.37 | 0.16 | 0.6159 | 281.35 | −0.03 | 0.9477 | 288.26 | 0.01 |
| 0.1360 | 266.57 | −0.07 | 0.6453 | 281.44 | −0.03 | 1.0000 | 289.63 | 0.00 |
| 0.1943 | 269.60 | −0.11 | 0.6755 | 281.44 | 0.08 | | | |
| 0.2729 | 272.85 | −0.12 | 0.7073 | 281.09 | 0.12 | | | |

Table 6

Physical properties of the pure substances

| Compound | $T_{fus}$ (K) | $T_{fus(lit)}$ (K) | $\Delta_{fus}H$ (kJ mol$^{-1}$) | $\Delta_{fus}C_p$ (J mol$^{-1}$ K$^{-1}$) |
|---|---|---|---|---|
| Octan-1-ol | 258.03 | 258.35[a] | 23.70[a] | 41.33[a] |
| Nonan-1-ol | 268.10 | 268.00[b] | 24.54 | 55.78 |
| Decan-1-ol | 278.67 | 279.14[c] | 31.40 | 82.65 |
| Undecan-1-ol | 289.63 | 289.65[d] | 30.59 | 76.52 |
| Hexylamine | 252.15[e] | 251.90[f] | 25.04 | 69.71 |
| Octylamine | 273.37[g] | 273.15[h] | 34.74 | 72.51 |
| Decylamine | 289.16[i] | 289.26[j] | 42.70 | 33.40 |
| 1.3-Diaminopropane | 262.19 | 262.37[k] | 22.36 | 66.31 |

benzoic acid + 1-naphthol

Cheng-Chia Huang, Yan-Ping Chen, Measurements and model prediction of the solid}liquid equilibria oforganic binary mixtures, Chemical Engineering Science 55 (2000) 3175}3185

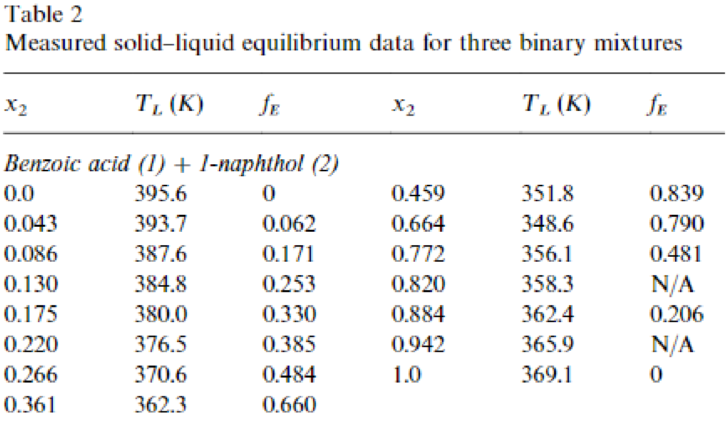


Table 2
Measured solid–liquid equilibrium data for three binary mixtures

| $x_2$ | $T_L$ (K) | $f_E$ | $x_2$ | $T_L$ (K) | $f_E$ |
|---|---|---|---|---|---|
| *Benzoic acid (1) + 1-naphthol (2)* | | | | | |
| 0.0 | 395.6 | 0 | 0.459 | 351.8 | 0.839 |
| 0.043 | 393.7 | 0.062 | 0.664 | 348.6 | 0.790 |
| 0.086 | 387.6 | 0.171 | 0.772 | 356.1 | 0.481 |
| 0.130 | 384.8 | 0.253 | 0.820 | 358.3 | N/A |
| 0.175 | 380.0 | 0.330 | 0.884 | 362.4 | 0.206 |
| 0.220 | 376.5 | 0.385 | 0.942 | 365.9 | N/A |
| 0.266 | 370.6 | 0.484 | 1.0 | 369.1 | 0 |
| 0.361 | 362.3 | 0.660 | | | |

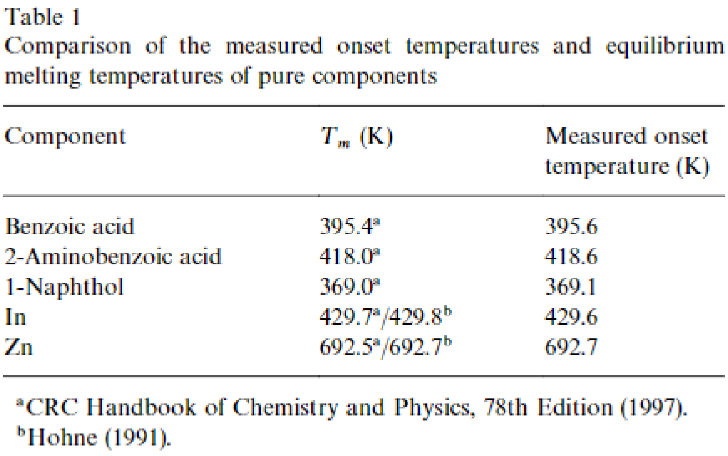


Table 1
Comparison of the measured onset temperatures and equilibrium melting temperatures of pure components

| Component | $T_m$ (K) | Measured onset temperature (K) |
|---|---|---|
| Benzoic acid | 395.4[a] | 395.6 |
| 2-Aminobenzoic acid | 418.0[a] | 418.6 |
| 1-Naphthol | 369.0[a] | 369.1 |
| In | 429.7[a]/429.8[b] | 429.6 |
| Zn | 692.5[a]/692.7[b] | 692.7 |

[a] CRC Handbook of Chemistry and Physics, 78th Edition (1997).
[b] Hohne (1991).

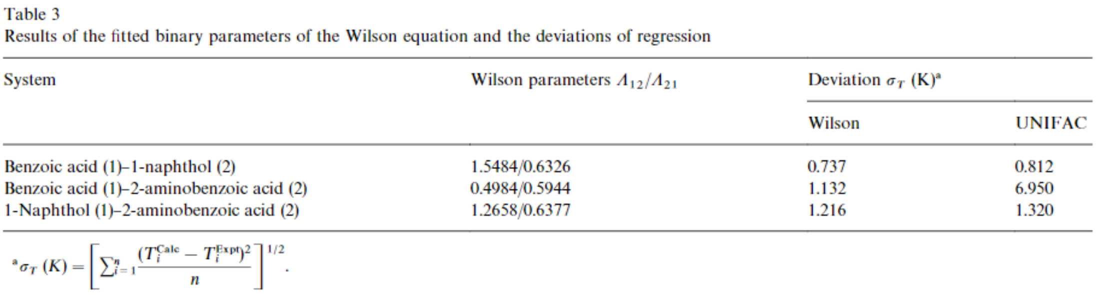


Table 3
Results of the fitted binary parameters of the Wilson equation and the deviations of regression

| System | Wilson parameters $\Lambda_{12}/\Lambda_{21}$ | Deviation $\sigma_T$ (K)[a] | |
|---|---|---|---|
| | | Wilson | UNIFAC |
| Benzoic acid (1)–1-naphthol (2) | 1.5484/0.6326 | 0.737 | 0.812 |
| Benzoic acid (1)–2-aminobenzoic acid (2) | 0.4984/0.5944 | 1.132 | 6.950 |
| 1-Naphthol (1)–2-aminobenzoic acid (2) | 1.2658/0.6377 | 1.216 | 1.320 |

[a] $\sigma_T\ (K) = \left[\sum_{i=1}^{n} \frac{(T_i^{\mathrm{Calc}} - T_i^{\mathrm{Expt}})^2}{n}\right]^{1/2}$.

benzoic acid + 2-aminobenzoic acid

Cheng-Chia Huang, Yan-Ping Chen, Measurements and model prediction of the solid}liquid equilibria oforganic binary mixtures, Chemical Engineering Science 55 (2000) 3175}3185

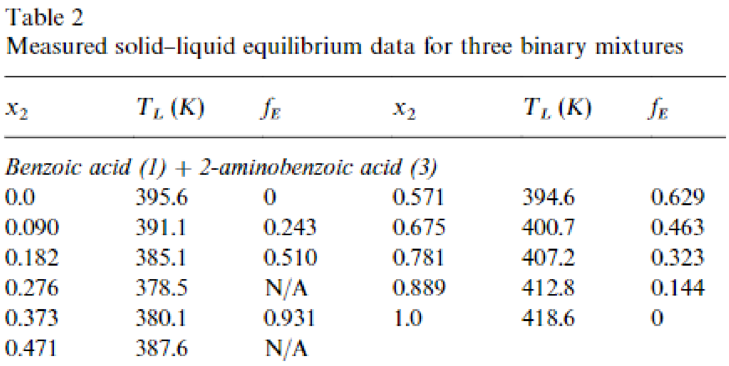


Table 2
Measured solid–liquid equilibrium data for three binary mixtures

| $x_2$ | $T_L$ (K) | $f_E$ | $x_2$ | $T_L$ (K) | $f_E$ |
|---|---|---|---|---|---|
| *Benzoic acid (1) + 2-aminobenzoic acid (3)* | | | | | |
| 0.0 | 395.6 | 0 | 0.571 | 394.6 | 0.629 |
| 0.090 | 391.1 | 0.243 | 0.675 | 400.7 | 0.463 |
| 0.182 | 385.1 | 0.510 | 0.781 | 407.2 | 0.323 |
| 0.276 | 378.5 | N/A | 0.889 | 412.8 | 0.144 |
| 0.373 | 380.1 | 0.931 | 1.0 | 418.6 | 0 |
| 0.471 | 387.6 | N/A | | | |

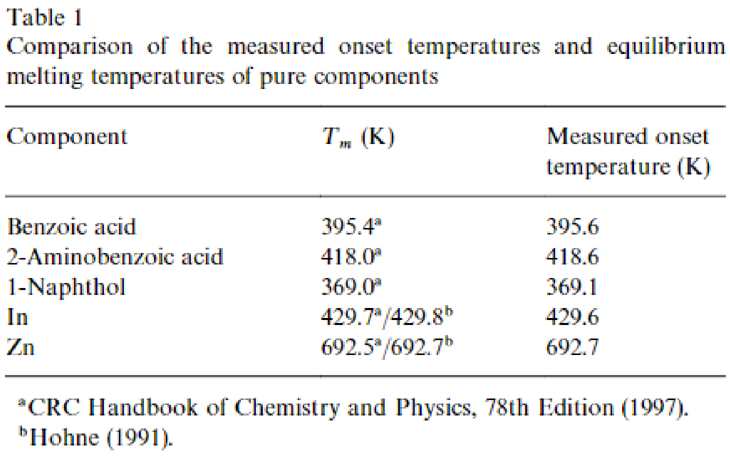


Table 1
Comparison of the measured onset temperatures and equilibrium melting temperatures of pure components

| Component | $T_m$ (K) | Measured onset temperature (K) |
|---|---|---|
| Benzoic acid | 395.4[a] | 395.6 |
| 2-Aminobenzoic acid | 418.0[a] | 418.6 |
| 1-Naphthol | 369.0[a] | 369.1 |
| In | 429.7[a]/429.8[b] | 429.6 |
| Zn | 692.5[a]/692.7[b] | 692.7 |

[a] CRC Handbook of Chemistry and Physics, 78th Edition (1997).
[b] Hohne (1991).

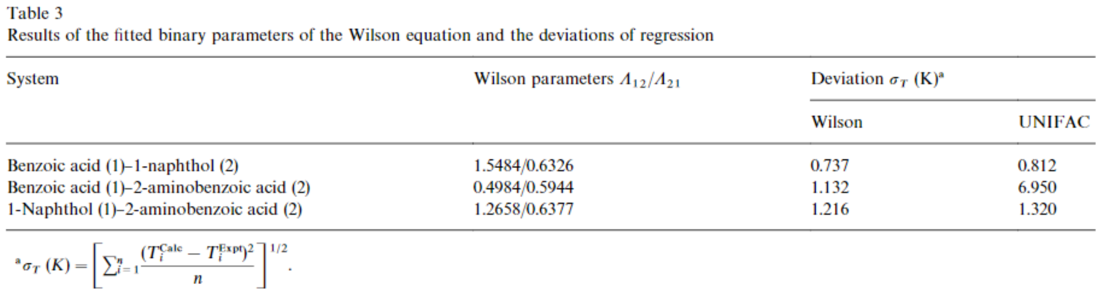


Table 3
Results of the fitted binary parameters of the Wilson equation and the deviations of regression

| System | Wilson parameters $\Lambda_{12}/\Lambda_{21}$ | Deviation $\sigma_T$ (K)[a] | |
|---|---|---|---|
| | | Wilson | UNIFAC |
| Benzoic acid (1)–1-naphthol (2) | 1.5484/0.6326 | 0.737 | 0.812 |
| Benzoic acid (1)–2-aminobenzoic acid (2) | 0.4984/0.5944 | 1.132 | 6.950 |
| 1-Naphthol (1)–2-aminobenzoic acid (2) | 1.2658/0.6377 | 1.216 | 1.320 |

[a] $\sigma_T\ (K) = \left[\sum_{i=1}^{n} \frac{(T_i^{\mathrm{Calc}} - T_i^{\mathrm{Expt}})^2}{n}\right]^{1/2}$.

1-naphthol + 2-aminobenzoic acid

Cheng-Chia Huang, Yan-Ping Chen, Measurements and model prediction of the solid}liquid equilibria oforganic binary mixtures, Chemical Engineering Science 55 (2000) 3175}3185

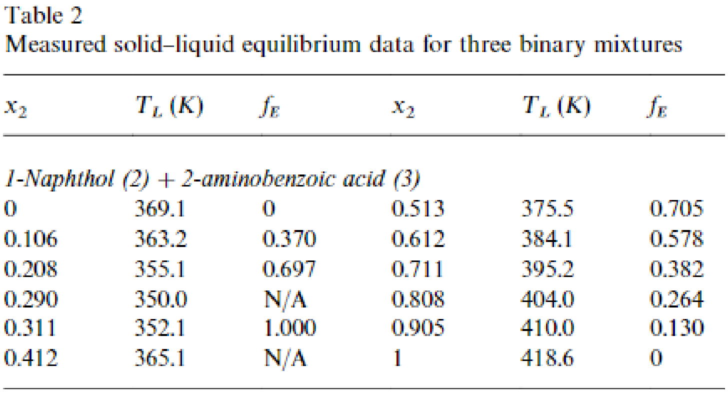


Table 2
Measured solid–liquid equilibrium data for three binary mixtures

| $x_2$ | $T_L$ (K) | $f_E$ | $x_2$ | $T_L$ (K) | $f_E$ |
|---|---|---|---|---|---|
| *1-Naphthol (2) + 2-aminobenzoic acid (3)* | | | | | |
| 0 | 369.1 | 0 | 0.513 | 375.5 | 0.705 |
| 0.106 | 363.2 | 0.370 | 0.612 | 384.1 | 0.578 |
| 0.208 | 355.1 | 0.697 | 0.711 | 395.2 | 0.382 |
| 0.290 | 350.0 | N/A | 0.808 | 404.0 | 0.264 |
| 0.311 | 352.1 | 1.000 | 0.905 | 410.0 | 0.130 |
| 0.412 | 365.1 | N/A | 1 | 418.6 | 0 |

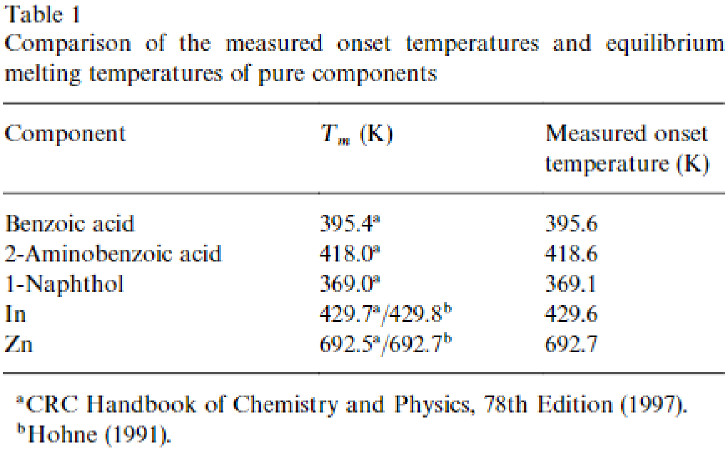


Table 1
Comparison of the measured onset temperatures and equilibrium melting temperatures of pure components

| Component | $T_m$ (K) | Measured onset temperature (K) |
|---|---|---|
| Benzoic acid | 395.4[a] | 395.6 |
| 2-Aminobenzoic acid | 418.0[a] | 418.6 |
| 1-Naphthol | 369.0[a] | 369.1 |
| In | 429.7[a]/429.8[b] | 429.6 |
| Zn | 692.5[a]/692.7[b] | 692.7 |

[a] CRC Handbook of Chemistry and Physics, 78th Edition (1997).
[b] Hohne (1991).

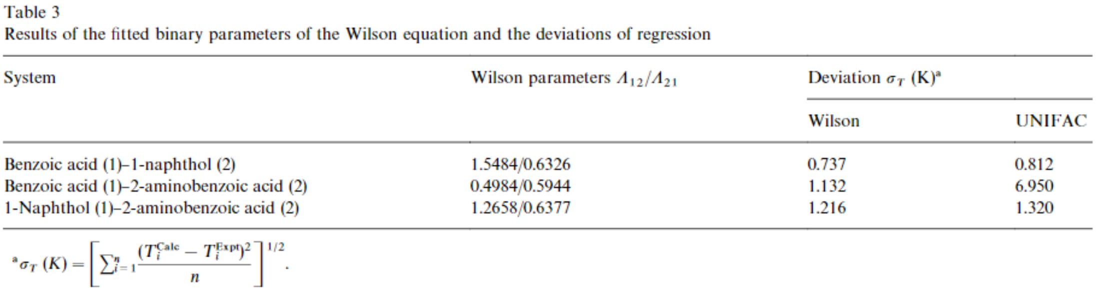


Table 3
Results of the fitted binary parameters of the Wilson equation and the deviations of regression

| System | Wilson parameters $\Lambda_{12}/\Lambda_{21}$ | Deviation $\sigma_T$ (K)[a] | |
|---|---|---|---|
| | | Wilson | UNIFAC |
| Benzoic acid (1)–1-naphthol (2) | 1.5484/0.6326 | 0.737 | 0.812 |
| Benzoic acid (1)–2-aminobenzoic acid (2) | 0.4984/0.5944 | 1.132 | 6.950 |
| 1-Naphthol (1)–2-aminobenzoic acid (2) | 1.2658/0.6377 | 1.216 | 1.320 |

[a] $\sigma_T\ (K) = \left[\sum_{i=1}^{n} \frac{(T_i^{\mathrm{Calc}} - T_i^{\mathrm{Expt}})^2}{n}\right]^{1/2}$.

pyrene + *n*-octadecane

R. Mahmoud, R. Solimando, M. Rogalski, Solid–liquid equilibria of systems containing pyrene and long chainnormal-alkanes, Fluid Phase Equilibria 148 (1998) 139–146

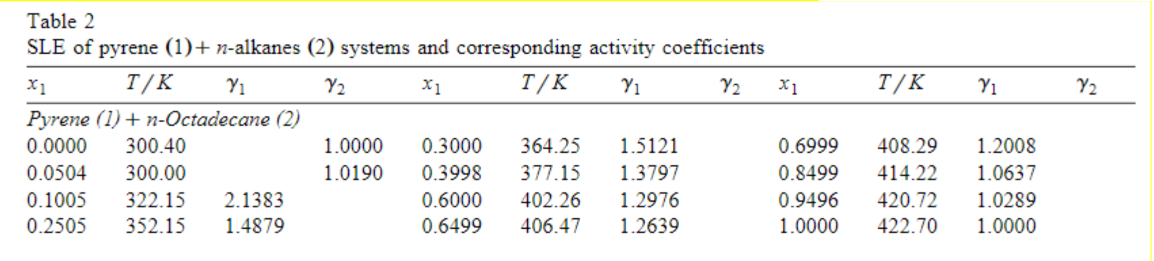


Table 2
SLE of pyrene (1) + *n*-alkanes (2) systems and corresponding activity coefficients

| $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ | $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ | $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *Pyrene (1) + n-Octadecane (2)* | | | | | | | | | | | |
| 0.0000 | 300.40 | | 1.0000 | 0.3000 | 364.25 | 1.5121 | | 0.6999 | 408.29 | 1.2008 | |
| 0.0504 | 300.00 | | 1.0190 | 0.3998 | 377.15 | 1.3797 | | 0.8499 | 414.22 | 1.0637 | |
| 0.1005 | 322.15 | 2.1383 | | 0.6000 | 402.26 | 1.2976 | | 0.9496 | 420.72 | 1.0289 | |
| 0.2505 | 352.15 | 1.4879 | | 0.6499 | 406.47 | 1.2639 | | 1.0000 | 422.70 | 1.0000 | |

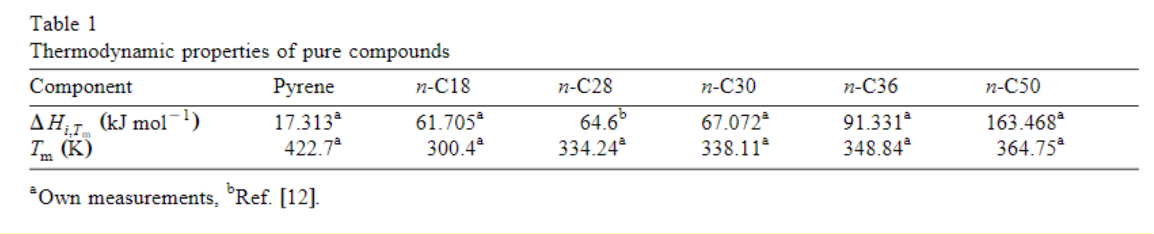


Table 1
Thermodynamic properties of pure compounds

| Component | Pyrene | *n*-C18 | *n*-C28 | *n*-C30 | *n*-C36 | *n*-C50 |
|---|---|---|---|---|---|---|
| $\Delta H_{i,T_m}$ (kJ mol$^{-1}$) | 17.313[a] | 61.705[a] | 64.6[b] | 67.072[a] | 91.331[a] | 163.468[a] |
| $T_m$ (K) | 422.7[a] | 300.4[a] | 334.24[a] | 338.11[a] | 348.84[a] | 364.75[a] |

[a] Own measurements, [b] Ref. [12].

pyrene + *n*-octacosane

R. Mahmoud, R. Solimando, M. Rogalski, Solid–liquid equilibria of systems containing pyrene and long chainnormal-alkanes, Fluid Phase Equilibria 148 (1998) 139–146

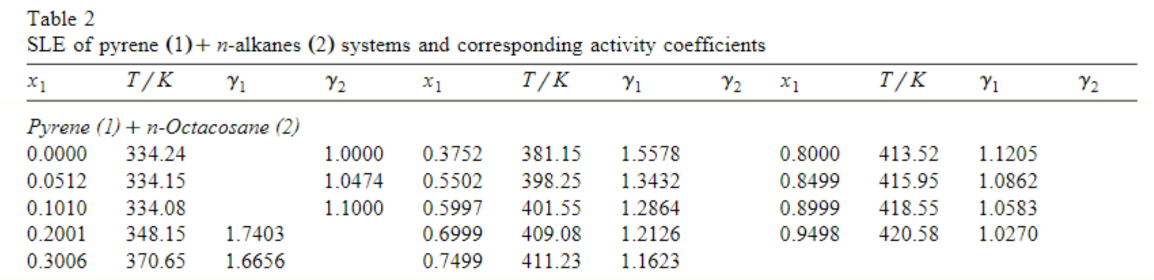


Table 2
SLE of pyrene (1) + *n*-alkanes (2) systems and corresponding activity coefficients

| $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ | $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ | $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *Pyrene (1) + n-Octacosane (2)* | | | | | | | | | | | |
| 0.0000 | 334.24 | | 1.0000 | 0.3752 | 381.15 | 1.5578 | | 0.8000 | 413.52 | 1.1205 | |
| 0.0512 | 334.15 | | 1.0474 | 0.5502 | 398.25 | 1.3432 | | 0.8499 | 415.95 | 1.0862 | |
| 0.1010 | 334.08 | | 1.1000 | 0.5997 | 401.55 | 1.2864 | | 0.8999 | 418.55 | 1.0583 | |
| 0.2001 | 348.15 | 1.7403 | | 0.6999 | 409.08 | 1.2126 | | 0.9498 | 420.58 | 1.0270 | |
| 0.3006 | 370.65 | 1.6656 | | 0.7499 | 411.23 | 1.1623 | | | | | |

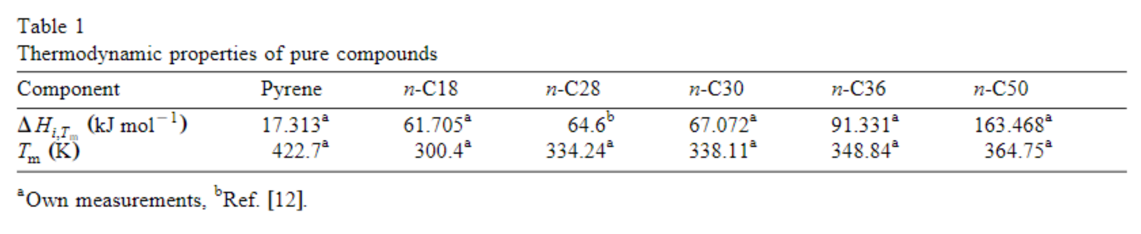


Table 1
Thermodynamic properties of pure compounds

| Component | Pyrene | *n*-C18 | *n*-C28 | *n*-C30 | *n*-C36 | *n*-C50 |
|---|---|---|---|---|---|---|
| $\Delta H_{i,T_m}$ (kJ mol$^{-1}$) | 17.313[a] | 61.705[a] | 64.6[b] | 67.072[a] | 91.331[a] | 163.468[a] |
| $T_m$ (K) | 422.7[a] | 300.4[a] | 334.24[a] | 338.11[a] | 348.84[a] | 364.75[a] |

[a] Own measurements, [b] Ref. [12].

pyrene + *n*-triacontane

R. Mahmoud, R. Solimando, M. Rogalski, Solid–liquid equilibria of systems containing pyrene and long chainnormal-alkanes, Fluid Phase Equilibria 148 (1998) 139–146

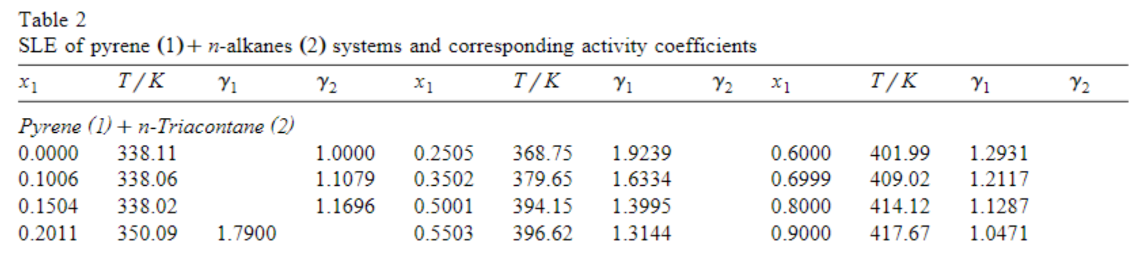


Table 2

SLE of pyrene (1) + *n*-alkanes (2) systems and corresponding activity coefficients

| $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ | $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ | $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *Pyrene (1) + n-Triacontane (2)* | | | | | | | | | | | |
| 0.0000 | 338.11 | | 1.0000 | 0.2505 | 368.75 | 1.9239 | | 0.6000 | 401.99 | 1.2931 | |
| 0.1006 | 338.06 | | 1.1079 | 0.3502 | 379.65 | 1.6334 | | 0.6999 | 409.02 | 1.2117 | |
| 0.1504 | 338.02 | | 1.1696 | 0.5001 | 394.15 | 1.3995 | | 0.8000 | 414.12 | 1.1287 | |
| 0.2011 | 350.09 | 1.7900 | | 0.5503 | 396.62 | 1.3144 | | 0.9000 | 417.67 | 1.0471 | |

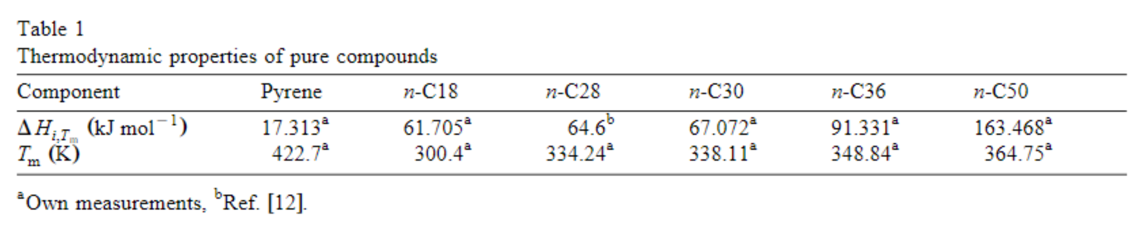


Table 1

Thermodynamic properties of pure compounds

| Component | Pyrene | *n*-C18 | *n*-C28 | *n*-C30 | *n*-C36 | *n*-C50 |
|---|---|---|---|---|---|---|
| $\Delta H_{i,T_m}$ (kJ mol$^{-1}$) | 17.313[a] | 61.705[a] | 64.6[b] | 67.072[a] | 91.331[a] | 163.468[a] |
| $T_m$ (K) | 422.7[a] | 300.4[a] | 334.24[a] | 338.11[a] | 348.84[a] | 364.75[a] |

[a] Own measurements, [b] Ref. [12].

pyrene + *n*-hexatriacontane

R. Mahmoud, R. Solimando, M. Rogalski, Solid–liquid equilibria of systems containing pyrene and long chainnormal-alkanes, Fluid Phase Equilibria 148 (1998) 139–146

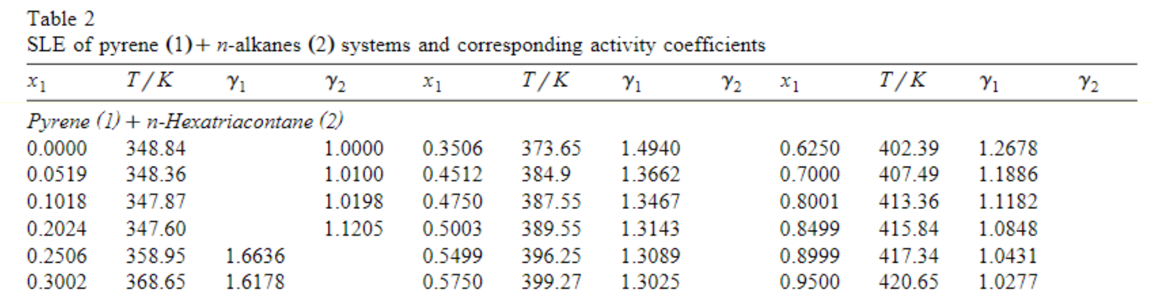


Table 2

SLE of pyrene (1) + *n*-alkanes (2) systems and corresponding activity coefficients

| $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ | $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ | $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *Pyrene (1) + n-Hexatriacontane (2)* | | | | | | | | | | | |
| 0.0000 | 348.84 | | 1.0000 | 0.3506 | 373.65 | 1.4940 | | 0.6250 | 402.39 | 1.2678 | |
| 0.0519 | 348.36 | | 1.0100 | 0.4512 | 384.9 | 1.3662 | | 0.7000 | 407.49 | 1.1886 | |
| 0.1018 | 347.87 | | 1.0198 | 0.4750 | 387.55 | 1.3467 | | 0.8001 | 413.36 | 1.1182 | |
| 0.2024 | 347.60 | | 1.1205 | 0.5003 | 389.55 | 1.3143 | | 0.8499 | 415.84 | 1.0848 | |
| 0.2506 | 358.95 | 1.6636 | | 0.5499 | 396.25 | 1.3089 | | 0.8999 | 417.34 | 1.0431 | |
| 0.3002 | 368.65 | 1.6178 | | 0.5750 | 399.27 | 1.3025 | | 0.9500 | 420.65 | 1.0277 | |

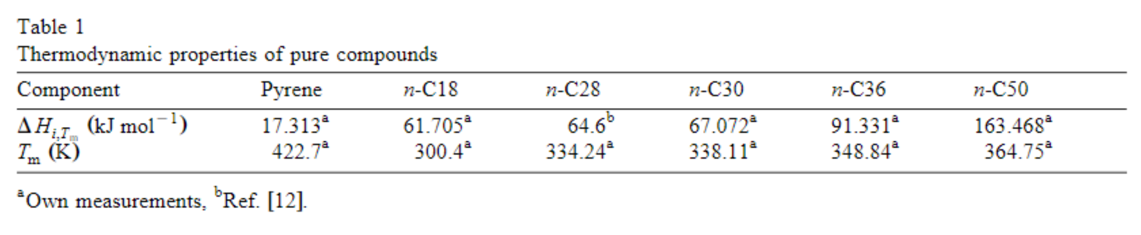


Table 1

Thermodynamic properties of pure compounds

| Component | Pyrene | *n*-C18 | *n*-C28 | *n*-C30 | *n*-C36 | *n*-C50 |
|---|---|---|---|---|---|---|
| $\Delta H_{i,T_m}$ (kJ mol$^{-1}$) | 17.313[a] | 61.705[a] | 64.6[b] | 67.072[a] | 91.331[a] | 163.468[a] |
| $T_m$ (K) | 422.7[a] | 300.4[a] | 334.24[a] | 338.11[a] | 348.84[a] | 364.75[a] |

[a] Own measurements, [b] Ref. [12].

pyrene + *n*-pentacontane

R. Mahmoud, R. Solimando, M. Rogalski, Solid–liquid equilibria of systems containing pyrene and long chainnormal-alkanes, Fluid Phase Equilibria 148 (1998) 139–146

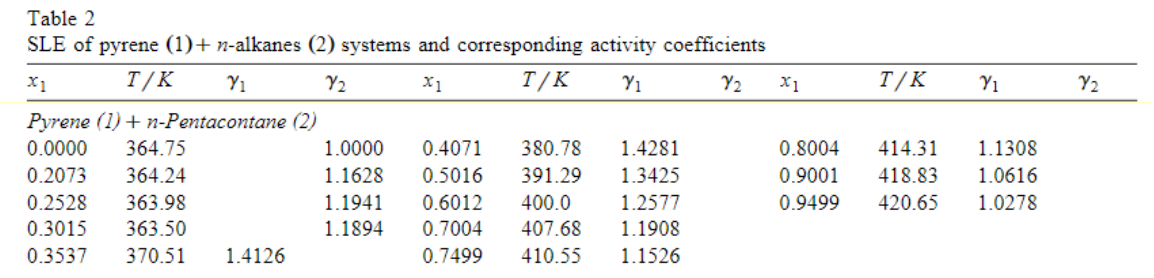


Table 2

SLE of pyrene (1) + *n*-alkanes (2) systems and corresponding activity coefficients

| $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ | $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ | $x_1$ | $T/K$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *Pyrene (1) + n-Pentacontane (2)* | | | | | | | | | | | |
| 0.0000 | 364.75 | | 1.0000 | 0.4071 | 380.78 | 1.4281 | | 0.8004 | 414.31 | 1.1308 | |
| 0.2073 | 364.24 | | 1.1628 | 0.5016 | 391.29 | 1.3425 | | 0.9001 | 418.83 | 1.0616 | |
| 0.2528 | 363.98 | | 1.1941 | 0.6012 | 400.0 | 1.2577 | | 0.9499 | 420.65 | 1.0278 | |
| 0.3015 | 363.50 | | 1.1894 | 0.7004 | 407.68 | 1.1908 | | | | | |
| 0.3537 | 370.51 | 1.4126 | | 0.7499 | 410.55 | 1.1526 | | | | | |

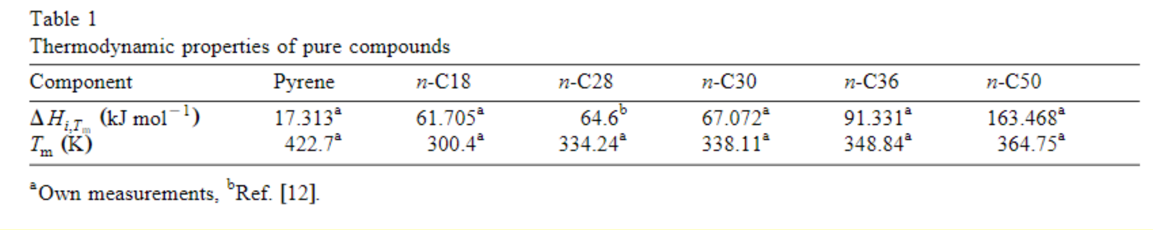


Table 1

Thermodynamic properties of pure compounds

| Component | Pyrene | *n*-C18 | *n*-C28 | *n*-C30 | *n*-C36 | *n*-C50 |
|---|---|---|---|---|---|---|
| $\Delta H_{i,T_m}$ (kJ mol$^{-1}$) | 17.313[a] | 61.705[a] | 64.6[b] | 67.072[a] | 91.331[a] | 163.468[a] |
| $T_m$ (K) | 422.7[a] | 300.4[a] | 334.24[a] | 338.11[a] | 348.84[a] | 364.75[a] |

[a] Own measurements, [b] Ref. [12].

eicosane + 1-octadecanol

Issam Boudouh, Juan Antonio González, Ismahane Djemai, Djamel Barkat, Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1-octadecanol, or + 1-eicosanol mixtures, Fluid Phase Equilibria Volume 442, 25 June 2017, Pages 28-37

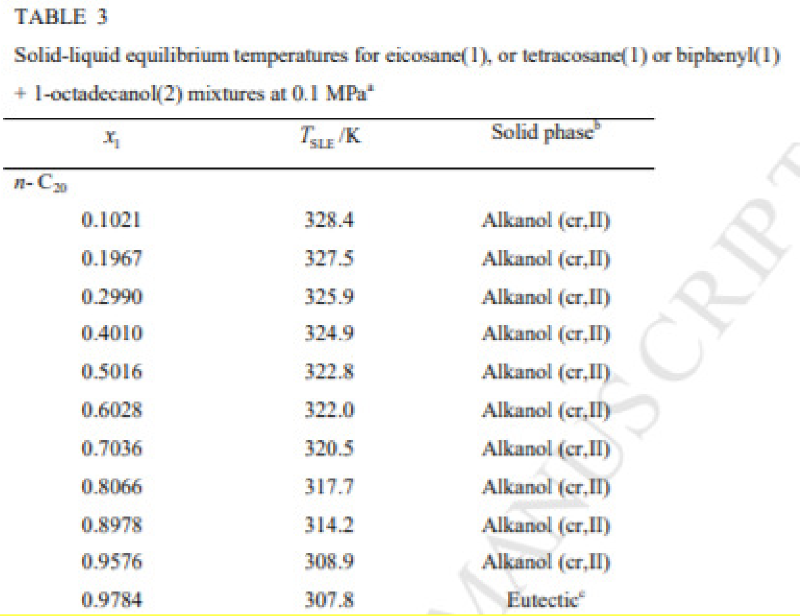


TABLE 3

Solid-liquid equilibrium temperatures for eicosane(1), or tetracosane(1) or biphenyl(1) + 1-octadecanol(2) mixtures at 0.1 MPa[a]

| $x_1$ | $T_{SLE}$ /K | Solid phase[b] |
|---|---|---|
| *n*- $C_{20}$ | | |
| 0.1021 | 328.4 | Alkanol (cr,II) |
| 0.1967 | 327.5 | Alkanol (cr,II) |
| 0.2990 | 325.9 | Alkanol (cr,II) |
| 0.4010 | 324.9 | Alkanol (cr,II) |
| 0.5016 | 322.8 | Alkanol (cr,II) |
| 0.6028 | 322.0 | Alkanol (cr,II) |
| 0.7036 | 320.5 | Alkanol (cr,II) |
| 0.8066 | 317.7 | Alkanol (cr,II) |
| 0.8978 | 314.2 | Alkanol (cr,II) |
| 0.9576 | 308.9 | Alkanol (cr,II) |
| 0.9784 | 307.8 | Eutectic[c] |

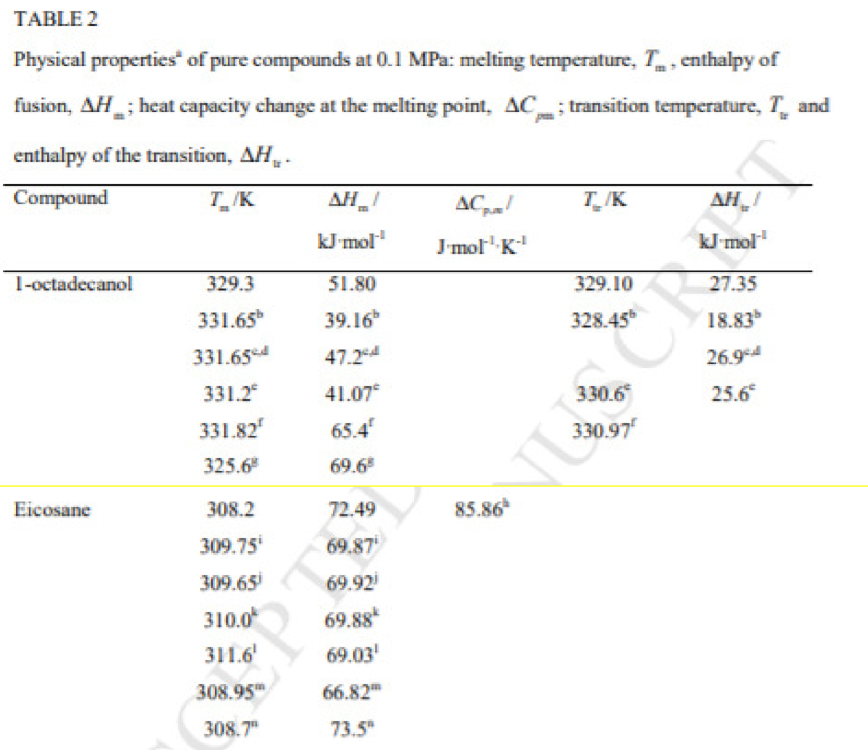


TABLE 2

Physical properties[a] of pure compounds at 0.1 MPa: melting temperature, $T_m$, enthalpy of fusion, $\Delta H_m$; heat capacity change at the melting point, $\Delta C_{pm}$; transition temperature, $T_{tr}$ and enthalpy of the transition, $\Delta H_{tr}$.

| Compound | $T_m$ /K | $\Delta H_m$ / kJ·mol$^{-1}$ | $\Delta C_{p,m}$ / J·mol$^{-1}$·K$^{-1}$ | $T_{tr}$ /K | $\Delta H_{tr}$ / kJ·mol$^{-1}$ |
|---|---|---|---|---|---|
| 1-octadecanol | 329.3 | 51.80 | | 329.10 | 27.35 |
| | 331.65[b] | 39.16[b] | | 328.45[b] | 18.83[b] |
| | 331.65[c,d] | 47.2[c,d] | | | 26.9[c,d] |
| | 331.2[e] | 41.07[e] | | 330.6[e] | 25.6[e] |
| | 331.82[f] | 65.4[f] | | 330.97[f] | |
| | 325.6[g] | 69.6[g] | | | |
| Eicosane | 308.2 | 72.49 | 85.86[h] | | |
| | 309.75[i] | 69.87[i] | | | |
| | 309.65[j] | 69.92[j] | | | |
| | 310.0[k] | 69.88[k] | | | |
| | 311.6[l] | 69.03[l] | | | |
| | 308.95[m] | 66.82[m] | | | |
| | 308.7[n] | 73.5[n] | | | |

tetracosane + 1-octadecanol
Issam Boudouh, Juan Antonio González, Ismahane Djemai, Djamel Barkat, Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1-octadecanol, or + 1-eicosanol mixtures, Fluid Phase Equilibria Volume 442, 25 June 2017, Pages 28-37

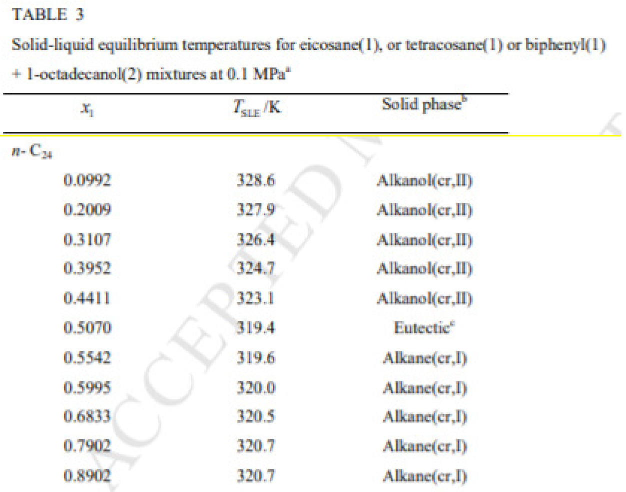


TABLE 3

Solid-liquid equilibrium temperatures for eicosane(1), or tetracosane(1) or biphenyl(1) + 1-octadecanol(2) mixtures at 0.1 MPa[a]

| $x_1$ | $T_{SLE}$ /K | Solid phase[b] |
|---|---|---|
| $n$- $C_{24}$ | | |
| 0.0992 | 328.6 | Alkanol(cr,II) |
| 0.2009 | 327.9 | Alkanol(cr,II) |
| 0.3107 | 326.4 | Alkanol(cr,II) |
| 0.3952 | 324.7 | Alkanol(cr,II) |
| 0.4411 | 323.1 | Alkanol(cr,II) |
| 0.5070 | 319.4 | Eutectic[c] |
| 0.5542 | 319.6 | Alkane(cr,I) |
| 0.5995 | 320.0 | Alkane(cr,I) |
| 0.6833 | 320.5 | Alkane(cr,I) |
| 0.7902 | 320.7 | Alkane(cr,I) |
| 0.8902 | 320.7 | Alkane(cr,I) |

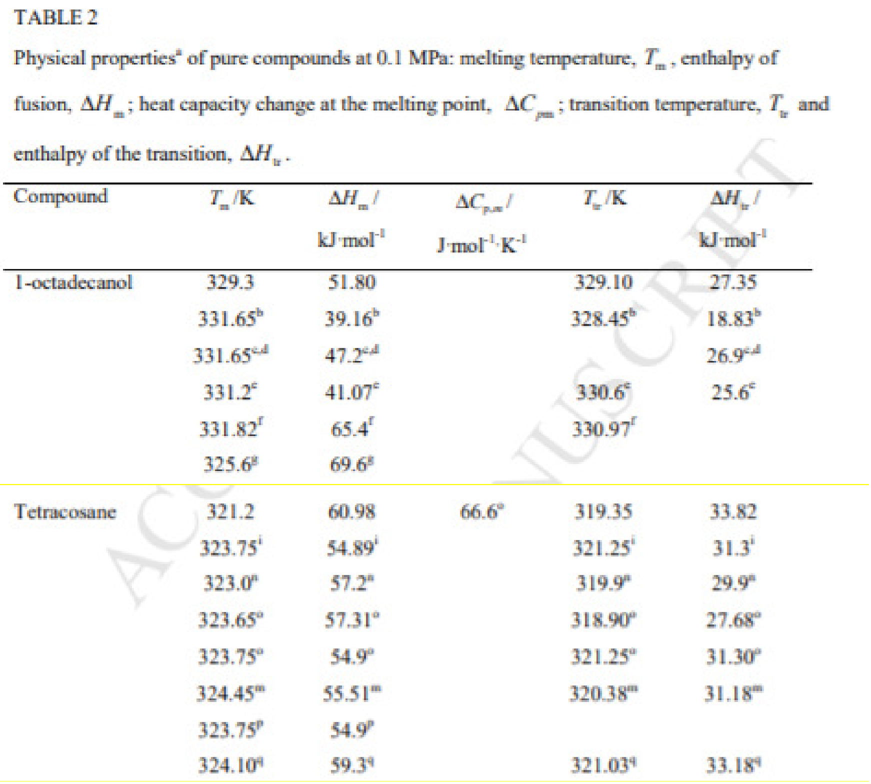


TABLE 2

Physical properties[a] of pure compounds at 0.1 MPa: melting temperature, $T_m$, enthalpy of fusion, $\Delta H_m$; heat capacity change at the melting point, $\Delta C_{pm}$; transition temperature, $T_{tr}$ and enthalpy of the transition, $\Delta H_{tr}$.

| Compound | $T_m$ /K | $\Delta H_m$ / kJ·mol$^{-1}$ | $\Delta C_{p,m}$ / J·mol$^{-1}$·K$^{-1}$ | $T_{tr}$ /K | $\Delta H_{tr}$ / kJ·mol$^{-1}$ |
|---|---|---|---|---|---|
| 1-octadecanol | 329.3 | 51.80 | | 329.10 | 27.35 |
| | 331.65[b] | 39.16[b] | | 328.45[b] | 18.83[b] |
| | 331.65[c,d] | 47.2[c,d] | | | 26.9[c,d] |
| | 331.2[e] | 41.07[e] | | 330.6[e] | 25.6[e] |
| | 331.82[f] | 65.4[f] | | 330.97[f] | |
| | 325.6[g] | 69.6[g] | | | |
| Tetracosane | 321.2 | 60.98 | 66.6[e] | 319.35 | 33.82 |
| | 323.75[i] | 54.89[i] | | 321.25[i] | 31.3[i] |
| | 323.0[n] | 57.2[n] | | 319.9[n] | 29.9[n] |
| | 323.65[o] | 57.31[o] | | 318.90[o] | 27.68[o] |
| | 323.75[o] | 54.9[o] | | 321.25[o] | 31.30[o] |
| | 324.45[m] | 55.51[m] | | 320.38[m] | 31.18[m] |
| | 323.75[p] | 54.9[p] | | | |
| | 324.10[q] | 59.3[q] | | 321.03[q] | 33.18[q] |

biphenyl + 1-octadecanol

Issam Boudouh, Juan Antonio González, Ismahane Djemai, Djamel Barkat, Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1-octadecanol, or + 1-eicosanol mixtures, Fluid Phase Equilibria Volume 442, 25 June 2017, Pages 28-37

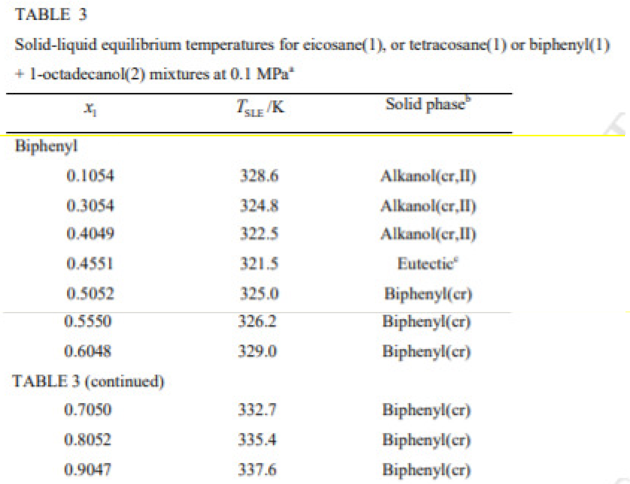


TABLE 3

Solid-liquid equilibrium temperatures for eicosane(1), or tetracosane(1) or biphenyl(1) + 1-octadecanol(2) mixtures at 0.1 MPa[a]

| $x_1$ | $T_{SLE}$ /K | Solid phase[b] |
|---|---|---|
| Biphenyl | | |
| 0.1054 | 328.6 | Alkanol(cr,II) |
| 0.3054 | 324.8 | Alkanol(cr,II) |
| 0.4049 | 322.5 | Alkanol(cr,II) |
| 0.4551 | 321.5 | Eutectic[c] |
| 0.5052 | 325.0 | Biphenyl(cr) |
| 0.5550 | 326.2 | Biphenyl(cr) |
| 0.6048 | 329.0 | Biphenyl(cr) |

TABLE 3 (continued)

| $x_1$ | $T_{SLE}$ /K | Solid phase[b] |
|---|---|---|
| 0.7050 | 332.7 | Biphenyl(cr) |
| 0.8052 | 335.4 | Biphenyl(cr) |
| 0.9047 | 337.6 | Biphenyl(cr) |

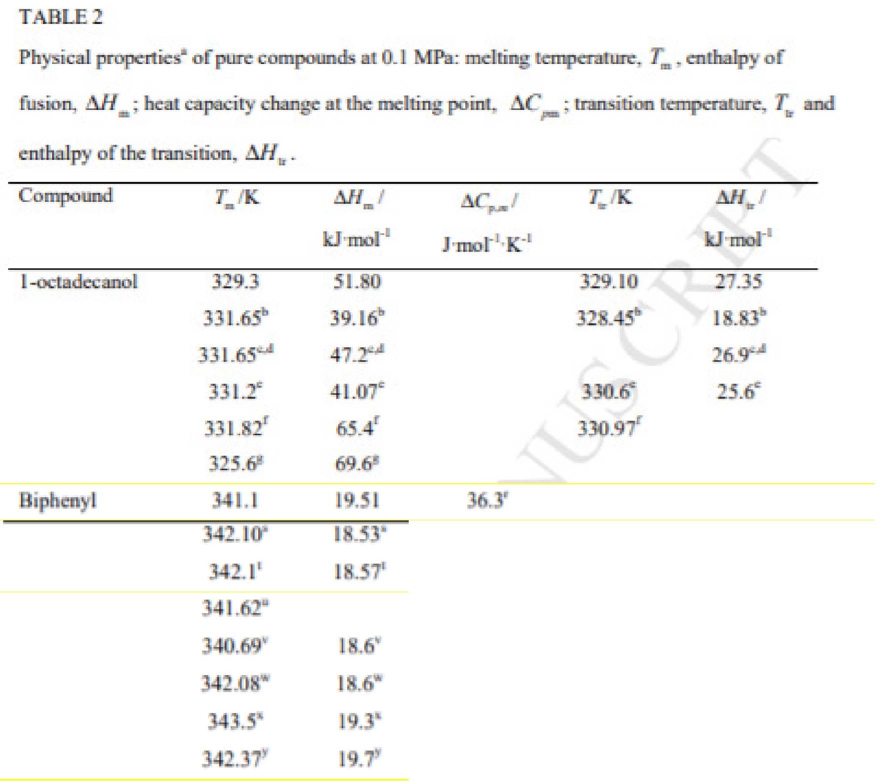


TABLE 2

Physical properties[a] of pure compounds at 0.1 MPa: melting temperature, $T_m$ , enthalpy of fusion, $\Delta H_m$ ; heat capacity change at the melting point, $\Delta C_{pm}$ ; transition temperature, $T_{tr}$ and enthalpy of the transition, $\Delta H_{tr}$ .

| Compound | $T_m$ /K | $\Delta H_m$ / kJ·mol$^{-1}$ | $\Delta C_{p,m}$ / J·mol$^{-1}$·K$^{-1}$ | $T_{tr}$ /K | $\Delta H_{tr}$ / kJ·mol$^{-1}$ |
|---|---|---|---|---|---|
| 1-octadecanol | 329.3 | 51.80 | | 329.10 | 27.35 |
| | 331.65[b] | 39.16[b] | | 328.45[b] | 18.83[b] |
| | 331.65[c,d] | 47.2[c,d] | | | 26.9[c,d] |
| | 331.2[e] | 41.07[e] | | 330.6[e] | 25.6[e] |
| | 331.82[f] | 65.4[f] | | 330.97[f] | |
| | 325.6[g] | 69.6[g] | | | |
| Biphenyl | 341.1 | 19.51 | 36.3[r] | | |
| | 342.10[s] | 18.53[s] | | | |
| | 342.1[t] | 18.57[t] | | | |
| | 341.62[u] | | | | |
| | 340.69[v] | 18.6[v] | | | |
| | 342.08[w] | 18.6[w] | | | |
| | 343.5[x] | 19.3[x] | | | |
| | 342.37[y] | 19.7[y] | | | |

eicosane + 1-eicosanol

Issam Boudouh, Juan Antonio González, Ismahane Djemai, Djamel Barkat, Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1-octadecanol, or + 1-eicosanol mixtures, Fluid Phase Equilibria Volume 442, 25 June 2017, Pages 28-37

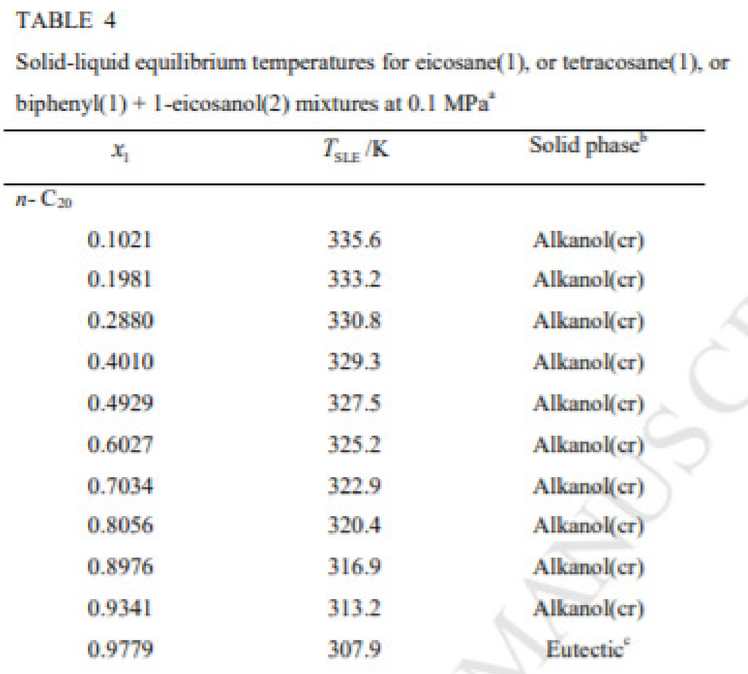


TABLE 4

Solid-liquid equilibrium temperatures for eicosane(1), or tetracosane(1), or biphenyl(1) + 1-eicosanol(2) mixtures at 0.1 MPa[a]

| $x_1$ | $T_{SLE}$ /K | Solid phase[b] |
|---|---|---|
| $n$- $C_{20}$ | | |
| 0.1021 | 335.6 | Alkanol(cr) |
| 0.1981 | 333.2 | Alkanol(cr) |
| 0.2880 | 330.8 | Alkanol(cr) |
| 0.4010 | 329.3 | Alkanol(cr) |
| 0.4929 | 327.5 | Alkanol(cr) |
| 0.6027 | 325.2 | Alkanol(cr) |
| 0.7034 | 322.9 | Alkanol(cr) |
| 0.8056 | 320.4 | Alkanol(cr) |
| 0.8976 | 316.9 | Alkanol(cr) |
| 0.9341 | 313.2 | Alkanol(cr) |
| 0.9779 | 307.9 | Eutectic[c] |

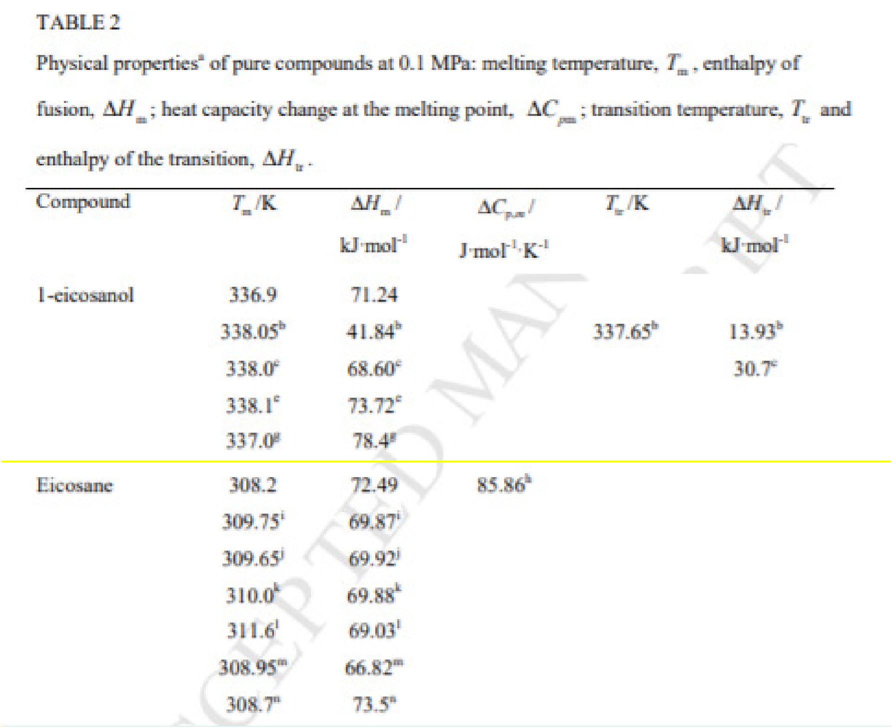


TABLE 2

Physical properties[a] of pure compounds at 0.1 MPa: melting temperature, $T_m$ , enthalpy of fusion, $\Delta H_m$ ; heat capacity change at the melting point, $\Delta C_{pm}$ ; transition temperature, $T_{tr}$ and enthalpy of the transition, $\Delta H_{tr}$ .

| Compound | $T_m$ /K | $\Delta H_m$ / kJ·mol$^{-1}$ | $\Delta C_{p,m}$ / J·mol$^{-1}$·K$^{-1}$ | $T_{tr}$ /K | $\Delta H_{tr}$ / kJ·mol$^{-1}$ |
|---|---|---|---|---|---|
| 1-eicosanol | 336.9 | 71.24 | | | |
| | 338.05[b] | 41.84[b] | | 337.65[b] | 13.93[b] |
| | 338.0[c] | 68.60[c] | | | 30.7[c] |
| | 338.1[e] | 73.72[e] | | | |
| | 337.0[g] | 78.4[g] | | | |
| Eicosane | 308.2 | 72.49 | 85.86[h] | | |
| | 309.75[i] | 69.87[i] | | | |
| | 309.65[j] | 69.92[j] | | | |
| | 310.0[k] | 69.88[k] | | | |
| | 311.6[l] | 69.03[l] | | | |
| | 308.95[m] | 66.82[m] | | | |
| | 308.7[n] | 73.5[n] | | | |

tetracosane + 1-eicosanol
Issam Boudouh, Juan Antonio González, Ismahane Djemai, Djamel Barkat, Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1-octadecanol, or + 1-eicosanol mixtures, Fluid Phase Equilibria Volume 442, 25 June 2017, Pages 28-37

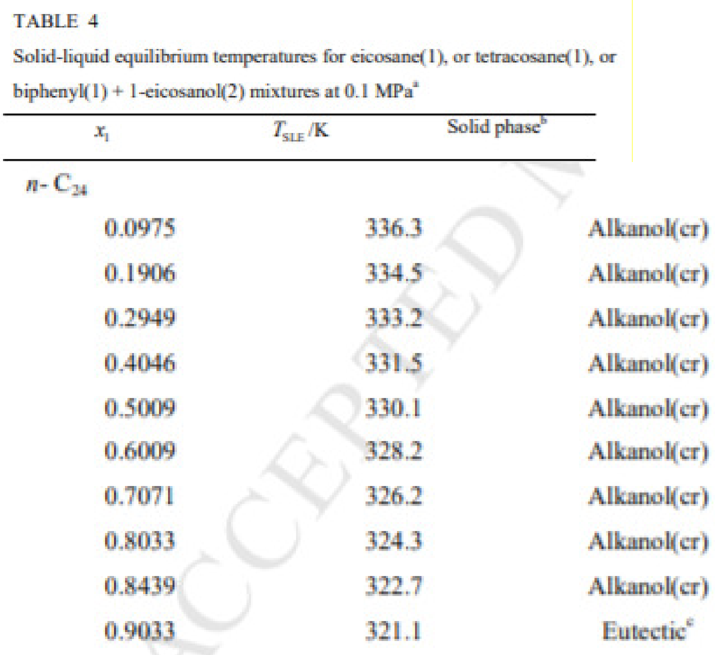


TABLE 4

Solid-liquid equilibrium temperatures for eicosane(1), or tetracosane(1), or biphenyl(1) + 1-eicosanol(2) mixtures at 0.1 MPa[a]

| $x_1$ | $T_{SLE}$ /K | Solid phase[b] |
|---|---|---|
| *n*- $C_{24}$ | | |
| 0.0975 | 336.3 | Alkanol(cr) |
| 0.1906 | 334.5 | Alkanol(cr) |
| 0.2949 | 333.2 | Alkanol(cr) |
| 0.4046 | 331.5 | Alkanol(cr) |
| 0.5009 | 330.1 | Alkanol(cr) |
| 0.6009 | 328.2 | Alkanol(cr) |
| 0.7071 | 326.2 | Alkanol(cr) |
| 0.8033 | 324.3 | Alkanol(cr) |
| 0.8439 | 322.7 | Alkanol(cr) |
| 0.9033 | 321.1 | Eutectic[c] |

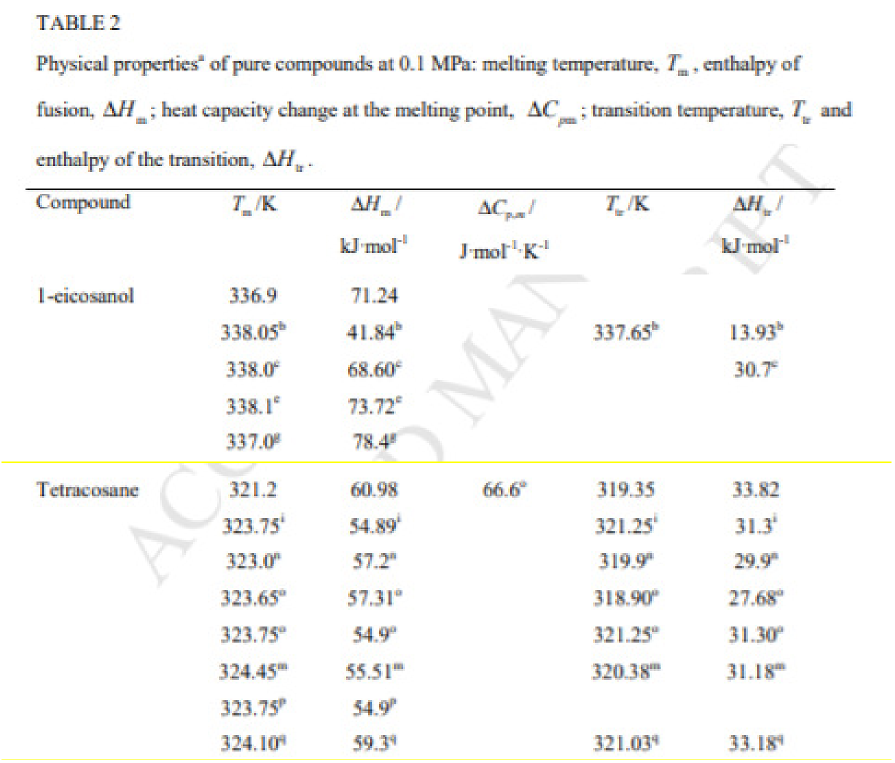


TABLE 2

Physical properties[a] of pure compounds at 0.1 MPa: melting temperature, $T_m$ , enthalpy of fusion, $\Delta H_m$ ; heat capacity change at the melting point, $\Delta C_{pm}$ ; transition temperature, $T_{tr}$ and enthalpy of the transition, $\Delta H_{tr}$ .

| Compound | $T_m$ /K | $\Delta H_m$ / kJ·mol⁻¹ | $\Delta C_{p,m}$ / J·mol⁻¹·K⁻¹ | $T_{tr}$ /K | $\Delta H_{tr}$ / kJ·mol⁻¹ |
|---|---|---|---|---|---|
| 1-eicosanol | 336.9 | 71.24 | | | |
| | 338.05[b] | 41.84[b] | | 337.65[b] | 13.93[b] |
| | 338.0[c] | 68.60[c] | | | 30.7[c] |
| | 338.1[e] | 73.72[e] | | | |
| | 337.0[g] | 78.4[g] | | | |
| Tetracosane | 321.2 | 60.98 | 66.6[e] | 319.35 | 33.82 |
| | 323.75[i] | 54.89[i] | | 321.25[i] | 31.3[i] |
| | 323.0[n] | 57.2[n] | | 319.9[n] | 29.9[n] |
| | 323.65[o] | 57.31[o] | | 318.90[o] | 27.68[o] |
| | 323.75[o] | 54.9[o] | | 321.25[o] | 31.30[o] |
| | 324.45[m] | 55.51[m] | | 320.38[m] | 31.18[m] |
| | 323.75[p] | 54.9[p] | | | |
| | 324.10[q] | 59.3[q] | | 321.03[q] | 33.18[q] |

biphenyl + 1-eicosanol

Issam Boudouh, Juan Antonio González, Ismahane Djemai, Djamel Barkat, Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1-octadecanol, or + 1-eicosanol mixtures, Fluid Phase Equilibria Volume 442, 25 June 2017, Pages 28-37

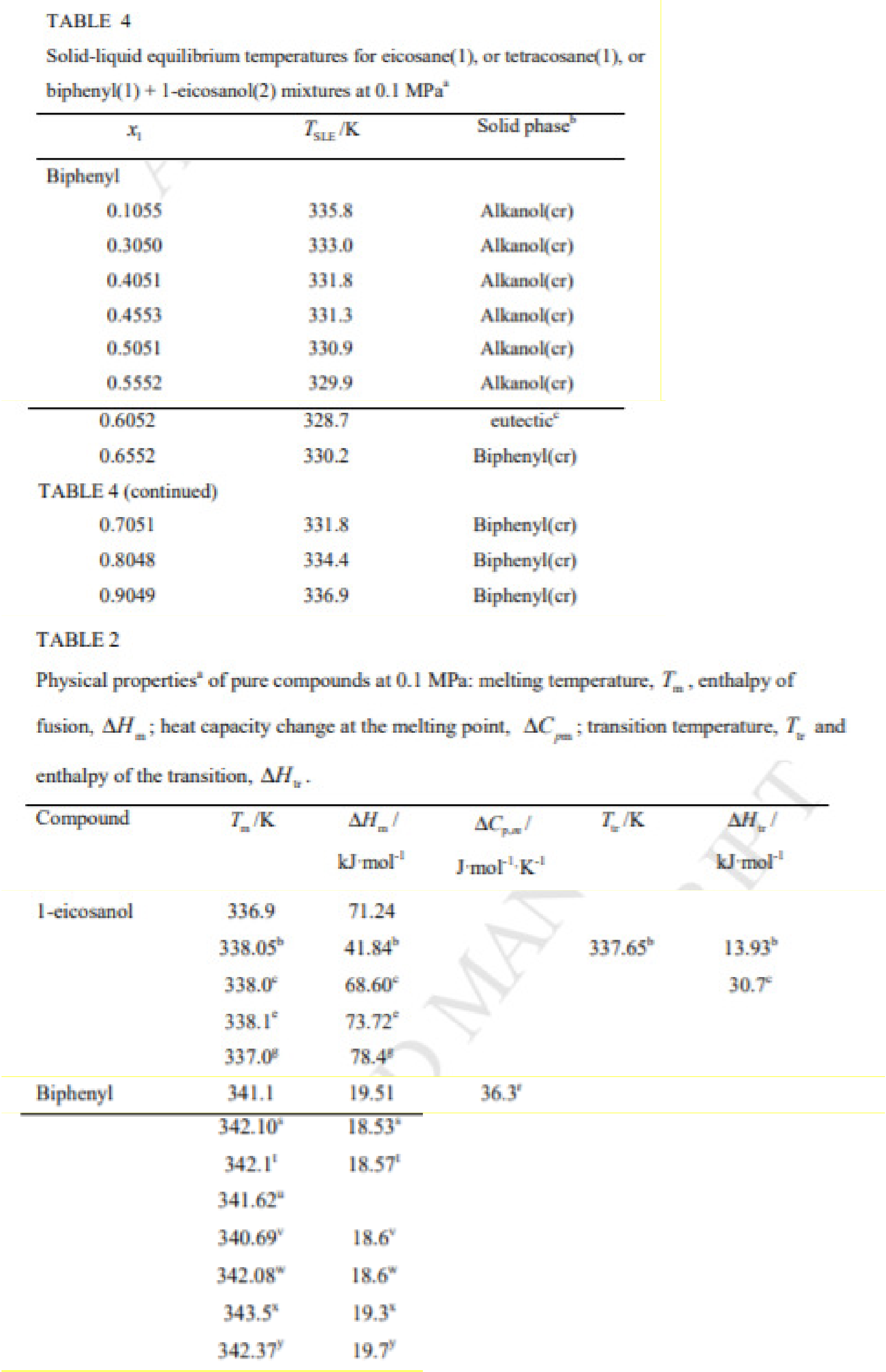


TABLE 4

Solid-liquid equilibrium temperatures for eicosane(1), or tetracosane(1), or biphenyl(1) + 1-eicosanol(2) mixtures at 0.1 MPa[a]

| $x_1$ | $T_{SLE}$ /K | Solid phase[b] |
|---|---|---|
| Biphenyl | | |
| 0.1055 | 335.8 | Alkanol(cr) |
| 0.3050 | 333.0 | Alkanol(cr) |
| 0.4051 | 331.8 | Alkanol(cr) |
| 0.4553 | 331.3 | Alkanol(cr) |
| 0.5051 | 330.9 | Alkanol(cr) |
| 0.5552 | 329.9 | Alkanol(cr) |
| 0.6052 | 328.7 | eutectic[c] |
| 0.6552 | 330.2 | Biphenyl(cr) |

TABLE 4 (continued)

| | | |
|---|---|---|
| 0.7051 | 331.8 | Biphenyl(cr) |
| 0.8048 | 334.4 | Biphenyl(cr) |
| 0.9049 | 336.9 | Biphenyl(cr) |

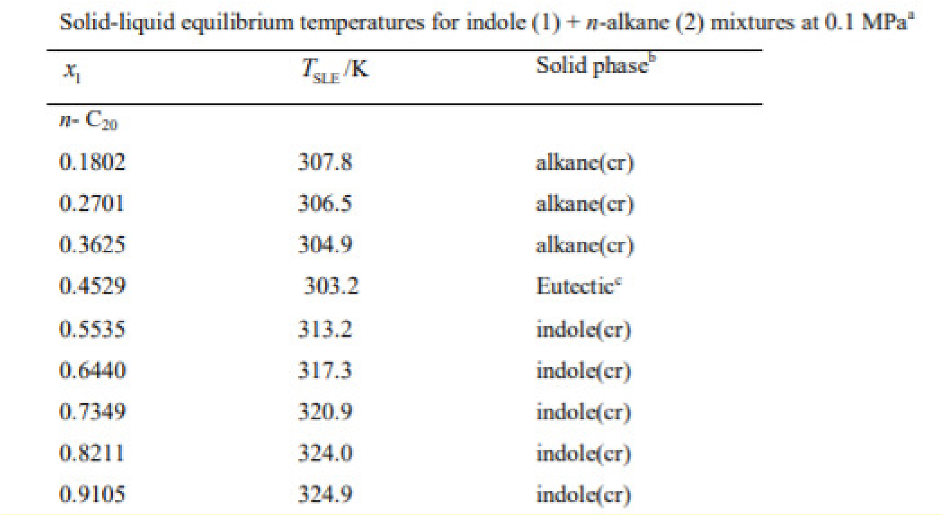
TABLE 2

Physical properties[a] of pure compounds at 0.1 MPa: melting temperature, $T_m$, enthalpy of fusion, $\Delta H_m$; heat capacity change at the melting point, $\Delta C_{pm}$; transition temperature, $T_{tr}$ and enthalpy of the transition, $\Delta H_{tr}$.

| Compound | $T_m$ /K | $\Delta H_m$ / kJ·mol$^{-1}$ | $\Delta C_{p,m}$ / J·mol$^{-1}$·K$^{-1}$ | $T_{tr}$ /K | $\Delta H_{tr}$ / kJ·mol$^{-1}$ |
|---|---|---|---|---|---|
| 1-eicosanol | 336.9 | 71.24 | | | |
| | 338.05[b] | 41.84[b] | | 337.65[b] | 13.93[b] |
| | 338.0[c] | 68.60[c] | | | 30.7[c] |
| | 338.1[e] | 73.72[e] | | | |
| | 337.0[g] | 78.4[g] | | | |
| Biphenyl | 341.1 | 19.51 | 36.3[r] | | |
| | 342.10[s] | 18.53[s] | | | |
| | 342.1[t] | 18.57[t] | | | |
| | 341.62[u] | | | | |
| | 340.69[v] | 18.6[v] | | | |
| | 342.08[w] | 18.6[w] | | | |
| | 343.5[x] | 19.3[x] | | | |
| | 342.37[y] | 19.7[y] | | | |

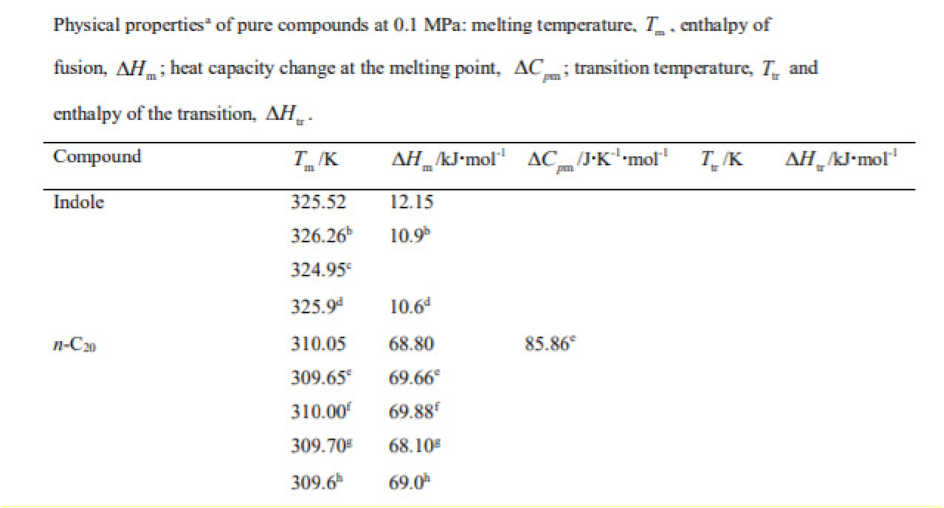
indole + eicosane

Issam Boudouh, Djamel Barkat, Juan Antonio González, Ismahane Djemai, Solid-liquid equilibria of indole binary systems, Thermochimica Acta, Volume 644, 20 November 2016, Pages 13-19



Solid-liquid equilibrium temperatures for indole (1) + *n*-alkane (2) mixtures at 0.1 MPa[a]

| $x_1$ | $T_{SLE}$/K | Solid phase[b] |
|---|---|---|
| *n*- $C_{20}$ | | |
| 0.1802 | 307.8 | alkane(cr) |
| 0.2701 | 306.5 | alkane(cr) |
| 0.3625 | 304.9 | alkane(cr) |
| 0.4529 | 303.2 | Eutectic[c] |
| 0.5535 | 313.2 | indole(cr) |
| 0.6440 | 317.3 | indole(cr) |
| 0.7349 | 320.9 | indole(cr) |
| 0.8211 | 324.0 | indole(cr) |
| 0.9105 | 324.9 | indole(cr) |

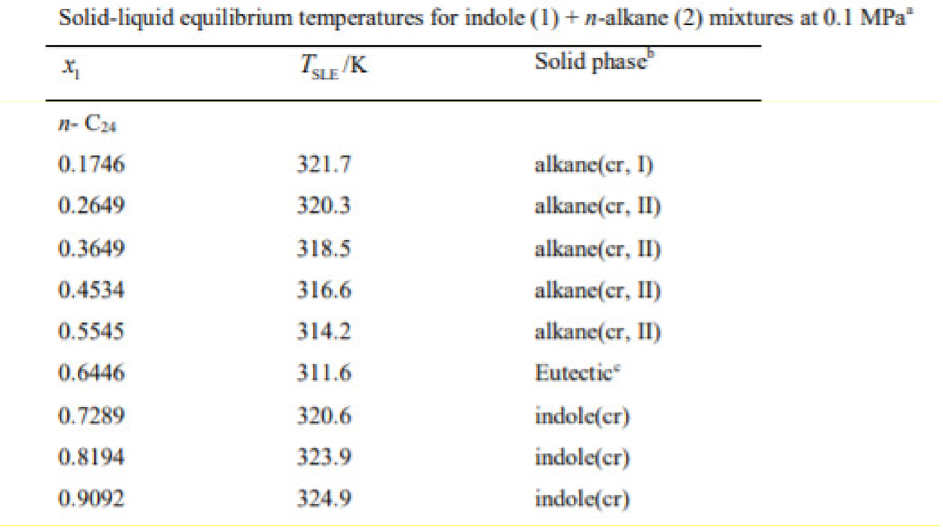


Physical properties[a] of pure compounds at 0.1 MPa: melting temperature, $T_m$, enthalpy of fusion, $\Delta H_m$; heat capacity change at the melting point, $\Delta C_{pm}$; transition temperature, $T_{tr}$ and enthalpy of the transition, $\Delta H_{tr}$.

| Compound | $T_m$/K | $\Delta H_m$/kJ·mol$^{-1}$ | $\Delta C_{pm}$/J·K$^{-1}$·mol$^{-1}$ | $T_{tr}$/K | $\Delta H_{tr}$/kJ·mol$^{-1}$ |
|---|---|---|---|---|---|
| Indole | 325.52 | 12.15 | | | |
| | 326.26[b] | 10.9[b] | | | |
| | 324.95[c] | | | | |
| | 325.9[d] | 10.6[d] | | | |
| *n*-$C_{20}$ | 310.05 | 68.80 | 85.86[e] | | |
| | 309.65[e] | 69.66[e] | | | |
| | 310.00[f] | 69.88[f] | | | |
| | 309.70[g] | 68.10[g] | | | |
| | 309.6[h] | 69.0[h] | | | |

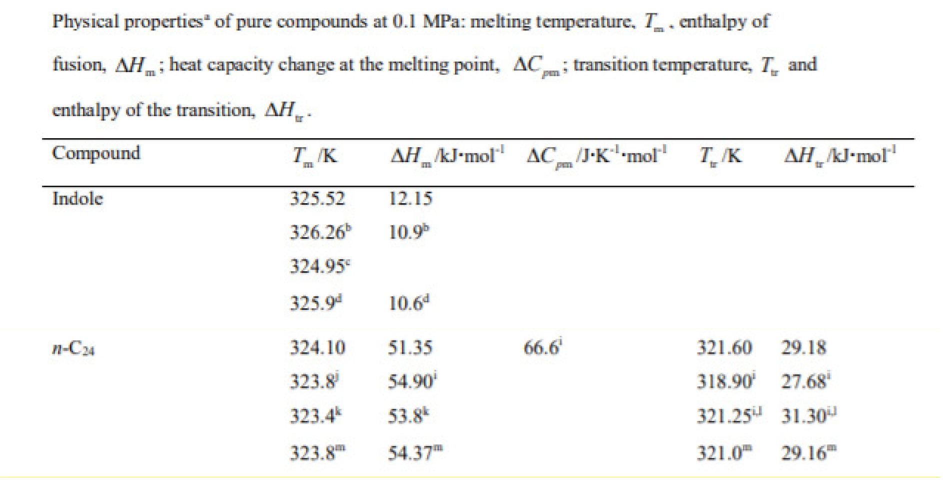
indole + tetracosane

Issam Boudouh, Djamel Barkat, Juan Antonio González, Ismahane Djemai, Solid-liquid equilibria of indole binary systems, Thermochimica Acta, Volume 644, 20 November 2016, Pages 13-19



Solid-liquid equilibrium temperatures for indole (1) + *n*-alkane (2) mixtures at 0.1 MPa[a]

| $x_1$ | $T_{SLE}$ /K | Solid phase[b] |
|---|---|---|
| *n*- $C_{24}$ | | |
| 0.1746 | 321.7 | alkane(cr, I) |
| 0.2649 | 320.3 | alkane(cr, II) |
| 0.3649 | 318.5 | alkane(cr, II) |
| 0.4534 | 316.6 | alkane(cr, II) |
| 0.5545 | 314.2 | alkane(cr, II) |
| 0.6446 | 311.6 | Eutectic[c] |
| 0.7289 | 320.6 | indole(cr) |
| 0.8194 | 323.9 | indole(cr) |
| 0.9092 | 324.9 | indole(cr) |

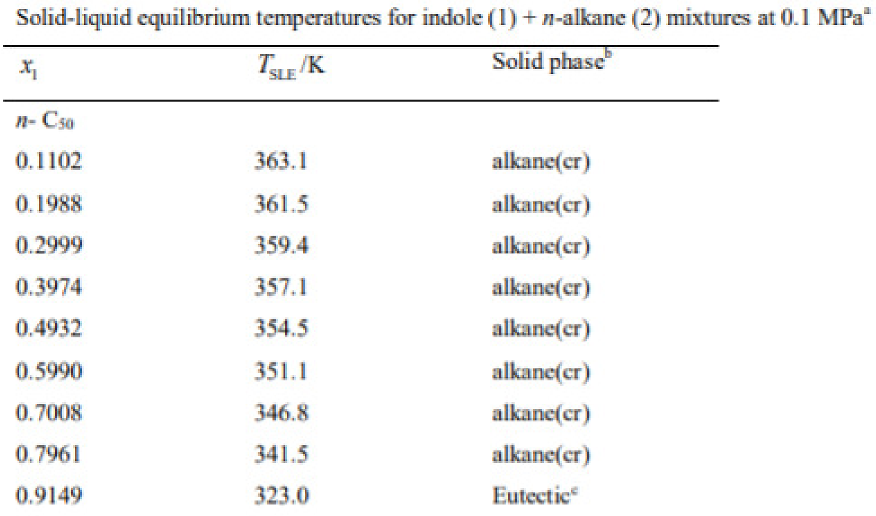


Physical properties[a] of pure compounds at 0.1 MPa: melting temperature, $T_m$, enthalpy of fusion, $\Delta H_m$; heat capacity change at the melting point, $\Delta C_{pm}$; transition temperature, $T_{tr}$ and enthalpy of the transition, $\Delta H_{tr}$.

| Compound | $T_m$ /K | $\Delta H_m$ /kJ·mol$^{-1}$ | $\Delta C_{pm}$ /J·K$^{-1}$·mol$^{-1}$ | $T_{tr}$ /K | $\Delta H_{tr}$ /kJ·mol$^{-1}$ |
|---|---|---|---|---|---|
| Indole | 325.52 | 12.15 | | | |
| | 326.26[b] | 10.9[b] | | | |
| | 324.95[c] | | | | |
| | 325.9[d] | 10.6[d] | | | |
| *n*-$C_{24}$ | 324.10 | 51.35 | 66.6[i] | 321.60 | 29.18 |
| | 323.8[j] | 54.90[i] | | 318.90[i] | 27.68[i] |
| | 323.4[k] | 53.8[k] | | 321.25[i,l] | 31.30[i,l] |
| | 323.8[m] | 54.37[m] | | 321.0[m] | 29.16[m] |

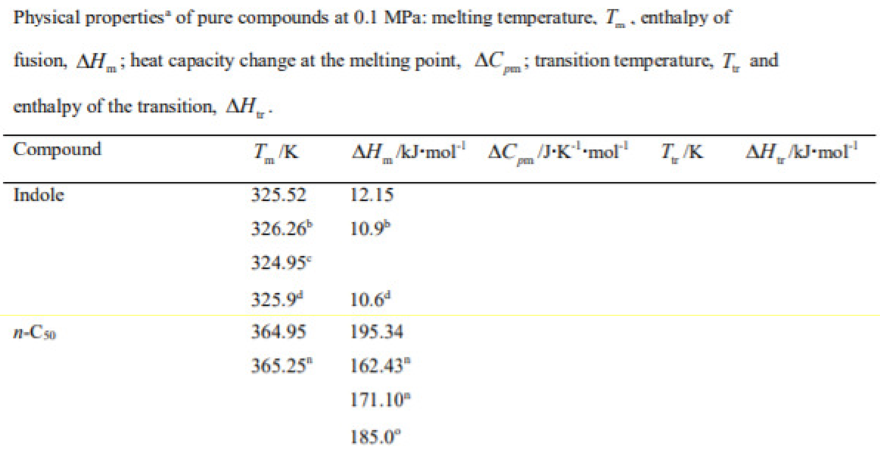
indole + pentacontane

Issam Boudouh, Djamel Barkat, Juan Antonio González, Ismahane Djemai, Solid-liquid equilibria of indole binary systems, Thermochimica Acta, Volume 644, 20 November 2016, Pages 13-19



Solid-liquid equilibrium temperatures for indole (1) + *n*-alkane (2) mixtures at 0.1 MPa[a]

| $x_1$ | $T_{SLE}$ /K | Solid phase[b] |
|---|---|---|
| *n*- $C_{50}$ | | |
| 0.1102 | 363.1 | alkane(cr) |
| 0.1988 | 361.5 | alkane(cr) |
| 0.2999 | 359.4 | alkane(cr) |
| 0.3974 | 357.1 | alkane(cr) |
| 0.4932 | 354.5 | alkane(cr) |
| 0.5990 | 351.1 | alkane(cr) |
| 0.7008 | 346.8 | alkane(cr) |
| 0.7961 | 341.5 | alkane(cr) |
| 0.9149 | 323.0 | Eutectic[c] |



Physical properties[a] of pure compounds at 0.1 MPa: melting temperature, $T_m$ , enthalpy of fusion, $\Delta H_m$ ; heat capacity change at the melting point, $\Delta C_{pm}$ ; transition temperature, $T_{tr}$ and enthalpy of the transition, $\Delta H_{tr}$ .

| Compound | $T_m$ /K | $\Delta H_m$ /kJ·mol$^{-1}$ | $\Delta C_{pm}$ /J·K$^{-1}$·mol$^{-1}$ | $T_{tr}$ /K | $\Delta H_{tr}$ /kJ·mol$^{-1}$ |
|---|---|---|---|---|---|
| Indole | 325.52 | 12.15 | | | |
| | 326.26[b] | 10.9[b] | | | |
| | 324.95[c] | | | | |
| | 325.9[d] | 10.6[d] | | | |
| *n*-$C_{50}$ | 364.95 | 195.34 | | | |
| | 365.25[n] | 162.43[n] | | | |
| | | 171.10[n] | | | |
| | | 185.0[o] | | | |

*N*-methyl-2-pyrrolidinone + 2-methyl-2-propanol

U. Domanska, J. Łachwa, (Solid + liquid) phase equilibria ofbinary mixtures containingN-methyl-2-pyrrolidinone and alcoholat atmospheric pressure, J. Chem. Thermodynamics 35 (2003) 1215–1224

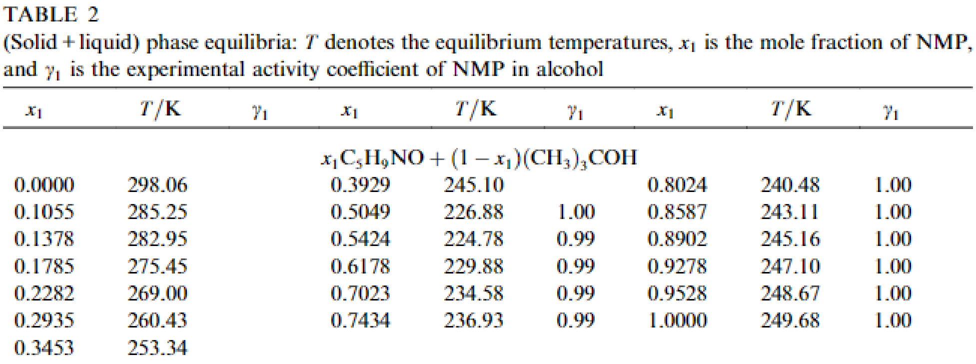


TABLE 2

(Solid + liquid) phase equilibria: $T$ denotes the equilibrium temperatures, $x_1$ is the mole fraction of NMP, and $\gamma_1$ is the experimental activity coefficient of NMP in alcohol

| $x_1$ | $T$/K | $\gamma_1$ | $x_1$ | $T$/K | $\gamma_1$ | $x_1$ | $T$/K | $\gamma_1$ |
|---|---|---|---|---|---|---|---|---|
| $x_1C_5H_9NO + (1-x_1)(CH_3)_3COH$ | | | | | | | | |
| 0.0000 | 298.06 | | 0.3929 | 245.10 | | 0.8024 | 240.48 | 1.00 |
| 0.1055 | 285.25 | | 0.5049 | 226.88 | 1.00 | 0.8587 | 243.11 | 1.00 |
| 0.1378 | 282.95 | | 0.5424 | 224.78 | 0.99 | 0.8902 | 245.16 | 1.00 |
| 0.1785 | 275.45 | | 0.6178 | 229.88 | 0.99 | 0.9278 | 247.10 | 1.00 |
| 0.2282 | 269.00 | | 0.7023 | 234.58 | 0.99 | 0.9528 | 248.67 | 1.00 |
| 0.2935 | 260.43 | | 0.7434 | 236.93 | 0.99 | 1.0000 | 249.68 | 1.00 |
| 0.3453 | 253.34 | | | | | | | |

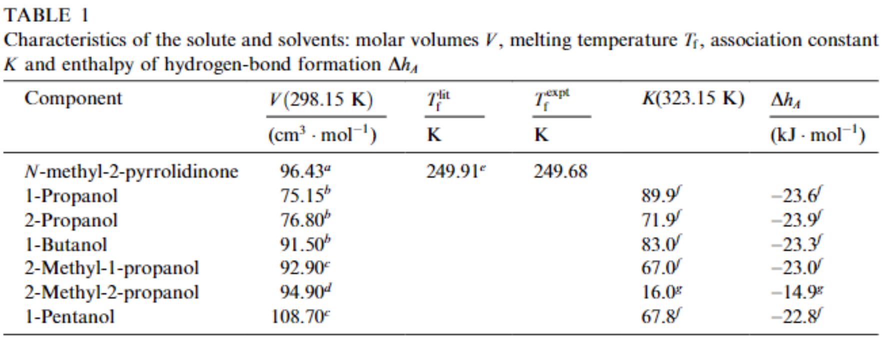


TABLE 1

Characteristics of the solute and solvents: molar volumes $V$, melting temperature $T_f$, association constant $K$ and enthalpy of hydrogen-bond formation $\Delta h_A$

| Component | $V$(298.15 K) (cm$^3$ · mol$^{-1}$) | $T_f^{lit}$ K | $T_f^{expt}$ K | $K$(323.15 K) | $\Delta h_A$ (kJ · mol$^{-1}$) |
|---|---|---|---|---|---|
| *N*-methyl-2-pyrrolidinone | 96.43[a] | 249.91[e] | 249.68 | | |
| 1-Propanol | 75.15[b] | | | 89.9[f] | −23.6[f] |
| 2-Propanol | 76.80[b] | | | 71.9[f] | −23.9[f] |
| 1-Butanol | 91.50[b] | | | 83.0[f] | −23.3[f] |
| 2-Methyl-1-propanol | 92.90[c] | | | 67.0[f] | −23.0[f] |
| 2-Methyl-2-propanol | 94.90[d] | | | 16.0[g] | −14.9[g] |
| 1-Pentanol | 108.70[c] | | | 67.8[f] | −22.8[f] |

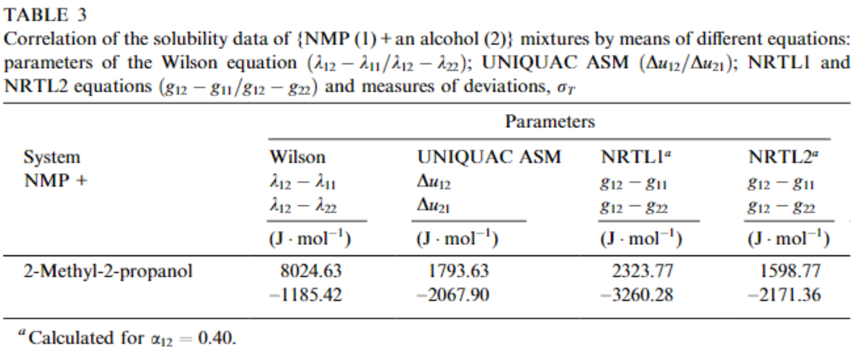


TABLE 3

Correlation of the solubility data of {NMP (1) + an alcohol (2)} mixtures by means of different equations: parameters of the Wilson equation ($\lambda_{12}-\lambda_{11}/\lambda_{12}-\lambda_{22}$); UNIQUAC ASM ($\Delta u_{12}/\Delta u_{21}$); NRTL1 and NRTL2 equations ($g_{12}-g_{11}/g_{12}-g_{22}$) and measures of deviations, $\sigma_T$

| | Parameters | | | |
|---|---|---|---|---|
| System NMP + | Wilson<br>$\lambda_{12}-\lambda_{11}$<br>$\lambda_{12}-\lambda_{22}$<br>(J · mol$^{-1}$) | UNIQUAC ASM<br>$\Delta u_{12}$<br>$\Delta u_{21}$<br>(J · mol$^{-1}$) | NRTL1[a]<br>$g_{12}-g_{11}$<br>$g_{12}-g_{22}$<br>(J · mol$^{-1}$) | NRTL2[a]<br>$g_{12}-g_{11}$<br>$g_{12}-g_{22}$<br>(J · mol$^{-1}$) |
| 2-Methyl-2-propanol | 8024.63 | 1793.63 | 2323.77 | 1598.77 |
| | −1185.42 | −2067.90 | −3260.28 | −2171.36 |

[a] Calculated for $\alpha_{12} = 0.40$.

ODABRATI JEDAN MODEL

## 1,3,5-trioxane + *n*-heptane

U. Domanska, J. A. González, Solid–liquid and liquid–liquid equilibria for 1,3,5-trioxane, or 1,4,7,10,13,16-hexaoxacyclooctadecane+selectedn-alkane mixturesAnalysis in terms of DISQUAC, Fluid Phase Equilibria 205 (2003) 317–338

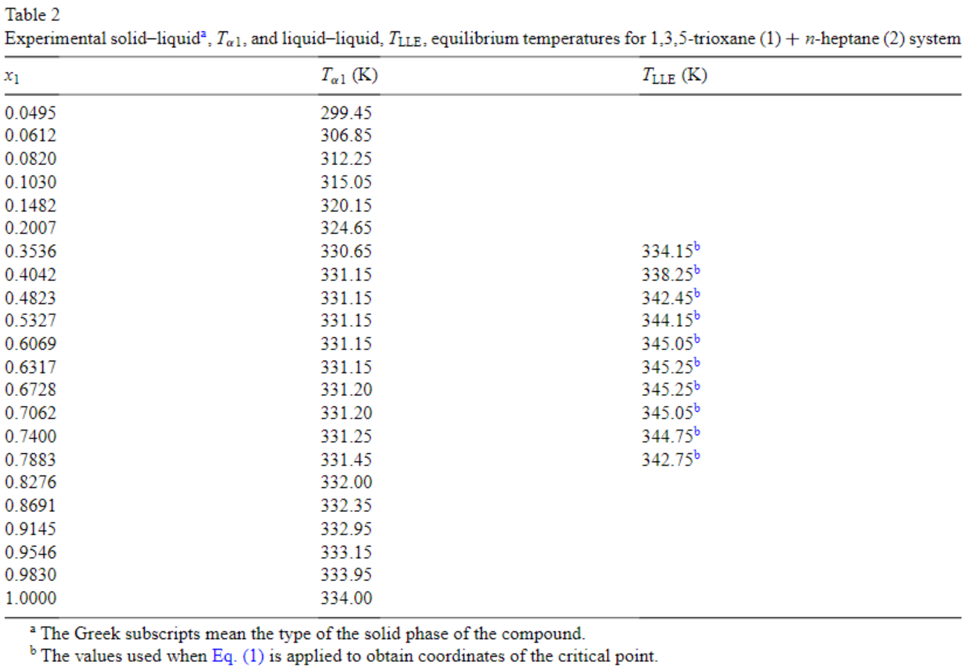


Table 2
Experimental solid–liquid[a], $T_{\alpha 1}$, and liquid–liquid, $T_{LLE}$, equilibrium temperatures for 1,3,5-trioxane (1) + *n*-heptane (2) system

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{LLE}$ (K) |
|---|---|---|
| 0.0495 | 299.45 | |
| 0.0612 | 306.85 | |
| 0.0820 | 312.25 | |
| 0.1030 | 315.05 | |
| 0.1482 | 320.15 | |
| 0.2007 | 324.65 | |
| 0.3536 | 330.65 | 334.15[b] |
| 0.4042 | 331.15 | 338.25[b] |
| 0.4823 | 331.15 | 342.45[b] |
| 0.5327 | 331.15 | 344.15[b] |
| 0.6069 | 331.15 | 345.05[b] |
| 0.6317 | 331.15 | 345.25[b] |
| 0.6728 | 331.20 | 345.25[b] |
| 0.7062 | 331.20 | 345.05[b] |
| 0.7400 | 331.25 | 344.75[b] |
| 0.7883 | 331.45 | 342.75[b] |
| 0.8276 | 332.00 | |
| 0.8691 | 332.35 | |
| 0.9145 | 332.95 | |
| 0.9546 | 333.15 | |
| 0.9830 | 333.95 | |
| 1.0000 | 334.00 | |

[a] The Greek subscripts mean the type of the solid phase of the compound.

[b] The values used when Eq. (1) is applied to obtain coordinates of the critical point.

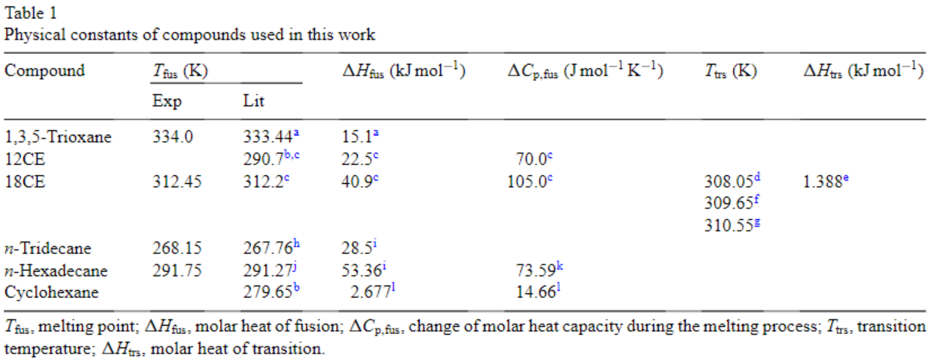


Table 1
Physical constants of compounds used in this work

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$ (kJ mol$^{-1}$) | $\Delta C_{p,fus}$ (J mol$^{-1}$ K$^{-1}$) | $T_{trs}$ (K) | $\Delta H_{trs}$ (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|
| | Exp | Lit | | | | |
| 1,3,5-Trioxane | 334.0 | 333.44[a] | 15.1[a] | | | |
| 12CE | | 290.7[b,c] | 22.5[c] | 70.0[c] | | |
| 18CE | 312.45 | 312.2[c] | 40.9[c] | 105.0[c] | 308.05[d]<br>309.65[f]<br>310.55[g] | 1.388[e] |
| *n*-Tridecane | 268.15 | 267.76[h] | 28.5[i] | | | |
| *n*-Hexadecane | 291.75 | 291.27[j] | 53.36[i] | 73.59[k] | | |
| Cyclohexane | | 279.65[b] | 2.677[l] | 14.66[l] | | |

$T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion; $\Delta C_{p,fus}$, change of molar heat capacity during the melting process; $T_{trs}$, transition temperature; $\Delta H_{trs}$, molar heat of transition.

1,3,5-trioxane + *n*-tridecane
U. Domanska, J. A. González, Solid–liquid and liquid–liquid equilibria for 1,3,5-trioxane, or 1,4,7,10,13,16-hexaoxacyclooctadecane+selectedn-alkane mixturesAnalysis in terms of DISQUAC, Fluid Phase Equilibria 205 (2003) 317–338

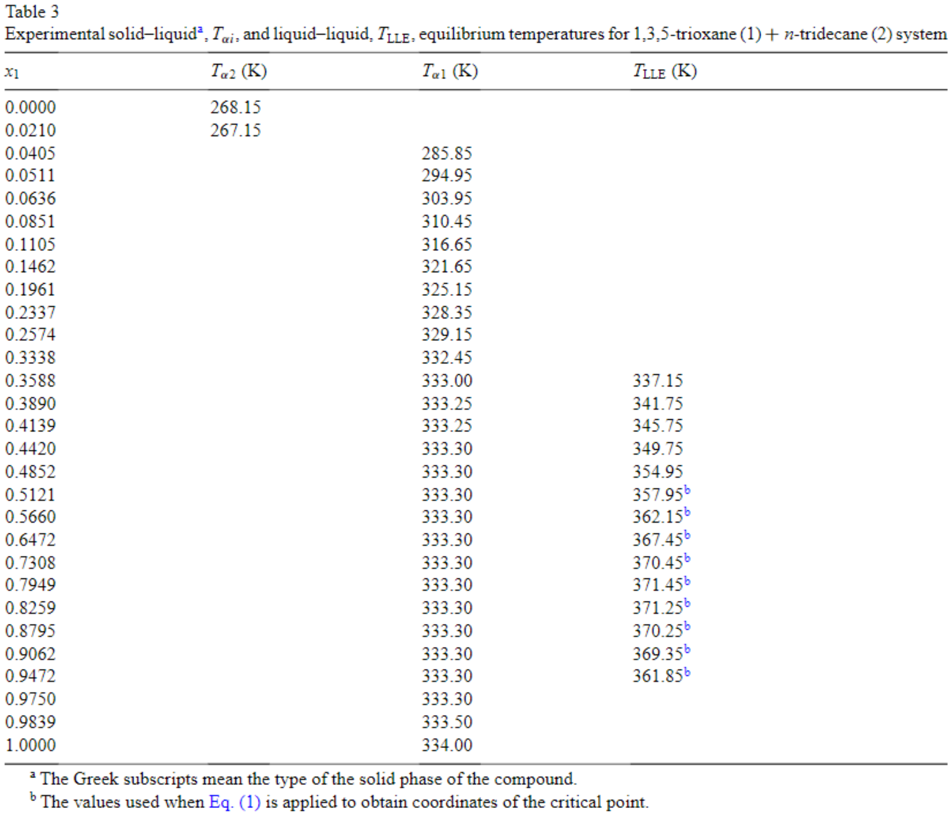


Table 3
Experimental solid–liquid[a], $T_{\alpha i}$, and liquid–liquid, $T_{LLE}$, equilibrium temperatures for 1,3,5-trioxane (1) + *n*-tridecane (2) system

| $x_1$ | $T_{\alpha 2}$ (K) | $T_{\alpha 1}$ (K) | $T_{LLE}$ (K) |
|---|---|---|---|
| 0.0000 | 268.15 | | |
| 0.0210 | 267.15 | | |
| 0.0405 | | 285.85 | |
| 0.0511 | | 294.95 | |
| 0.0636 | | 303.95 | |
| 0.0851 | | 310.45 | |
| 0.1105 | | 316.65 | |
| 0.1462 | | 321.65 | |
| 0.1961 | | 325.15 | |
| 0.2337 | | 328.35 | |
| 0.2574 | | 329.15 | |
| 0.3338 | | 332.45 | |
| 0.3588 | | 333.00 | 337.15 |
| 0.3890 | | 333.25 | 341.75 |
| 0.4139 | | 333.25 | 345.75 |
| 0.4420 | | 333.30 | 349.75 |
| 0.4852 | | 333.30 | 354.95 |
| 0.5121 | | 333.30 | 357.95[b] |
| 0.5660 | | 333.30 | 362.15[b] |
| 0.6472 | | 333.30 | 367.45[b] |
| 0.7308 | | 333.30 | 370.45[b] |
| 0.7949 | | 333.30 | 371.45[b] |
| 0.8259 | | 333.30 | 371.25[b] |
| 0.8795 | | 333.30 | 370.25[b] |
| 0.9062 | | 333.30 | 369.35[b] |
| 0.9472 | | 333.30 | 361.85[b] |
| 0.9750 | | 333.30 | |
| 0.9839 | | 333.50 | |
| 1.0000 | | 334.00 | |

[a] The Greek subscripts mean the type of the solid phase of the compound.
[b] The values used when Eq. (1) is applied to obtain coordinates of the critical point.

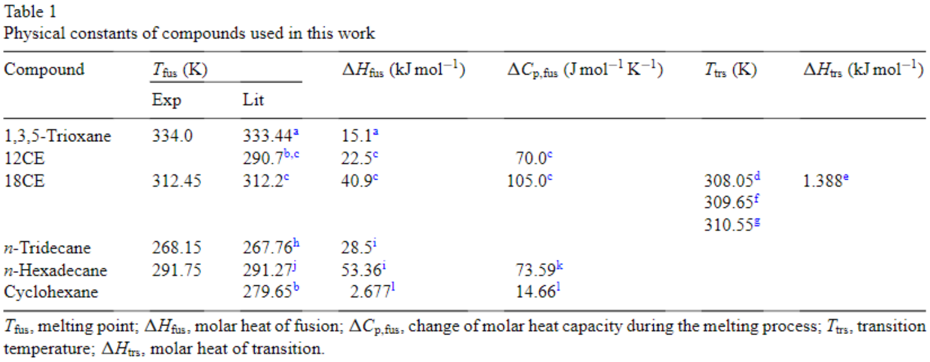


Table 1
Physical constants of compounds used in this work

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$ (kJ mol$^{-1}$) | $\Delta C_{p,fus}$ (J mol$^{-1}$ K$^{-1}$) | $T_{trs}$ (K) | $\Delta H_{trs}$ (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|
| | Exp | Lit | | | | |
| 1,3,5-Trioxane | 334.0 | 333.44[a] | 15.1[a] | | | |
| 12CE | | 290.7[b,c] | 22.5[c] | 70.0[c] | | |
| 18CE | 312.45 | 312.2[c] | 40.9[c] | 105.0[c] | 308.05[d]<br>309.65[f]<br>310.55[g] | 1.388[e] |
| *n*-Tridecane | 268.15 | 267.76[h] | 28.5[i] | | | |
| *n*-Hexadecane | 291.75 | 291.27[j] | 53.36[i] | 73.59[k] | | |
| Cyclohexane | | 279.65[b] | 2.677[l] | 14.66[l] | | |

$T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion; $\Delta C_{p,fus}$, change of molar heat capacity during the melting process; $T_{trs}$, transition temperature; $\Delta H_{trs}$, molar heat of transition.

1,3,5-trioxane + *n*-hexadecane
U. Domanska, J. A. González, Solid–liquid and liquid–liquid equilibria for 1,3,5-trioxane, or 1,4,7,10,13,16-hexaoxacyclooctadecane+selectedn-alkane mixturesAnalysis in terms of DISQUAC, Fluid Phase Equilibria 205 (2003) 317–338

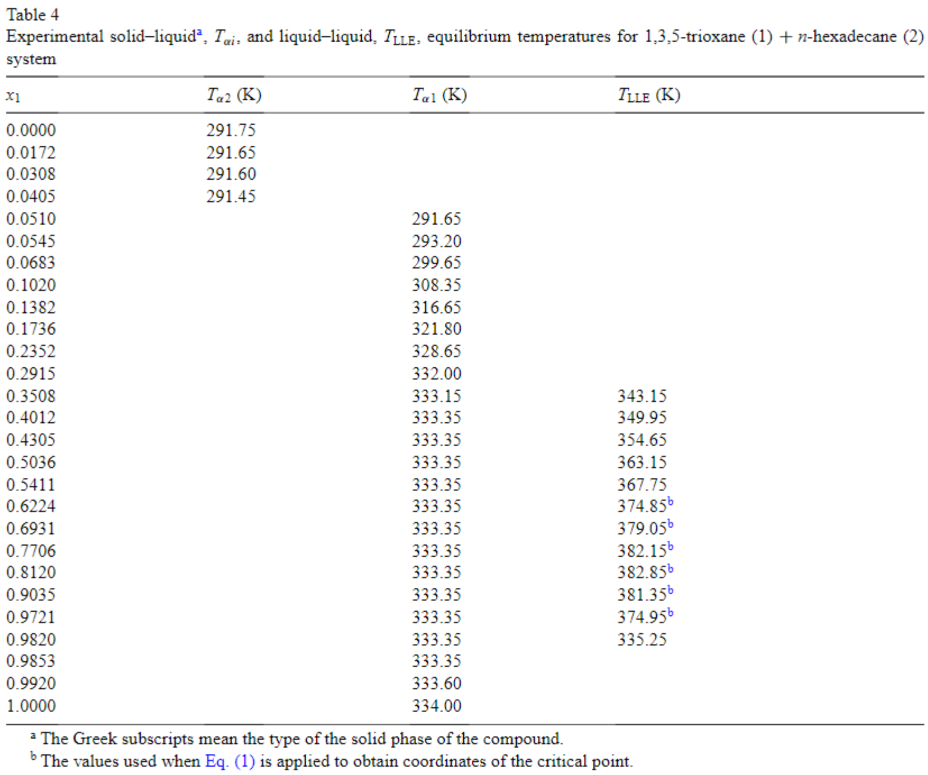


Table 4
Experimental solid–liquid[a], $T_{\alpha i}$, and liquid–liquid, $T_{LLE}$, equilibrium temperatures for 1,3,5-trioxane (1) + *n*-hexadecane (2) system

| $x_1$ | $T_{\alpha 2}$ (K) | $T_{\alpha 1}$ (K) | $T_{LLE}$ (K) |
|---|---|---|---|
| 0.0000 | 291.75 | | |
| 0.0172 | 291.65 | | |
| 0.0308 | 291.60 | | |
| 0.0405 | 291.45 | | |
| 0.0510 | | 291.65 | |
| 0.0545 | | 293.20 | |
| 0.0683 | | 299.65 | |
| 0.1020 | | 308.35 | |
| 0.1382 | | 316.65 | |
| 0.1736 | | 321.80 | |
| 0.2352 | | 328.65 | |
| 0.2915 | | 332.00 | |
| 0.3508 | | 333.15 | 343.15 |
| 0.4012 | | 333.35 | 349.95 |
| 0.4305 | | 333.35 | 354.65 |
| 0.5036 | | 333.35 | 363.15 |
| 0.5411 | | 333.35 | 367.75 |
| 0.6224 | | 333.35 | 374.85[b] |
| 0.6931 | | 333.35 | 379.05[b] |
| 0.7706 | | 333.35 | 382.15[b] |
| 0.8120 | | 333.35 | 382.85[b] |
| 0.9035 | | 333.35 | 381.35[b] |
| 0.9721 | | 333.35 | 374.95[b] |
| 0.9820 | | 333.35 | 335.25 |
| 0.9853 | | 333.35 | |
| 0.9920 | | 333.60 | |
| 1.0000 | | 334.00 | |

[a] The Greek subscripts mean the type of the solid phase of the compound.

[b] The values used when Eq. (1) is applied to obtain coordinates of the critical point.

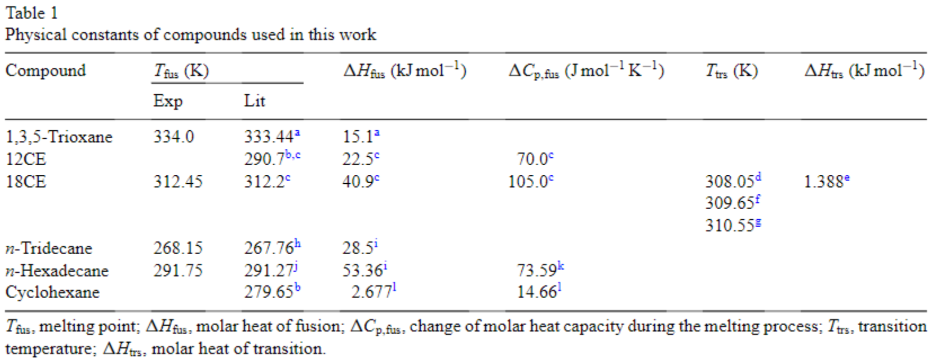


Table 1
Physical constants of compounds used in this work

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$ (kJ mol$^{-1}$) | $\Delta C_{p,fus}$ (J mol$^{-1}$ K$^{-1}$) | $T_{trs}$ (K) | $\Delta H_{trs}$ (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|
| | Exp | Lit | | | | |
| 1,3,5-Trioxane | 334.0 | 333.44[a] | 15.1[a] | | | |
| 12CE | | 290.7[b,c] | 22.5[c] | 70.0[c] | | |
| 18CE | 312.45 | 312.2[c] | 40.9[c] | 105.0[c] | 308.05[d]<br>309.65[f]<br>310.55[g] | 1.388[e] |
| *n*-Tridecane | 268.15 | 267.76[h] | 28.5[i] | | | |
| *n*-Hexadecane | 291.75 | 291.27[j] | 53.36[i] | 73.59[k] | | |
| Cyclohexane | | 279.65[b] | 2.677[l] | 14.66[l] | | |

$T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion; $\Delta C_{p,fus}$, change of molar heat capacity during the melting process; $T_{trs}$, transition temperature; $\Delta H_{trs}$, molar heat of transition.

18-crown-6 ether + *n*-heptane

U. Domanska, J. A. González, Solid–liquid and liquid–liquid equilibria for 1,3,5-trioxane, or 1,4,7,10,13,16-hexaoxacyclooctadecane+selectedn-alkane mixturesAnalysis in terms of DISQUAC, Fluid Phase Equilibria 205 (2003) 317–338

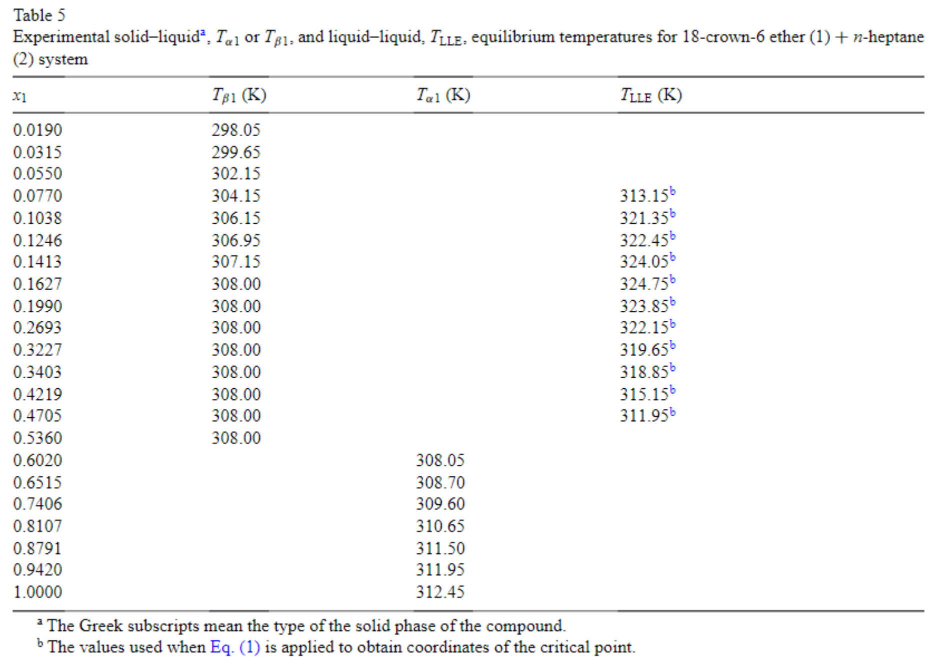


Table 5

Experimental solid–liquid[a], $T_{\alpha 1}$ or $T_{\beta 1}$, and liquid–liquid, $T_{LLE}$, equilibrium temperatures for 18-crown-6 ether (1) + *n*-heptane (2) system

| $x_1$ | $T_{\beta 1}$ (K) | $T_{\alpha 1}$ (K) | $T_{LLE}$ (K) |
|---|---|---|---|
| 0.0190 | 298.05 | | |
| 0.0315 | 299.65 | | |
| 0.0550 | 302.15 | | |
| 0.0770 | 304.15 | | 313.15$^{b}$ |
| 0.1038 | 306.15 | | 321.35$^{b}$ |
| 0.1246 | 306.95 | | 322.45$^{b}$ |
| 0.1413 | 307.15 | | 324.05$^{b}$ |
| 0.1627 | 308.00 | | 324.75$^{b}$ |
| 0.1990 | 308.00 | | 323.85$^{b}$ |
| 0.2693 | 308.00 | | 322.15$^{b}$ |
| 0.3227 | 308.00 | | 319.65$^{b}$ |
| 0.3403 | 308.00 | | 318.85$^{b}$ |
| 0.4219 | 308.00 | | 315.15$^{b}$ |
| 0.4705 | 308.00 | | 311.95$^{b}$ |
| 0.5360 | 308.00 | | |
| 0.6020 | | 308.05 | |
| 0.6515 | | 308.70 | |
| 0.7406 | | 309.60 | |
| 0.8107 | | 310.65 | |
| 0.8791 | | 311.50 | |
| 0.9420 | | 311.95 | |
| 1.0000 | | 312.45 | |

[a] The Greek subscripts mean the type of the solid phase of the compound.

[b] The values used when Eq. (1) is applied to obtain coordinates of the critical point.

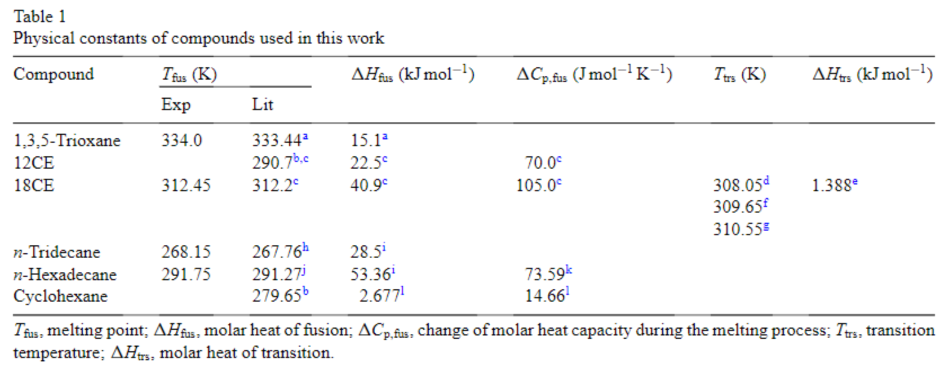


Table 1

Physical constants of compounds used in this work

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$ (kJ mol$^{-1}$) | $\Delta C_{p,fus}$ (J mol$^{-1}$ K$^{-1}$) | $T_{trs}$ (K) | $\Delta H_{trs}$ (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|
| | Exp | Lit | | | | |
| 1,3,5-Trioxane | 334.0 | 333.44$^{a}$ | 15.1$^{a}$ | | | |
| 12CE | | 290.7$^{b,c}$ | 22.5$^{c}$ | 70.0$^{c}$ | | |
| 18CE | 312.45 | 312.2$^{c}$ | 40.9$^{c}$ | 105.0$^{c}$ | 308.05$^{d}$<br>309.65$^{f}$<br>310.55$^{g}$ | 1.388$^{e}$ |
| *n*-Tridecane | 268.15 | 267.76$^{h}$ | 28.5$^{i}$ | | | |
| *n*-Hexadecane | 291.75 | 291.27$^{j}$ | 53.36$^{i}$ | 73.59$^{k}$ | | |
| Cyclohexane | | 279.65$^{b}$ | 2.677$^{l}$ | 14.66$^{l}$ | | |

$T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion; $\Delta C_{p,fus}$, change of molar heat capacity during the melting process; $T_{trs}$, transition temperature; $\Delta H_{trs}$, molar heat of transition.

18-crown-6 ether + *n*-tridecane

U. Domanska, J. A. González, Solid–liquid and liquid–liquid equilibria for 1,3,5-trioxane, or 1,4,7,10,13,16-hexaoxacyclooctadecane+selectedn-alkane mixturesAnalysis in terms of DISQUAC, Fluid Phase Equilibria 205 (2003) 317–338

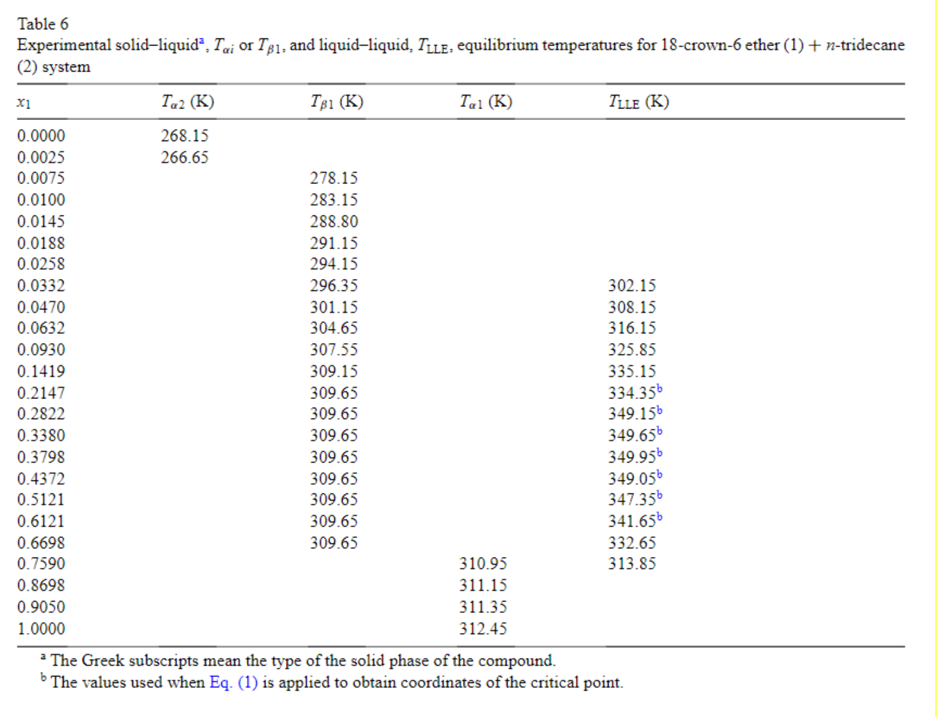


Table 6
Experimental solid–liquid[a], $T_{\alpha i}$ or $T_{\beta 1}$, and liquid–liquid, $T_{LLE}$, equilibrium temperatures for 18-crown-6 ether (1) + *n*-tridecane (2) system

| $x_1$ | $T_{\alpha 2}$ (K) | $T_{\beta 1}$ (K) | $T_{\alpha 1}$ (K) | $T_{LLE}$ (K) |
|---|---|---|---|---|
| 0.0000 | 268.15 | | | |
| 0.0025 | 266.65 | | | |
| 0.0075 | | 278.15 | | |
| 0.0100 | | 283.15 | | |
| 0.0145 | | 288.80 | | |
| 0.0188 | | 291.15 | | |
| 0.0258 | | 294.15 | | |
| 0.0332 | | 296.35 | | 302.15 |
| 0.0470 | | 301.15 | | 308.15 |
| 0.0632 | | 304.65 | | 316.15 |
| 0.0930 | | 307.55 | | 325.85 |
| 0.1419 | | 309.15 | | 335.15 |
| 0.2147 | | 309.65 | | 334.35[b] |
| 0.2822 | | 309.65 | | 349.15[b] |
| 0.3380 | | 309.65 | | 349.65[b] |
| 0.3798 | | 309.65 | | 349.95[b] |
| 0.4372 | | 309.65 | | 349.05[b] |
| 0.5121 | | 309.65 | | 347.35[b] |
| 0.6121 | | 309.65 | | 341.65[b] |
| 0.6698 | | 309.65 | | 332.65 |
| 0.7590 | | | 310.95 | 313.85 |
| 0.8698 | | | 311.15 | |
| 0.9050 | | | 311.35 | |
| 1.0000 | | | 312.45 | |

[a] The Greek subscripts mean the type of the solid phase of the compound.

[b] The values used when Eq. (1) is applied to obtain coordinates of the critical point.

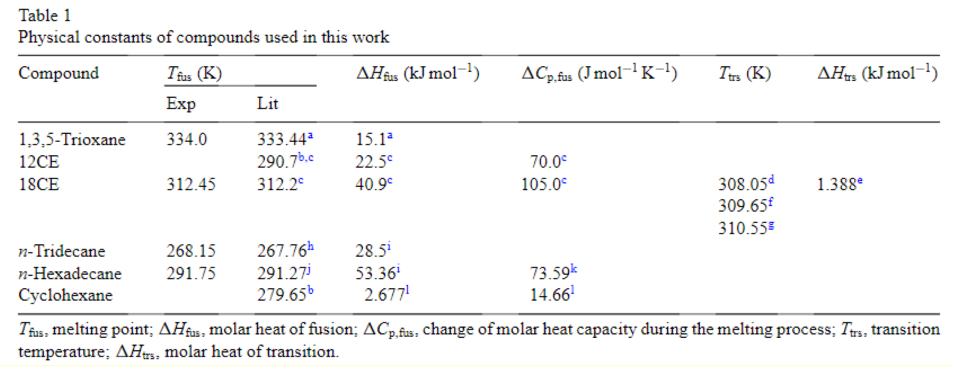


Table 1
Physical constants of compounds used in this work

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$ (kJ mol$^{-1}$) | $\Delta C_{p,fus}$ (J mol$^{-1}$ K$^{-1}$) | $T_{trs}$ (K) | $\Delta H_{trs}$ (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|
| | Exp | Lit | | | | |
| 1,3,5-Trioxane | 334.0 | 333.44[a] | 15.1[a] | | | |
| 12CE | | 290.7[b,c] | 22.5[c] | 70.0[c] | | |
| 18CE | 312.45 | 312.2[c] | 40.9[c] | 105.0[c] | 308.05[d]<br>309.65[f]<br>310.55[g] | 1.388[e] |
| *n*-Tridecane | 268.15 | 267.76[h] | 28.5[i] | | | |
| *n*-Hexadecane | 291.75 | 291.27[j] | 53.36[i] | 73.59[k] | | |
| Cyclohexane | | 279.65[b] | 2.677[l] | 14.66[l] | | |

$T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion; $\Delta C_{p,fus}$, change of molar heat capacity during the melting process; $T_{trs}$, transition temperature; $\Delta H_{trs}$, molar heat of transition.

1-tetradecanol + dimethyl carbonate
J. A. Gonzalez, M. Szurgocinska, U. Domanska, Thermodynamics of mixtures containing organic carbonatesPart XIII. Solid–liquid equilibria of long-chain 1-alkanol+dimethyl or diethyl carbonate systems: DISQUAC and ERASanalysis of the hydroxyl/carbonate interactions, Fluid Phase Equilibria 200 (2002) 349–374

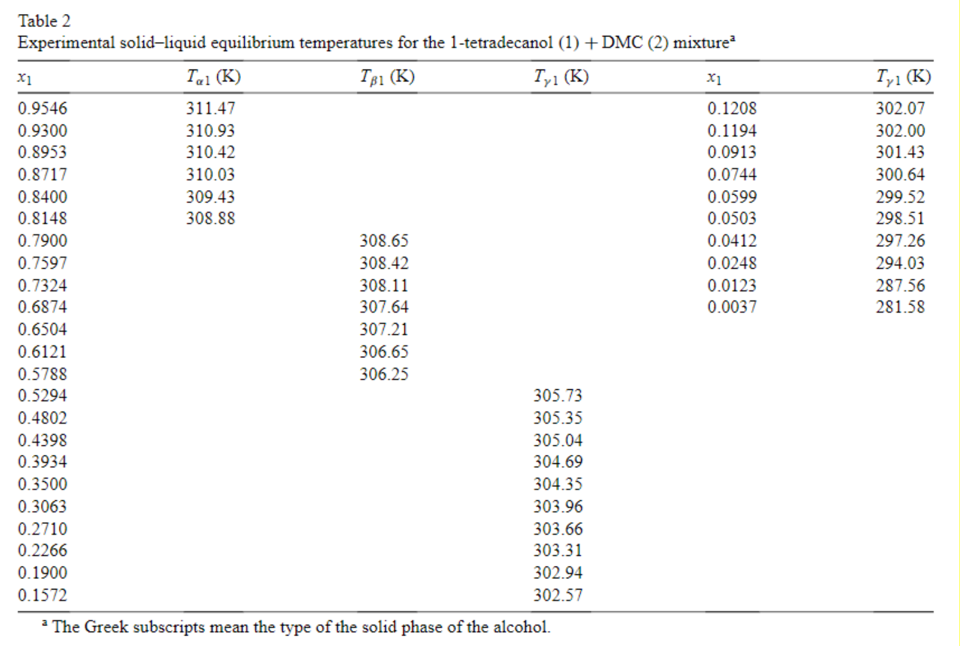


Table 2
Experimental solid–liquid equilibrium temperatures for the 1-tetradecanol (1) + DMC (2) mixture[a]

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{\beta 1}$ (K) | $T_{\gamma 1}$ (K) | $x_1$ | $T_{\gamma 1}$ (K) |
|---|---|---|---|---|---|
| 0.9546 | 311.47 | | | 0.1208 | 302.07 |
| 0.9300 | 310.93 | | | 0.1194 | 302.00 |
| 0.8953 | 310.42 | | | 0.0913 | 301.43 |
| 0.8717 | 310.03 | | | 0.0744 | 300.64 |
| 0.8400 | 309.43 | | | 0.0599 | 299.52 |
| 0.8148 | 308.88 | | | 0.0503 | 298.51 |
| 0.7900 | | 308.65 | | 0.0412 | 297.26 |
| 0.7597 | | 308.42 | | 0.0248 | 294.03 |
| 0.7324 | | 308.11 | | 0.0123 | 287.56 |
| 0.6874 | | 307.64 | | 0.0037 | 281.58 |
| 0.6504 | | 307.21 | | | |
| 0.6121 | | 306.65 | | | |
| 0.5788 | | 306.25 | | | |
| 0.5294 | | | 305.73 | | |
| 0.4802 | | | 305.35 | | |
| 0.4398 | | | 305.04 | | |
| 0.3934 | | | 304.69 | | |
| 0.3500 | | | 304.35 | | |
| 0.3063 | | | 303.96 | | |
| 0.2710 | | | 303.66 | | |
| 0.2266 | | | 303.31 | | |
| 0.1900 | | | 302.94 | | |
| 0.1572 | | | 302.57 | | |

[a] The Greek subscripts mean the type of the solid phase of the alcohol.

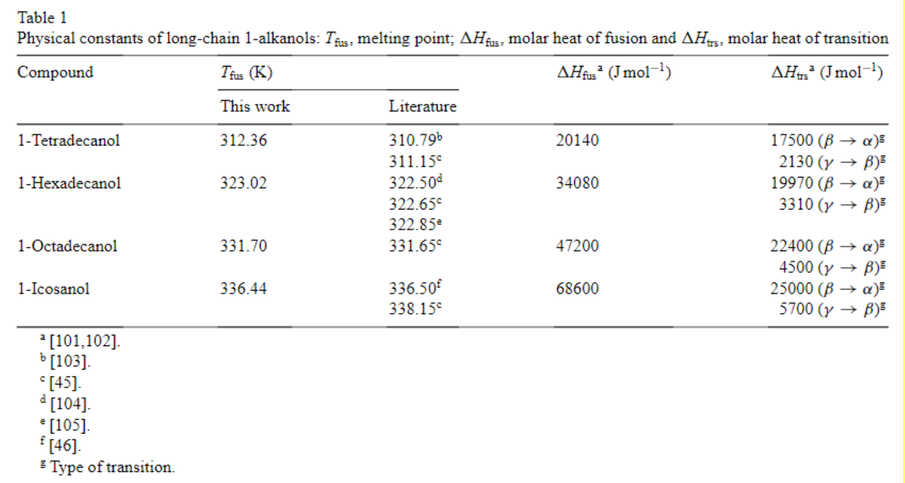


Table 1
Physical constants of long-chain 1-alkanols: $T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion and $\Delta H_{trs}$, molar heat of transition

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$[a] (J mol$^{-1}$) | $\Delta H_{trs}$[a] (J mol$^{-1}$) |
|---|---|---|---|---|
| | This work | Literature | | |
| 1-Tetradecanol | 312.36 | 310.79[b]<br>311.15[c] | 20140 | 17500 ($\beta \rightarrow \alpha$)[g]<br>2130 ($\gamma \rightarrow \beta$)[g] |
| 1-Hexadecanol | 323.02 | 322.50[d]<br>322.65[c]<br>322.85[e] | 34080 | 19970 ($\beta \rightarrow \alpha$)[g]<br>3310 ($\gamma \rightarrow \beta$)[g] |
| 1-Octadecanol | 331.70 | 331.65[c] | 47200 | 22400 ($\beta \rightarrow \alpha$)[g]<br>4500 ($\gamma \rightarrow \beta$)[g] |
| 1-Icosanol | 336.44 | 336.50[f]<br>338.15[c] | 68600 | 25000 ($\beta \rightarrow \alpha$)[g]<br>5700 ($\gamma \rightarrow \beta$)[g] |

[a] [101,102].
[b] [103].
[c] [45].
[d] [104].
[e] [105].
[f] [46].
[g] Type of transition.

1-hexadecanol + dimethyl carbonate

J. A. Gonzalez, M. Szurgocinska, U. Domanska, Thermodynamics of mixtures containing organic carbonatesPart XIII. Solid–liquid equilibria of long-chain 1-alkanol+dimethyl or diethyl carbonate systems: DISQUAC and ERASanalysis of the hydroxyl/carbonate interactions, Fluid Phase Equilibria 200 (2002) 349–374

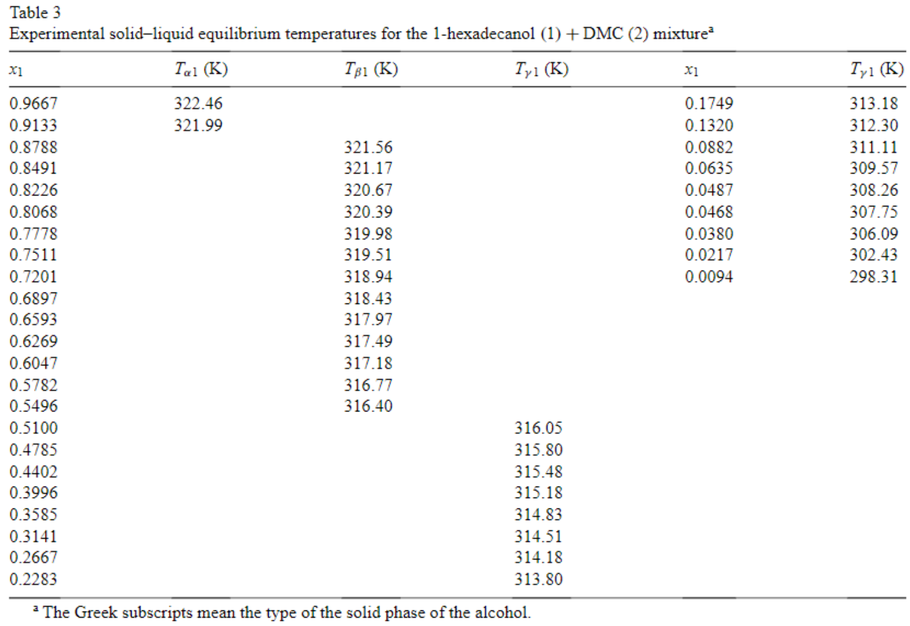


Table 3

Experimental solid–liquid equilibrium temperatures for the 1-hexadecanol (1) + DMC (2) mixture[a]

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{\beta 1}$ (K) | $T_{\gamma 1}$ (K) | $x_1$ | $T_{\gamma 1}$ (K) |
|---|---|---|---|---|---|
| 0.9667 | 322.46 | | | 0.1749 | 313.18 |
| 0.9133 | 321.99 | | | 0.1320 | 312.30 |
| 0.8788 | | 321.56 | | 0.0882 | 311.11 |
| 0.8491 | | 321.17 | | 0.0635 | 309.57 |
| 0.8226 | | 320.67 | | 0.0487 | 308.26 |
| 0.8068 | | 320.39 | | 0.0468 | 307.75 |
| 0.7778 | | 319.98 | | 0.0380 | 306.09 |
| 0.7511 | | 319.51 | | 0.0217 | 302.43 |
| 0.7201 | | 318.94 | | 0.0094 | 298.31 |
| 0.6897 | | 318.43 | | | |
| 0.6593 | | 317.97 | | | |
| 0.6269 | | 317.49 | | | |
| 0.6047 | | 317.18 | | | |
| 0.5782 | | 316.77 | | | |
| 0.5496 | | 316.40 | | | |
| 0.5100 | | | 316.05 | | |
| 0.4785 | | | 315.80 | | |
| 0.4402 | | | 315.48 | | |
| 0.3996 | | | 315.18 | | |
| 0.3585 | | | 314.83 | | |
| 0.3141 | | | 314.51 | | |
| 0.2667 | | | 314.18 | | |
| 0.2283 | | | 313.80 | | |

[a] The Greek subscripts mean the type of the solid phase of the alcohol.

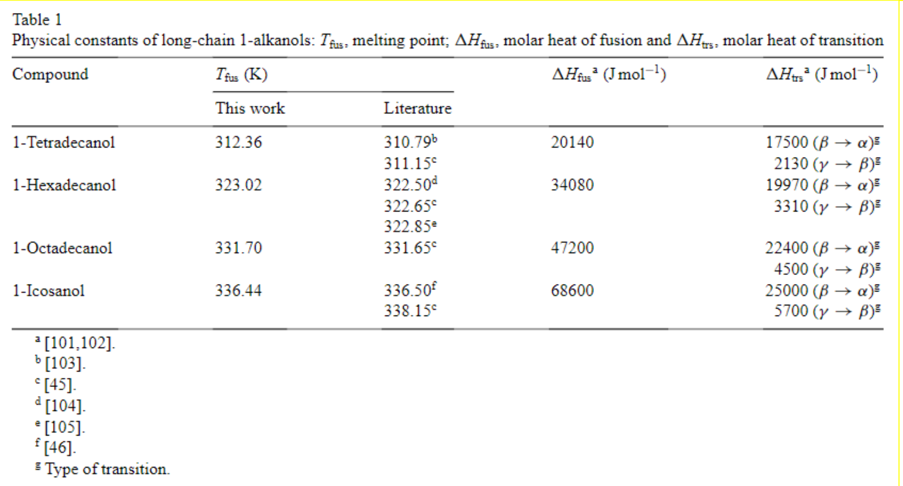


Table 1

Physical constants of long-chain 1-alkanols: $T_{\text{fus}}$, melting point; $\Delta H_{\text{fus}}$, molar heat of fusion and $\Delta H_{\text{trs}}$, molar heat of transition

| Compound | $T_{\text{fus}}$ (K) | | $\Delta H_{\text{fus}}$[a] (J mol$^{-1}$) | $\Delta H_{\text{trs}}$[a] (J mol$^{-1}$) |
|---|---|---|---|---|
| | This work | Literature | | |
| 1-Tetradecanol | 312.36 | 310.79[b]<br>311.15[c] | 20140 | 17500 ($\beta \rightarrow \alpha$)[g]<br>2130 ($\gamma \rightarrow \beta$)[g] |
| 1-Hexadecanol | 323.02 | 322.50[d]<br>322.65[c]<br>322.85[e] | 34080 | 19970 ($\beta \rightarrow \alpha$)[g]<br>3310 ($\gamma \rightarrow \beta$)[g] |
| 1-Octadecanol | 331.70 | 331.65[c] | 47200 | 22400 ($\beta \rightarrow \alpha$)[g]<br>4500 ($\gamma \rightarrow \beta$)[g] |
| 1-Icosanol | 336.44 | 336.50[f]<br>338.15[c] | 68600 | 25000 ($\beta \rightarrow \alpha$)[g]<br>5700 ($\gamma \rightarrow \beta$)[g] |

[a] [101,102].

[b] [103].

[c] [45].

[d] [104].

[e] [105].

[f] [46].

[g] Type of transition.

1-octadecanol + dimethyl carbonate

J. A. Gonzalez, M. Szurgocinska, U. Domanska, Thermodynamics of mixtures containing organic carbonatesPart XIII. Solid–liquid equilibria of long-chain 1-alkanol+dimethyl or diethyl carbonate systems: DISQUAC and ERASanalysis of the hydroxyl/carbonate interactions, Fluid Phase Equilibria 200 (2002) 349–374

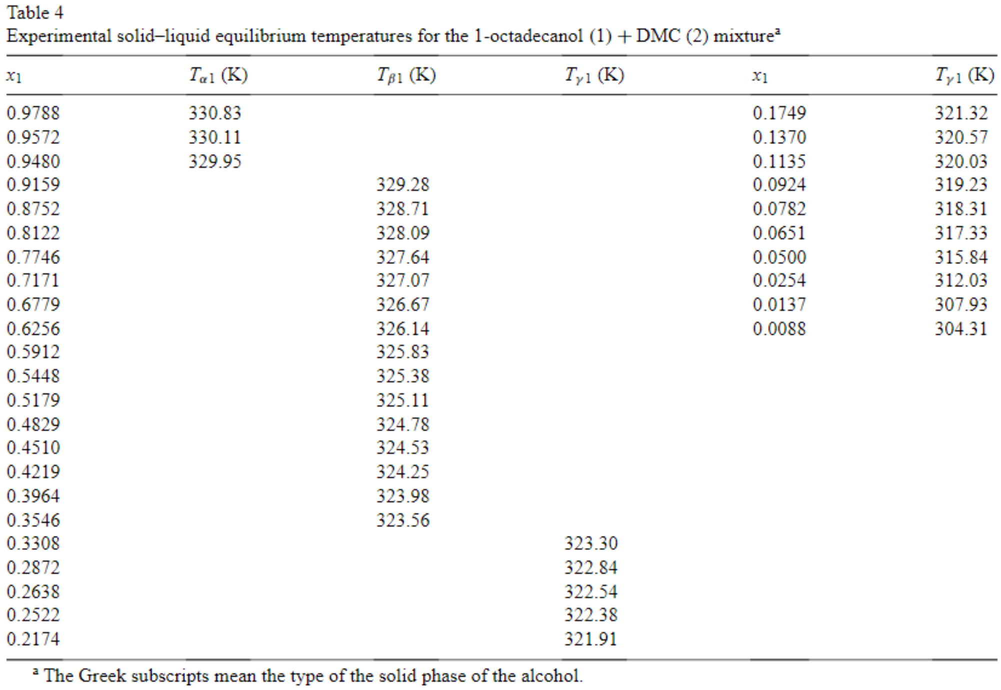


Table 4
Experimental solid–liquid equilibrium temperatures for the 1-octadecanol (1) + DMC (2) mixture[a]

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{\beta 1}$ (K) | $T_{\gamma 1}$ (K) | $x_1$ | $T_{\gamma 1}$ (K) |
|---|---|---|---|---|---|
| 0.9788 | 330.83 | | | 0.1749 | 321.32 |
| 0.9572 | 330.11 | | | 0.1370 | 320.57 |
| 0.9480 | 329.95 | | | 0.1135 | 320.03 |
| 0.9159 | | 329.28 | | 0.0924 | 319.23 |
| 0.8752 | | 328.71 | | 0.0782 | 318.31 |
| 0.8122 | | 328.09 | | 0.0651 | 317.33 |
| 0.7746 | | 327.64 | | 0.0500 | 315.84 |
| 0.7171 | | 327.07 | | 0.0254 | 312.03 |
| 0.6779 | | 326.67 | | 0.0137 | 307.93 |
| 0.6256 | | 326.14 | | 0.0088 | 304.31 |
| 0.5912 | | 325.83 | | | |
| 0.5448 | | 325.38 | | | |
| 0.5179 | | 325.11 | | | |
| 0.4829 | | 324.78 | | | |
| 0.4510 | | 324.53 | | | |
| 0.4219 | | 324.25 | | | |
| 0.3964 | | 323.98 | | | |
| 0.3546 | | 323.56 | | | |
| 0.3308 | | | 323.30 | | |
| 0.2872 | | | 322.84 | | |
| 0.2638 | | | 322.54 | | |
| 0.2522 | | | 322.38 | | |
| 0.2174 | | | 321.91 | | |

[a] The Greek subscripts mean the type of the solid phase of the alcohol.

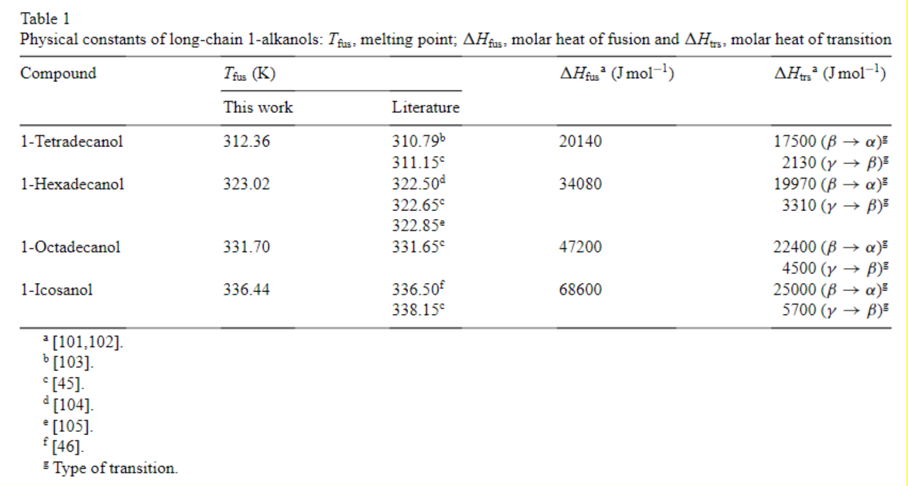


Table 1
Physical constants of long-chain 1-alkanols: $T_{\text{fus}}$, melting point; $\Delta H_{\text{fus}}$, molar heat of fusion and $\Delta H_{\text{trs}}$, molar heat of transition

| Compound | $T_{\text{fus}}$ (K) | | $\Delta H_{\text{fus}}$[a] (J mol$^{-1}$) | $\Delta H_{\text{trs}}$[a] (J mol$^{-1}$) |
|---|---|---|---|---|
| | This work | Literature | | |
| 1-Tetradecanol | 312.36 | 310.79[b]<br>311.15[c] | 20140 | 17500 ($\beta \rightarrow \alpha$)[g]<br>2130 ($\gamma \rightarrow \beta$)[g] |
| 1-Hexadecanol | 323.02 | 322.50[d]<br>322.65[c]<br>322.85[e] | 34080 | 19970 ($\beta \rightarrow \alpha$)[g]<br>3310 ($\gamma \rightarrow \beta$)[g] |
| 1-Octadecanol | 331.70 | 331.65[c] | 47200 | 22400 ($\beta \rightarrow \alpha$)[g]<br>4500 ($\gamma \rightarrow \beta$)[g] |
| 1-Icosanol | 336.44 | 336.50[f]<br>338.15[c] | 68600 | 25000 ($\beta \rightarrow \alpha$)[g]<br>5700 ($\gamma \rightarrow \beta$)[g] |

[a] [101,102].
[b] [103].
[c] [45].
[d] [104].
[e] [105].
[f] [46].
[g] Type of transition.

1-icosanol + dimethyl carbonate
J. A. Gonzalez, M. Szurgocinska, U. Domanska, Thermodynamics of mixtures containing organic carbonatesPart XIII. Solid–liquid equilibria of long-chain 1-alkanol+dimethyl or diethyl carbonate systems: DISQUAC and ERASanalysis of the hydroxyl/carbonate interactions, Fluid Phase Equilibria 200 (2002) 349–374

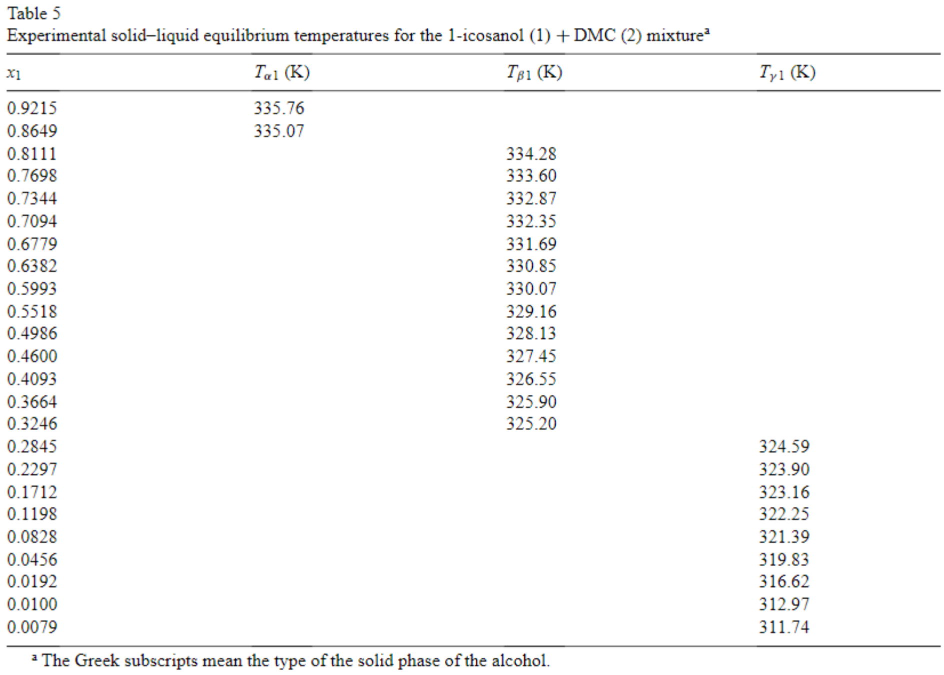


Table 5
Experimental solid–liquid equilibrium temperatures for the 1-icosanol (1) + DMC (2) mixture[a]

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{\beta 1}$ (K) | $T_{\gamma 1}$ (K) |
|---|---|---|---|
| 0.9215 | 335.76 | | |
| 0.8649 | 335.07 | | |
| 0.8111 | | 334.28 | |
| 0.7698 | | 333.60 | |
| 0.7344 | | 332.87 | |
| 0.7094 | | 332.35 | |
| 0.6779 | | 331.69 | |
| 0.6382 | | 330.85 | |
| 0.5993 | | 330.07 | |
| 0.5518 | | 329.16 | |
| 0.4986 | | 328.13 | |
| 0.4600 | | 327.45 | |
| 0.4093 | | 326.55 | |
| 0.3664 | | 325.90 | |
| 0.3246 | | 325.20 | |
| 0.2845 | | | 324.59 |
| 0.2297 | | | 323.90 |
| 0.1712 | | | 323.16 |
| 0.1198 | | | 322.25 |
| 0.0828 | | | 321.39 |
| 0.0456 | | | 319.83 |
| 0.0192 | | | 316.62 |
| 0.0100 | | | 312.97 |
| 0.0079 | | | 311.74 |

[a] The Greek subscripts mean the type of the solid phase of the alcohol.

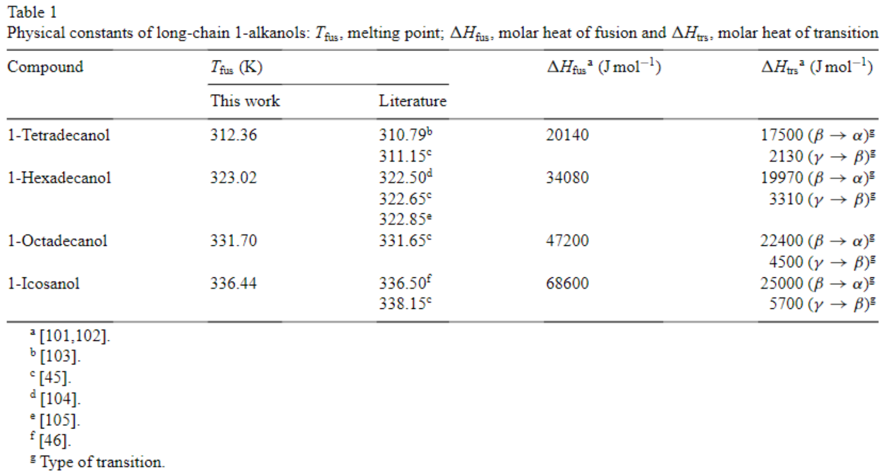


Table 1
Physical constants of long-chain 1-alkanols: $T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion and $\Delta H_{trs}$, molar heat of transition

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$[a] (J mol$^{-1}$) | $\Delta H_{trs}$[a] (J mol$^{-1}$) |
|---|---|---|---|---|
| | This work | Literature | | |
| 1-Tetradecanol | 312.36 | 310.79[b]<br>311.15[c] | 20140 | 17500 ($\beta \rightarrow \alpha$)[g]<br>2130 ($\gamma \rightarrow \beta$)[g] |
| 1-Hexadecanol | 323.02 | 322.50[d]<br>322.65[c]<br>322.85[e] | 34080 | 19970 ($\beta \rightarrow \alpha$)[g]<br>3310 ($\gamma \rightarrow \beta$)[g] |
| 1-Octadecanol | 331.70 | 331.65[c] | 47200 | 22400 ($\beta \rightarrow \alpha$)[g]<br>4500 ($\gamma \rightarrow \beta$)[g] |
| 1-Icosanol | 336.44 | 336.50[f]<br>338.15[c] | 68600 | 25000 ($\beta \rightarrow \alpha$)[g]<br>5700 ($\gamma \rightarrow \beta$)[g] |

[a] [101,102].
[b] [103].
[c] [45].
[d] [104].
[e] [105].
[f] [46].
[g] Type of transition.

1-tetradecanol + diethyl carbonate

J. A. Gonzalez, M. Szurgocinska, U. Domanska, Thermodynamics of mixtures containing organic carbonatesPart XIII. Solid–liquid equilibria of long-chain 1-alkanol+dimethyl or diethyl carbonate systems: DISQUAC and ERASanalysis of the hydroxyl/carbonate interactions, Fluid Phase Equilibria 200 (2002) 349–374

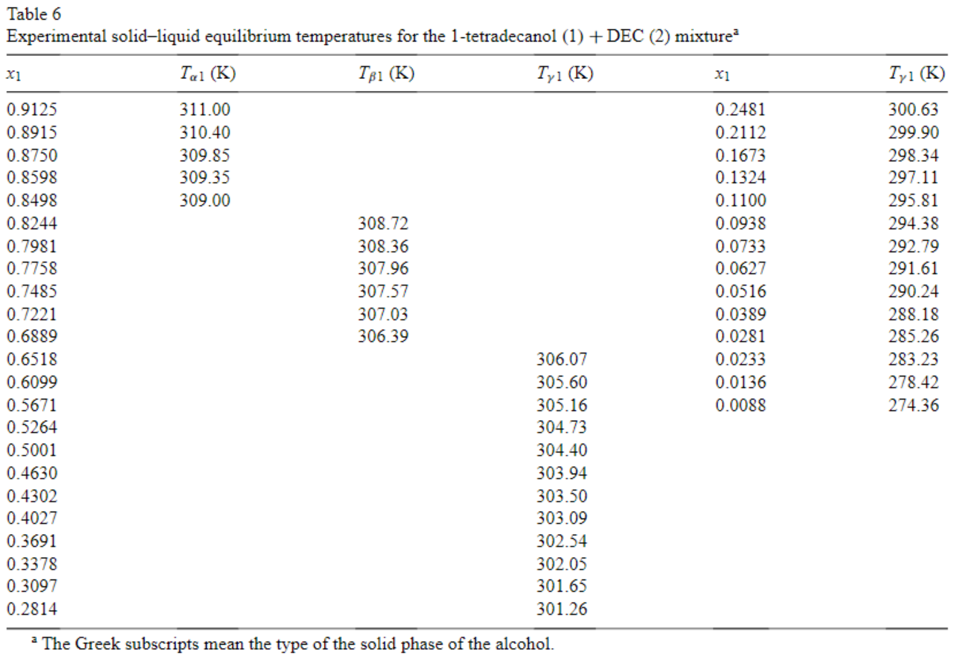


Table 6
Experimental solid–liquid equilibrium temperatures for the 1-tetradecanol (1) + DEC (2) mixture[a]

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{\beta 1}$ (K) | $T_{\gamma 1}$ (K) | $x_1$ | $T_{\gamma 1}$ (K) |
|---|---|---|---|---|---|
| 0.9125 | 311.00 | | | 0.2481 | 300.63 |
| 0.8915 | 310.40 | | | 0.2112 | 299.90 |
| 0.8750 | 309.85 | | | 0.1673 | 298.34 |
| 0.8598 | 309.35 | | | 0.1324 | 297.11 |
| 0.8498 | 309.00 | | | 0.1100 | 295.81 |
| 0.8244 | | 308.72 | | 0.0938 | 294.38 |
| 0.7981 | | 308.36 | | 0.0733 | 292.79 |
| 0.7758 | | 307.96 | | 0.0627 | 291.61 |
| 0.7485 | | 307.57 | | 0.0516 | 290.24 |
| 0.7221 | | 307.03 | | 0.0389 | 288.18 |
| 0.6889 | | 306.39 | | 0.0281 | 285.26 |
| 0.6518 | | | 306.07 | 0.0233 | 283.23 |
| 0.6099 | | | 305.60 | 0.0136 | 278.42 |
| 0.5671 | | | 305.16 | 0.0088 | 274.36 |
| 0.5264 | | | 304.73 | | |
| 0.5001 | | | 304.40 | | |
| 0.4630 | | | 303.94 | | |
| 0.4302 | | | 303.50 | | |
| 0.4027 | | | 303.09 | | |
| 0.3691 | | | 302.54 | | |
| 0.3378 | | | 302.05 | | |
| 0.3097 | | | 301.65 | | |
| 0.2814 | | | 301.26 | | |

[a] The Greek subscripts mean the type of the solid phase of the alcohol.

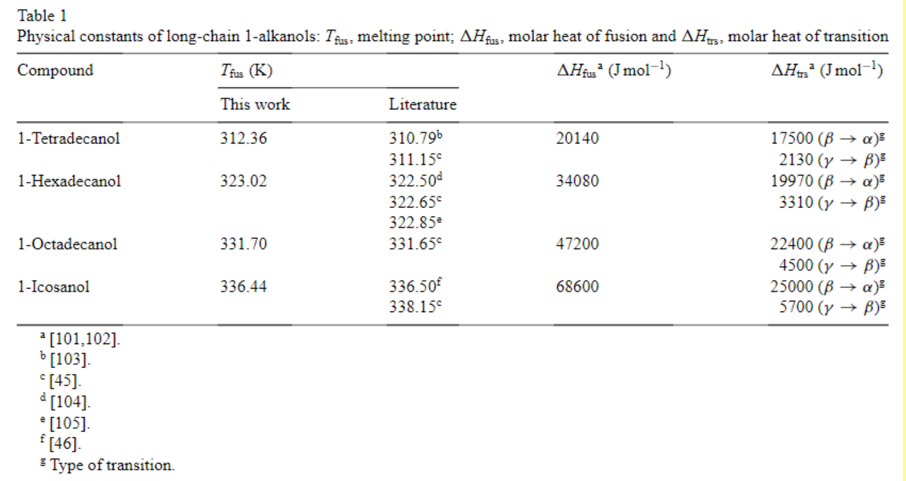


Table 1
Physical constants of long-chain 1-alkanols: $T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion and $\Delta H_{trs}$, molar heat of transition

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$[a] (J mol$^{-1}$) | $\Delta H_{trs}$[a] (J mol$^{-1}$) |
|---|---|---|---|---|
| | This work | Literature | | |
| 1-Tetradecanol | 312.36 | 310.79[b]<br>311.15[c] | 20140 | 17500 ($\beta \rightarrow \alpha$)[g]<br>2130 ($\gamma \rightarrow \beta$)[g] |
| 1-Hexadecanol | 323.02 | 322.50[d]<br>322.65[c]<br>322.85[e] | 34080 | 19970 ($\beta \rightarrow \alpha$)[g]<br>3310 ($\gamma \rightarrow \beta$)[g] |
| 1-Octadecanol | 331.70 | 331.65[c] | 47200 | 22400 ($\beta \rightarrow \alpha$)[g]<br>4500 ($\gamma \rightarrow \beta$)[g] |
| 1-Icosanol | 336.44 | 336.50[f]<br>338.15[c] | 68600 | 25000 ($\beta \rightarrow \alpha$)[g]<br>5700 ($\gamma \rightarrow \beta$)[g] |

[a] [101,102].
[b] [103].
[c] [45].
[d] [104].
[e] [105].
[f] [46].
[g] Type of transition.

1-hexadecanol + diethyl carbonate

J. A. Gonzalez, M. Szurgocinska, U. Domanska, Thermodynamics of mixtures containing organic carbonatesPart XIII. Solid–liquid equilibria of long-chain 1-alkanol+dimethyl or diethyl carbonate systems: DISQUAC and ERASanalysis of the hydroxyl/carbonate interactions, Fluid Phase Equilibria 200 (2002) 349–374

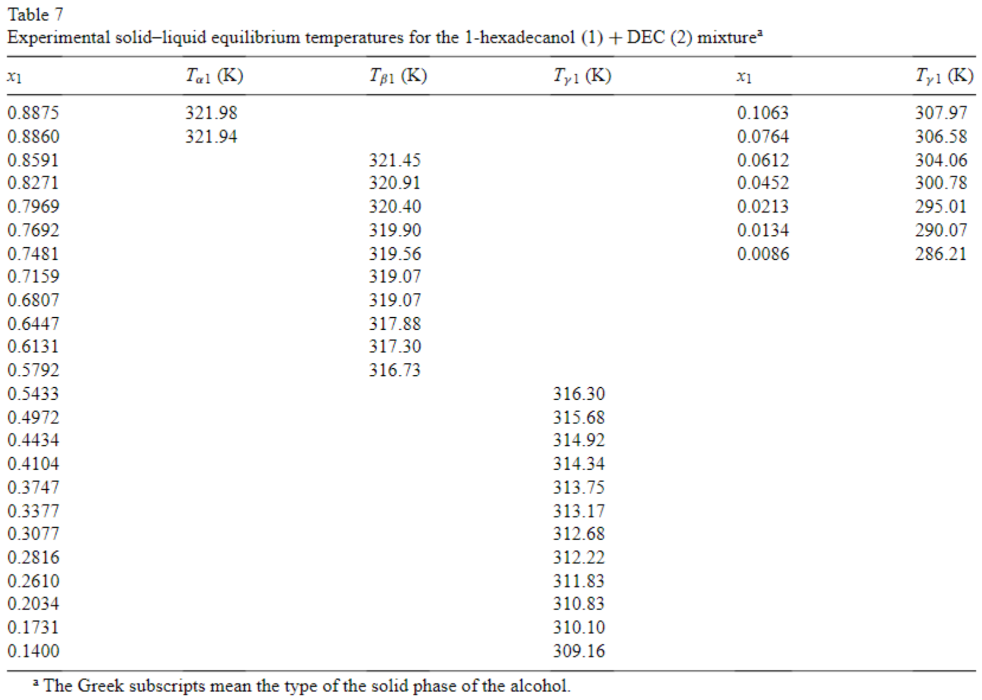


Table 7
Experimental solid–liquid equilibrium temperatures for the 1-hexadecanol (1) + DEC (2) mixture[a]

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{\beta 1}$ (K) | $T_{\gamma 1}$ (K) | $x_1$ | $T_{\gamma 1}$ (K) |
|---|---|---|---|---|---|
| 0.8875 | 321.98 | | | 0.1063 | 307.97 |
| 0.8860 | 321.94 | | | 0.0764 | 306.58 |
| 0.8591 | | 321.45 | | 0.0612 | 304.06 |
| 0.8271 | | 320.91 | | 0.0452 | 300.78 |
| 0.7969 | | 320.40 | | 0.0213 | 295.01 |
| 0.7692 | | 319.90 | | 0.0134 | 290.07 |
| 0.7481 | | 319.56 | | 0.0086 | 286.21 |
| 0.7159 | | 319.07 | | | |
| 0.6807 | | 319.07 | | | |
| 0.6447 | | 317.88 | | | |
| 0.6131 | | 317.30 | | | |
| 0.5792 | | 316.73 | | | |
| 0.5433 | | | 316.30 | | |
| 0.4972 | | | 315.68 | | |
| 0.4434 | | | 314.92 | | |
| 0.4104 | | | 314.34 | | |
| 0.3747 | | | 313.75 | | |
| 0.3377 | | | 313.17 | | |
| 0.3077 | | | 312.68 | | |
| 0.2816 | | | 312.22 | | |
| 0.2610 | | | 311.83 | | |
| 0.2034 | | | 310.83 | | |
| 0.1731 | | | 310.10 | | |
| 0.1400 | | | 309.16 | | |

[a] The Greek subscripts mean the type of the solid phase of the alcohol.

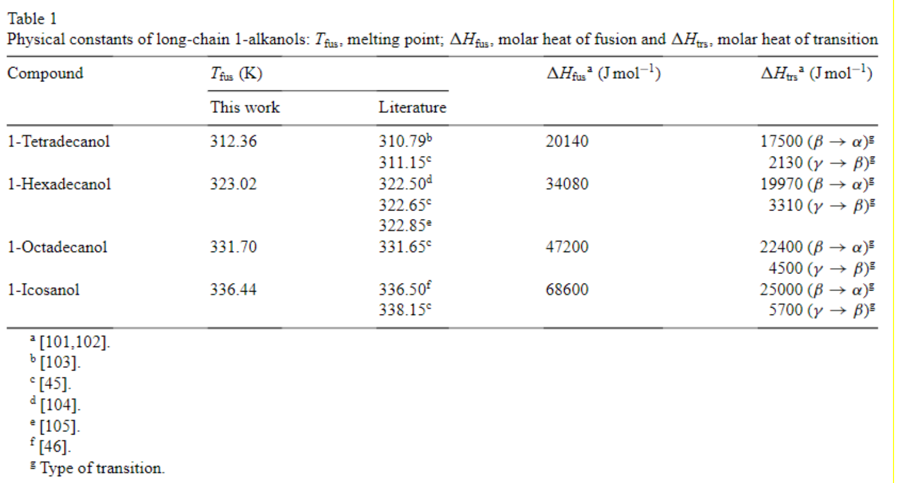


Table 1
Physical constants of long-chain 1-alkanols: $T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion and $\Delta H_{trs}$, molar heat of transition

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$[a] (J mol$^{-1}$) | $\Delta H_{trs}$[a] (J mol$^{-1}$) |
|---|---|---|---|---|
| | This work | Literature | | |
| 1-Tetradecanol | 312.36 | 310.79[b]<br>311.15[c] | 20140 | 17500 ($\beta \rightarrow \alpha$)[g]<br>2130 ($\gamma \rightarrow \beta$)[g] |
| 1-Hexadecanol | 323.02 | 322.50[d]<br>322.65[c]<br>322.85[e] | 34080 | 19970 ($\beta \rightarrow \alpha$)[g]<br>3310 ($\gamma \rightarrow \beta$)[g] |
| 1-Octadecanol | 331.70 | 331.65[c] | 47200 | 22400 ($\beta \rightarrow \alpha$)[g]<br>4500 ($\gamma \rightarrow \beta$)[g] |
| 1-Icosanol | 336.44 | 336.50[f]<br>338.15[c] | 68600 | 25000 ($\beta \rightarrow \alpha$)[g]<br>5700 ($\gamma \rightarrow \beta$)[g] |

[a] [101,102].
[b] [103].
[c] [45].
[d] [104].
[e] [105].
[f] [46].
[g] Type of transition.

1-octadecanol + diethyl carbonate

J. A. Gonzalez, M. Szurgocinska, U. Domanska, Thermodynamics of mixtures containing organic carbonatesPart XIII. Solid–liquid equilibria of long-chain 1-alkanol+dimethyl or diethyl carbonate systems: DISQUAC and ERASanalysis of the hydroxyl/carbonate interactions, Fluid Phase Equilibria 200 (2002) 349–374

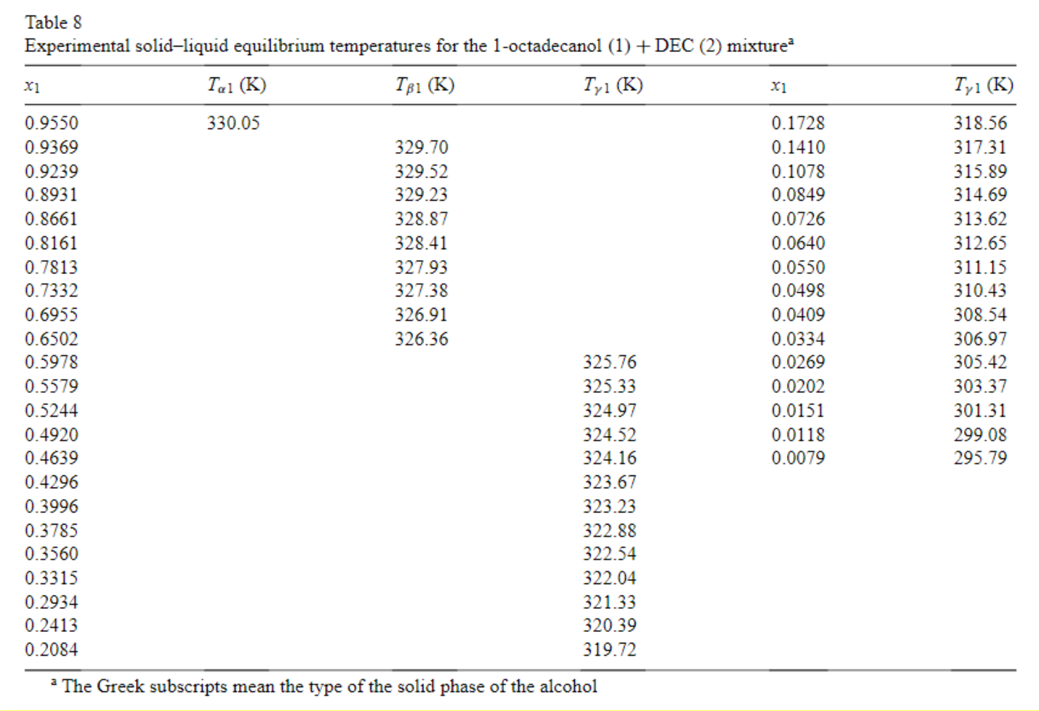


Table 8

Experimental solid–liquid equilibrium temperatures for the 1-octadecanol (1) + DEC (2) mixture[a]

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{\beta 1}$ (K) | $T_{\gamma 1}$ (K) | $x_1$ | $T_{\gamma 1}$ (K) |
|---|---|---|---|---|---|
| 0.9550 | 330.05 | | | 0.1728 | 318.56 |
| 0.9369 | | 329.70 | | 0.1410 | 317.31 |
| 0.9239 | | 329.52 | | 0.1078 | 315.89 |
| 0.8931 | | 329.23 | | 0.0849 | 314.69 |
| 0.8661 | | 328.87 | | 0.0726 | 313.62 |
| 0.8161 | | 328.41 | | 0.0640 | 312.65 |
| 0.7813 | | 327.93 | | 0.0550 | 311.15 |
| 0.7332 | | 327.38 | | 0.0498 | 310.43 |
| 0.6955 | | 326.91 | | 0.0409 | 308.54 |
| 0.6502 | | 326.36 | | 0.0334 | 306.97 |
| 0.5978 | | | 325.76 | 0.0269 | 305.42 |
| 0.5579 | | | 325.33 | 0.0202 | 303.37 |
| 0.5244 | | | 324.97 | 0.0151 | 301.31 |
| 0.4920 | | | 324.52 | 0.0118 | 299.08 |
| 0.4639 | | | 324.16 | 0.0079 | 295.79 |
| 0.4296 | | | 323.67 | | |
| 0.3996 | | | 323.23 | | |
| 0.3785 | | | 322.88 | | |
| 0.3560 | | | 322.54 | | |
| 0.3315 | | | 322.04 | | |
| 0.2934 | | | 321.33 | | |
| 0.2413 | | | 320.39 | | |
| 0.2084 | | | 319.72 | | |

[a] The Greek subscripts mean the type of the solid phase of the alcohol

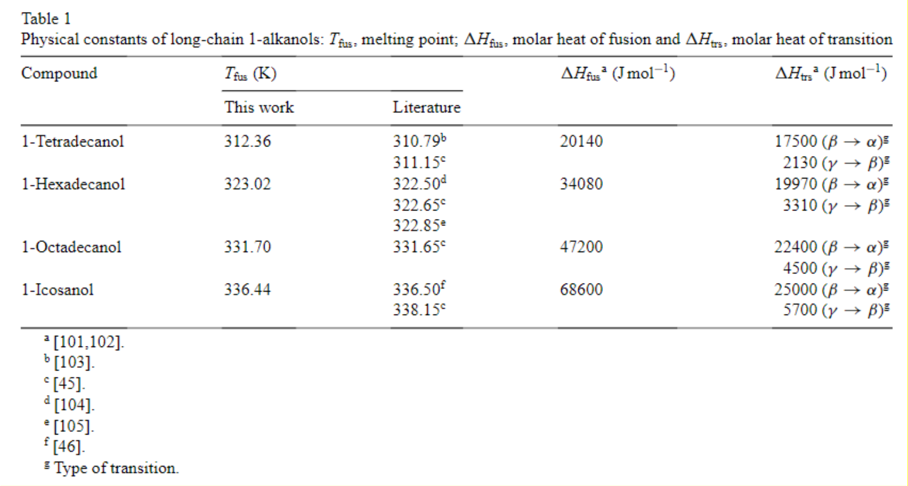


Table 1

Physical constants of long-chain 1-alkanols: $T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion and $\Delta H_{trs}$, molar heat of transition

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$[a] (J mol$^{-1}$) | $\Delta H_{trs}$[a] (J mol$^{-1}$) |
|---|---|---|---|---|
| | This work | Literature | | |
| 1-Tetradecanol | 312.36 | 310.79[b]<br>311.15[c] | 20140 | 17500 ($\beta \rightarrow \alpha$)[g]<br>2130 ($\gamma \rightarrow \beta$)[g] |
| 1-Hexadecanol | 323.02 | 322.50[d]<br>322.65[c]<br>322.85[e] | 34080 | 19970 ($\beta \rightarrow \alpha$)[g]<br>3310 ($\gamma \rightarrow \beta$)[g] |
| 1-Octadecanol | 331.70 | 331.65[c] | 47200 | 22400 ($\beta \rightarrow \alpha$)[g]<br>4500 ($\gamma \rightarrow \beta$)[g] |
| 1-Icosanol | 336.44 | 336.50[f]<br>338.15[c] | 68600 | 25000 ($\beta \rightarrow \alpha$)[g]<br>5700 ($\gamma \rightarrow \beta$)[g] |

[a] [101,102].
[b] [103].
[c] [45].
[d] [104].
[e] [105].
[f] [46].
[g] Type of transition.

1-icosanol + diethyl carbonate
J. A. Gonzalez, M. Szurgocinska, U. Domanska, Thermodynamics of mixtures containing organic carbonatesPart XIII. Solid–liquid equilibria of long-chain 1-alkanol+dimethyl or diethyl carbonate systems: DISQUAC and ERASanalysis of the hydroxyl/carbonate interactions, Fluid Phase Equilibria 200 (2002) 349–374

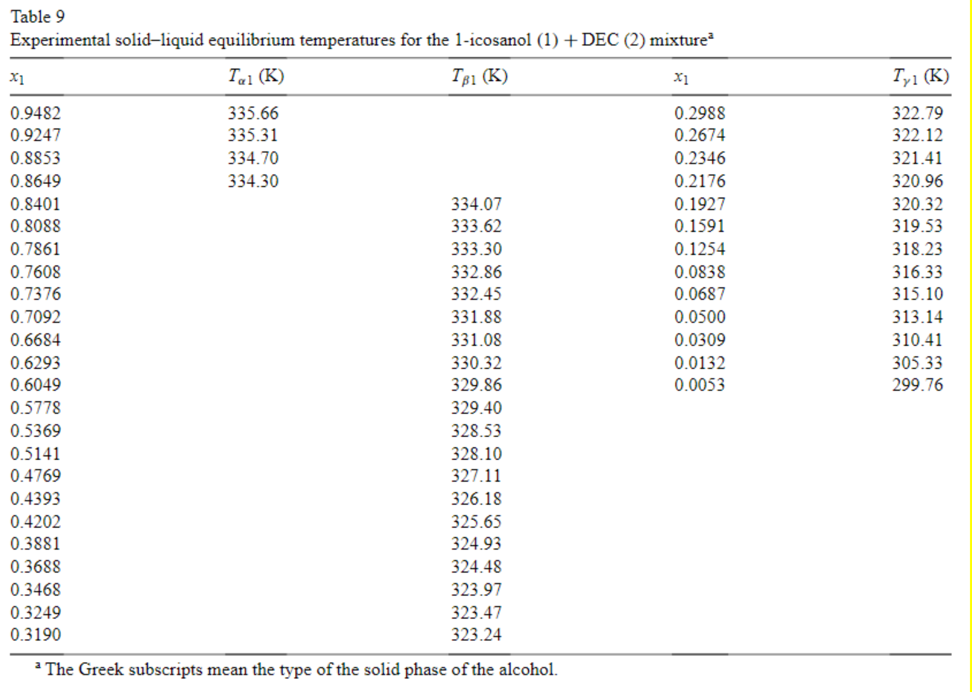


Table 9
Experimental solid–liquid equilibrium temperatures for the 1-icosanol (1) + DEC (2) mixture[a]

| $x_1$ | $T_{\alpha 1}$ (K) | $T_{\beta 1}$ (K) | $x_1$ | $T_{\gamma 1}$ (K) |
|---|---|---|---|---|
| 0.9482 | 335.66 | | 0.2988 | 322.79 |
| 0.9247 | 335.31 | | 0.2674 | 322.12 |
| 0.8853 | 334.70 | | 0.2346 | 321.41 |
| 0.8649 | 334.30 | | 0.2176 | 320.96 |
| 0.8401 | | 334.07 | 0.1927 | 320.32 |
| 0.8088 | | 333.62 | 0.1591 | 319.53 |
| 0.7861 | | 333.30 | 0.1254 | 318.23 |
| 0.7608 | | 332.86 | 0.0838 | 316.33 |
| 0.7376 | | 332.45 | 0.0687 | 315.10 |
| 0.7092 | | 331.88 | 0.0500 | 313.14 |
| 0.6684 | | 331.08 | 0.0309 | 310.41 |
| 0.6293 | | 330.32 | 0.0132 | 305.33 |
| 0.6049 | | 329.86 | 0.0053 | 299.76 |
| 0.5778 | | 329.40 | | |
| 0.5369 | | 328.53 | | |
| 0.5141 | | 328.10 | | |
| 0.4769 | | 327.11 | | |
| 0.4393 | | 326.18 | | |
| 0.4202 | | 325.65 | | |
| 0.3881 | | 324.93 | | |
| 0.3688 | | 324.48 | | |
| 0.3468 | | 323.97 | | |
| 0.3249 | | 323.47 | | |
| 0.3190 | | 323.24 | | |

[a] The Greek subscripts mean the type of the solid phase of the alcohol.

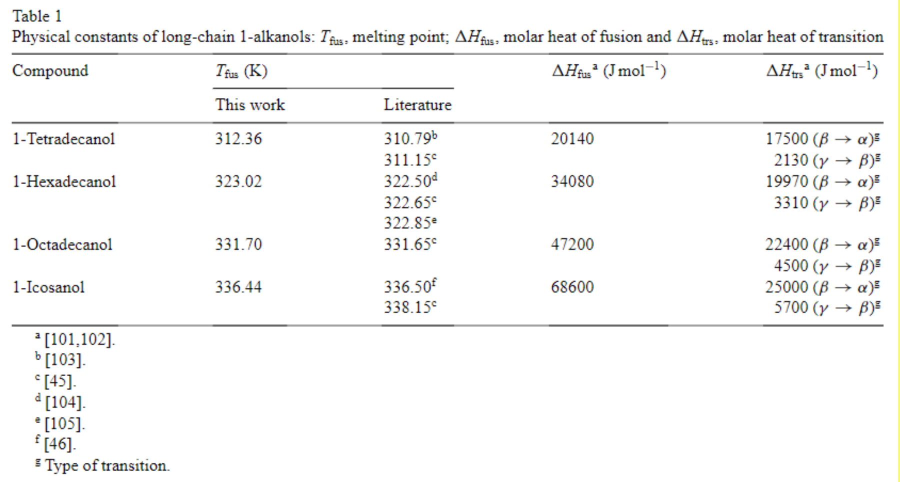


Table 1
Physical constants of long-chain 1-alkanols: $T_{fus}$, melting point; $\Delta H_{fus}$, molar heat of fusion and $\Delta H_{trs}$, molar heat of transition

| Compound | $T_{fus}$ (K) | | $\Delta H_{fus}$[a] (J mol$^{-1}$) | $\Delta H_{trs}$[a] (J mol$^{-1}$) |
|---|---|---|---|---|
| | This work | Literature | | |
| 1-Tetradecanol | 312.36 | 310.79[b]<br>311.15[c] | 20140 | 17500 ($\beta \rightarrow \alpha$)[g]<br>2130 ($\gamma \rightarrow \beta$)[g] |
| 1-Hexadecanol | 323.02 | 322.50[d]<br>322.65[c]<br>322.85[e] | 34080 | 19970 ($\beta \rightarrow \alpha$)[g]<br>3310 ($\gamma \rightarrow \beta$)[g] |
| 1-Octadecanol | 331.70 | 331.65[c] | 47200 | 22400 ($\beta \rightarrow \alpha$)[g]<br>4500 ($\gamma \rightarrow \beta$)[g] |
| 1-Icosanol | 336.44 | 336.50[f]<br>338.15[c] | 68600 | 25000 ($\beta \rightarrow \alpha$)[g]<br>5700 ($\gamma \rightarrow \beta$)[g] |

[a] [101,102].
[b] [103].
[c] [45].
[d] [104].
[e] [105].
[f] [46].
[g] Type of transition.

octan-1-ol + hexylamine

U. Domanska, M. Głoskowska, Experimental solid+liquid equilibria and excess molarvolumes of alkanol+hexylamine mixtures. Analysis in terms of the ERAS, DISQUAC and Mod. UNIFAC models, Fluid Phase Equilibria 216 (2004) 135–145

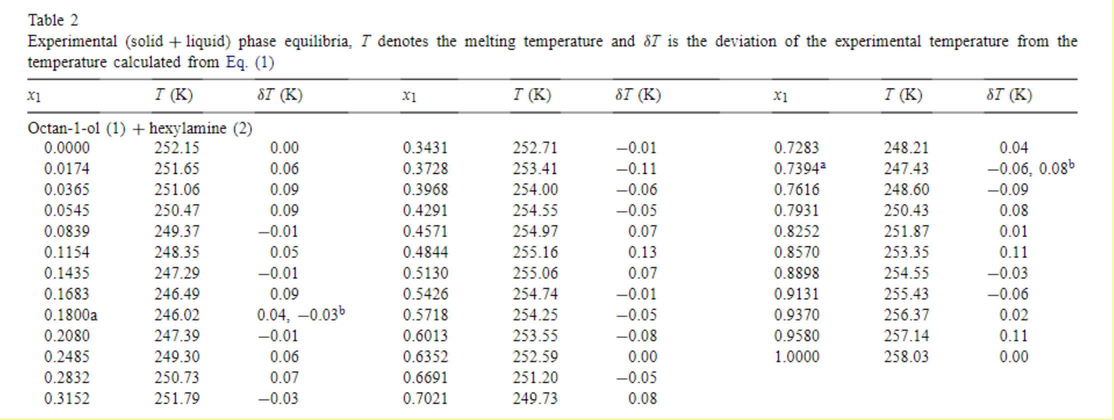


Table 2

Experimental (solid + liquid) phase equilibria, $T$ denotes the melting temperature and $\delta T$ is the deviation of the experimental temperature from the temperature calculated from Eq. (1)

| $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) |
|---|---|---|---|---|---|---|---|---|
| Octan-1-ol (1) + hexylamine (2) | | | | | | | | |
| 0.0000 | 252.15 | 0.00 | 0.3431 | 252.71 | −0.01 | 0.7283 | 248.21 | 0.04 |
| 0.0174 | 251.65 | 0.06 | 0.3728 | 253.41 | −0.11 | 0.7394[a] | 247.43 | −0.06, 0.08[b] |
| 0.0365 | 251.06 | 0.09 | 0.3968 | 254.00 | −0.06 | 0.7616 | 248.60 | −0.09 |
| 0.0545 | 250.47 | 0.09 | 0.4291 | 254.55 | −0.05 | 0.7931 | 250.43 | 0.08 |
| 0.0839 | 249.37 | −0.01 | 0.4571 | 254.97 | 0.07 | 0.8252 | 251.87 | 0.01 |
| 0.1154 | 248.35 | 0.05 | 0.4844 | 255.16 | 0.13 | 0.8570 | 253.35 | 0.11 |
| 0.1435 | 247.29 | −0.01 | 0.5130 | 255.06 | 0.07 | 0.8898 | 254.55 | −0.03 |
| 0.1683 | 246.49 | 0.09 | 0.5426 | 254.74 | −0.01 | 0.9131 | 255.43 | −0.06 |
| 0.1800a | 246.02 | 0.04, −0.03[b] | 0.5718 | 254.25 | −0.05 | 0.9370 | 256.37 | 0.02 |
| 0.2080 | 247.39 | −0.01 | 0.6013 | 253.55 | −0.08 | 0.9580 | 257.14 | 0.11 |
| 0.2485 | 249.30 | 0.06 | 0.6352 | 252.59 | 0.00 | 1.0000 | 258.03 | 0.00 |
| 0.2832 | 250.73 | 0.07 | 0.6691 | 251.20 | −0.05 | | | |
| 0.3152 | 251.79 | −0.03 | 0.7021 | 249.73 | 0.08 | | | |

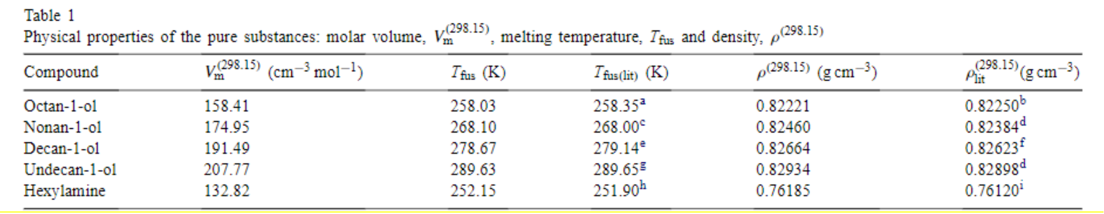


Table 1

Physical properties of the pure substances: molar volume, $V_m^{(298.15)}$, melting temperature, $T_{fus}$ and density, $\rho^{(298.15)}$

| Compound | $V_m^{(298.15)}$ ($cm^{-3}$ $mol^{-1}$) | $T_{fus}$ (K) | $T_{fus(lit)}$ (K) | $\rho^{(298.15)}$ (g $cm^{-3}$) | $\rho_{lit}^{(298.15)}$(g $cm^{-3}$) |
|---|---|---|---|---|---|
| Octan-1-ol | 158.41 | 258.03 | 258.35[a] | 0.82221 | 0.82250[b] |
| Nonan-1-ol | 174.95 | 268.10 | 268.00[c] | 0.82460 | 0.82384[d] |
| Decan-1-ol | 191.49 | 278.67 | 279.14[e] | 0.82664 | 0.82623[f] |
| Undecan-1-ol | 207.77 | 289.63 | 289.65[g] | 0.82934 | 0.82898[d] |
| Hexylamine | 132.82 | 252.15 | 251.90[h] | 0.76185 | 0.76120[i] |

nonan-1-ol + hexylamine

U. Domanska, M. Głoskowska, Experimental solid+liquid equilibria and excess molarvolumes of alkanol+hexylamine mixtures. Analysis in terms of the ERAS, DISQUAC and Mod. UNIFAC models, Fluid Phase Equilibria 216 (2004) 135–145

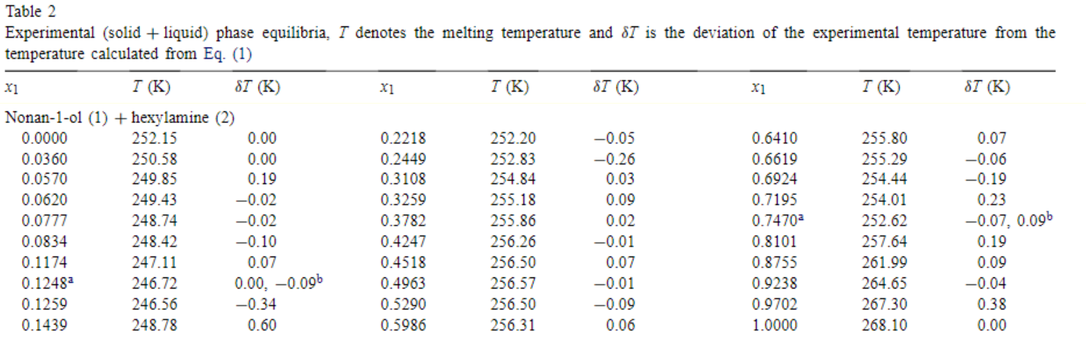


Table 2

Experimental (solid + liquid) phase equilibria, $T$ denotes the melting temperature and $\delta T$ is the deviation of the experimental temperature from the temperature calculated from Eq. (1)

| $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) |
|---|---|---|---|---|---|---|---|---|
| Nonan-1-ol (1) + hexylamine (2) | | | | | | | | |
| 0.0000 | 252.15 | 0.00 | 0.2218 | 252.20 | −0.05 | 0.6410 | 255.80 | 0.07 |
| 0.0360 | 250.58 | 0.00 | 0.2449 | 252.83 | −0.26 | 0.6619 | 255.29 | −0.06 |
| 0.0570 | 249.85 | 0.19 | 0.3108 | 254.84 | 0.03 | 0.6924 | 254.44 | −0.19 |
| 0.0620 | 249.43 | −0.02 | 0.3259 | 255.18 | 0.09 | 0.7195 | 254.01 | 0.23 |
| 0.0777 | 248.74 | −0.02 | 0.3782 | 255.86 | 0.02 | 0.7470[a] | 252.62 | −0.07, 0.09[b] |
| 0.0834 | 248.42 | −0.10 | 0.4247 | 256.26 | −0.01 | 0.8101 | 257.64 | 0.19 |
| 0.1174 | 247.11 | 0.07 | 0.4518 | 256.50 | 0.07 | 0.8755 | 261.99 | 0.09 |
| 0.1248[a] | 246.72 | 0.00, −0.09[b] | 0.4963 | 256.57 | −0.01 | 0.9238 | 264.65 | −0.04 |
| 0.1259 | 246.56 | −0.34 | 0.5290 | 256.50 | −0.09 | 0.9702 | 267.30 | 0.38 |
| 0.1439 | 248.78 | 0.60 | 0.5986 | 256.31 | 0.06 | 1.0000 | 268.10 | 0.00 |

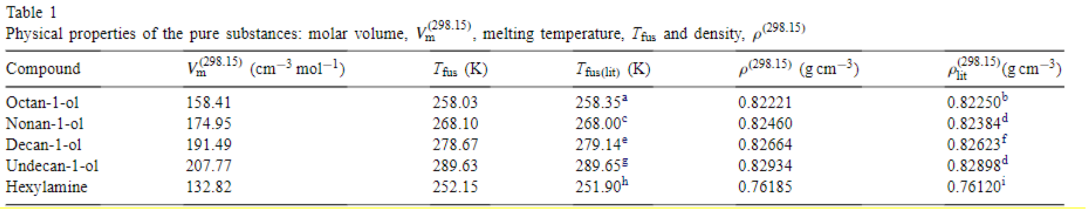


Table 1

Physical properties of the pure substances: molar volume, $V_m^{(298.15)}$, melting temperature, $T_{fus}$ and density, $\rho^{(298.15)}$

| Compound | $V_m^{(298.15)}$ ($cm^{-3}\,mol^{-1}$) | $T_{fus}$ (K) | $T_{fus(lit)}$ (K) | $\rho^{(298.15)}$ ($g\,cm^{-3}$) | $\rho_{lit}^{(298.15)}$($g\,cm^{-3}$) |
|---|---|---|---|---|---|
| Octan-1-ol | 158.41 | 258.03 | 258.35[a] | 0.82221 | 0.82250[b] |
| Nonan-1-ol | 174.95 | 268.10 | 268.00[c] | 0.82460 | 0.82384[d] |
| Decan-1-ol | 191.49 | 278.67 | 279.14[e] | 0.82664 | 0.82623[f] |
| Undecan-1-ol | 207.77 | 289.63 | 289.65[g] | 0.82934 | 0.82898[d] |
| Hexylamine | 132.82 | 252.15 | 251.90[h] | 0.76185 | 0.76120[i] |

decan-1-ol + hexylamine

U. Domanska, M. Głoskowska, Experimental solid+liquid equilibria and excess molarvolumes of alkanol+hexylamine mixtures. Analysis in terms of the ERAS, DISQUAC and Mod. UNIFAC models, Fluid Phase Equilibria 216 (2004) 135–145

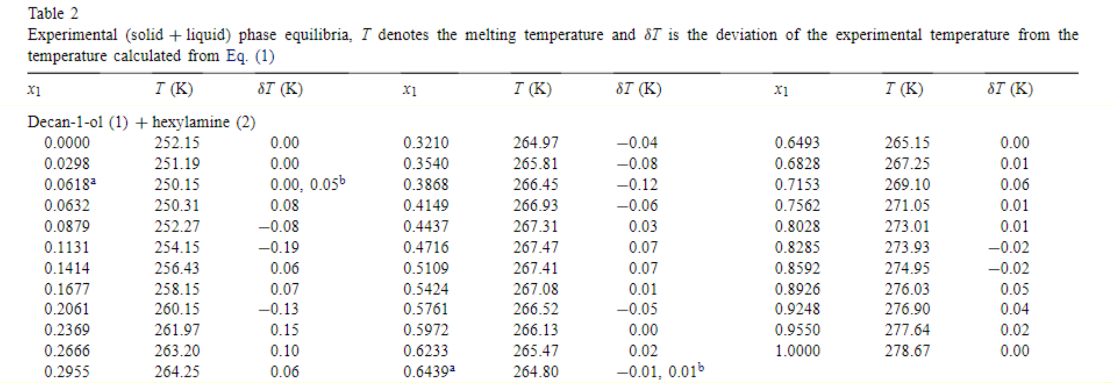


Table 2

Experimental (solid + liquid) phase equilibria, $T$ denotes the melting temperature and $\delta T$ is the deviation of the experimental temperature from the temperature calculated from Eq. (1)

| $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) |
|---|---|---|---|---|---|---|---|---|
| Decan-1-ol (1) + hexylamine (2) | | | | | | | | |
| 0.0000 | 252.15 | 0.00 | 0.3210 | 264.97 | −0.04 | 0.6493 | 265.15 | 0.00 |
| 0.0298 | 251.19 | 0.00 | 0.3540 | 265.81 | −0.08 | 0.6828 | 267.25 | 0.01 |
| 0.0618[a] | 250.15 | 0.00, 0.05[b] | 0.3868 | 266.45 | −0.12 | 0.7153 | 269.10 | 0.06 |
| 0.0632 | 250.31 | 0.08 | 0.4149 | 266.93 | −0.06 | 0.7562 | 271.05 | 0.01 |
| 0.0879 | 252.27 | −0.08 | 0.4437 | 267.31 | 0.03 | 0.8028 | 273.01 | 0.01 |
| 0.1131 | 254.15 | −0.19 | 0.4716 | 267.47 | 0.07 | 0.8285 | 273.93 | −0.02 |
| 0.1414 | 256.43 | 0.06 | 0.5109 | 267.41 | 0.07 | 0.8592 | 274.95 | −0.02 |
| 0.1677 | 258.15 | 0.07 | 0.5424 | 267.08 | 0.01 | 0.8926 | 276.03 | 0.05 |
| 0.2061 | 260.15 | −0.13 | 0.5761 | 266.52 | −0.05 | 0.9248 | 276.90 | 0.04 |
| 0.2369 | 261.97 | 0.15 | 0.5972 | 266.13 | 0.00 | 0.9550 | 277.64 | 0.02 |
| 0.2666 | 263.20 | 0.10 | 0.6233 | 265.47 | 0.02 | 1.0000 | 278.67 | 0.00 |
| 0.2955 | 264.25 | 0.06 | 0.6439[a] | 264.80 | −0.01, 0.01[b] | | | |

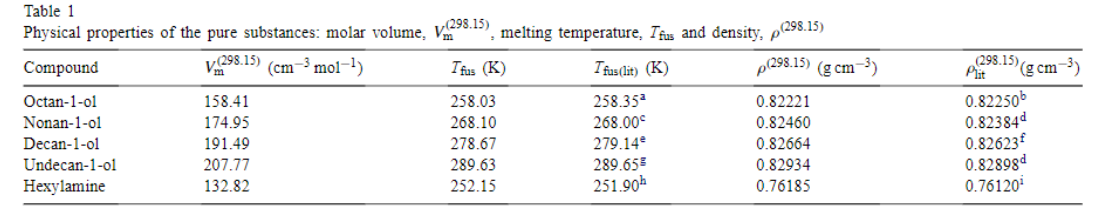


Table 1

Physical properties of the pure substances: molar volume, $V_m^{(298.15)}$, melting temperature, $T_{fus}$ and density, $\rho^{(298.15)}$

| Compound | $V_m^{(298.15)}$ (cm$^{-3}$ mol$^{-1}$) | $T_{fus}$ (K) | $T_{fus(lit)}$ (K) | $\rho^{(298.15)}$ (g cm$^{-3}$) | $\rho_{lit}^{(298.15)}$(g cm$^{-3}$) |
|---|---|---|---|---|---|
| Octan-1-ol | 158.41 | 258.03 | 258.35[a] | 0.82221 | 0.82250[b] |
| Nonan-1-ol | 174.95 | 268.10 | 268.00[c] | 0.82460 | 0.82384[d] |
| Decan-1-ol | 191.49 | 278.67 | 279.14[e] | 0.82664 | 0.82623[f] |
| Undecan-1-ol | 207.77 | 289.63 | 289.65[g] | 0.82934 | 0.82898[d] |
| Hexylamine | 132.82 | 252.15 | 251.90[h] | 0.76185 | 0.76120[i] |

undecan-1-ol + hexylamine
U. Domanska, M. Głoskowska, Experimental solid+liquid equilibria and excess molarvolumes of alkanol+hexylamine mixtures. Analysis in terms of the ERAS, DISQUAC and Mod. UNIFAC models, Fluid Phase Equilibria 216 (2004) 135–145

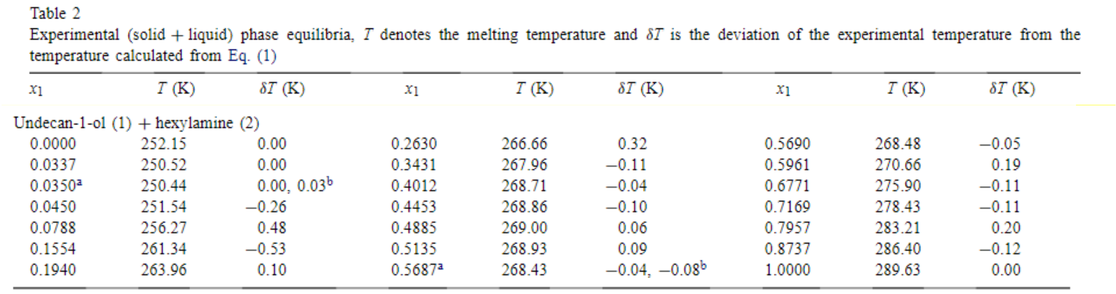


Table 2
Experimental (solid + liquid) phase equilibria, $T$ denotes the melting temperature and $\delta T$ is the deviation of the experimental temperature from the temperature calculated from Eq. (1)

| $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) | $x_1$ | $T$ (K) | $\delta T$ (K) |
|---|---|---|---|---|---|---|---|---|
| Undecan-1-ol (1) + hexylamine (2) | | | | | | | | |
| 0.0000 | 252.15 | 0.00 | 0.2630 | 266.66 | 0.32 | 0.5690 | 268.48 | −0.05 |
| 0.0337 | 250.52 | 0.00 | 0.3431 | 267.96 | −0.11 | 0.5961 | 270.66 | 0.19 |
| 0.0350[a] | 250.44 | 0.00, 0.03[b] | 0.4012 | 268.71 | −0.04 | 0.6771 | 275.90 | −0.11 |
| 0.0450 | 251.54 | −0.26 | 0.4453 | 268.86 | −0.10 | 0.7169 | 278.43 | −0.11 |
| 0.0788 | 256.27 | 0.48 | 0.4885 | 269.00 | 0.06 | 0.7957 | 283.21 | 0.20 |
| 0.1554 | 261.34 | −0.53 | 0.5135 | 268.93 | 0.09 | 0.8737 | 286.40 | −0.12 |
| 0.1940 | 263.96 | 0.10 | 0.5687[a] | 268.43 | −0.04, −0.08[b] | 1.0000 | 289.63 | 0.00 |

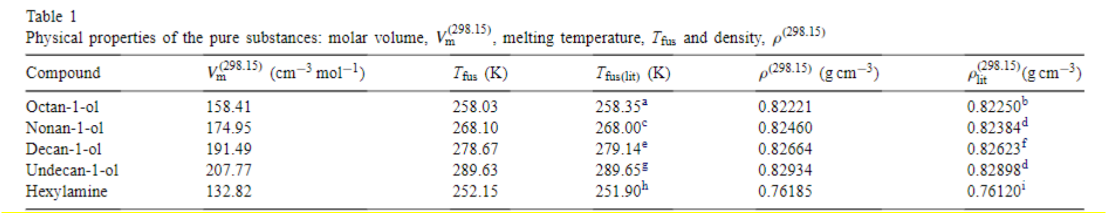


Table 1
Physical properties of the pure substances: molar volume, $V_m^{(298.15)}$, melting temperature, $T_{fus}$ and density, $\rho^{(298.15)}$

| Compound | $V_m^{(298.15)}$ ($cm^{-3}$ $mol^{-1}$) | $T_{fus}$ (K) | $T_{fus(lit)}$ (K) | $\rho^{(298.15)}$ (g $cm^{-3}$) | $\rho_{lit}^{(298.15)}$(g $cm^{-3}$) |
|---|---|---|---|---|---|
| Octan-1-ol | 158.41 | 258.03 | 258.35[a] | 0.82221 | 0.82250[b] |
| Nonan-1-ol | 174.95 | 268.10 | 268.00[c] | 0.82460 | 0.82384[d] |
| Decan-1-ol | 191.49 | 278.67 | 279.14[e] | 0.82664 | 0.82623[f] |
| Undecan-1-ol | 207.77 | 289.63 | 289.65[g] | 0.82934 | 0.82898[d] |
| Hexylamine | 132.82 | 252.15 | 251.90[h] | 0.76185 | 0.76120[i] |

*m*-chlorophenol + *p*-chlorophenol

Tze-Min Her, Liang-Sun Lee, Shih-Chieh Hsu, Solid–liquid equilibria of mixtures containingtert-butanol,m-chlorophenol, andp-chlorophenol and development ofadductive crystallization processes, Fluid Phase Equilibria 237 (2005) 152–161

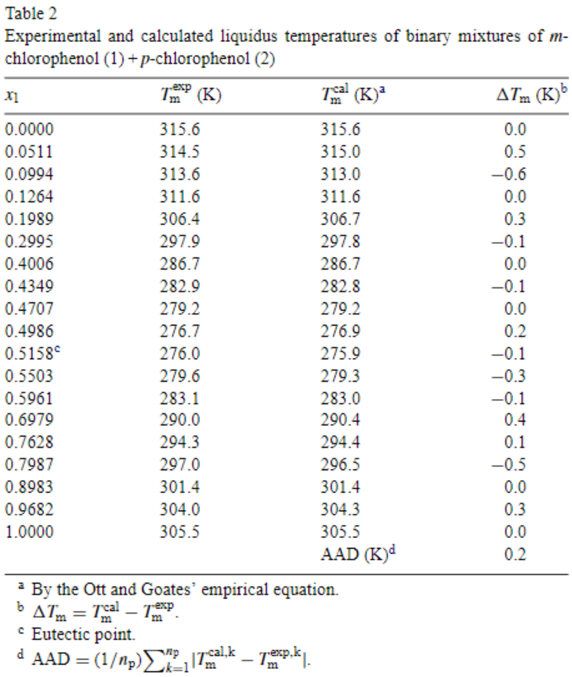


Table 2
Experimental and calculated liquidus temperatures of binary mixtures of *m*-chlorophenol (1) + *p*-chlorophenol (2)

| $x_1$ | $T_m^{exp}$ (K) | $T_m^{cal}$ (K)[a] | $\Delta T_m$ (K)[b] |
|---|---|---|---|
| 0.0000 | 315.6 | 315.6 | 0.0 |
| 0.0511 | 314.5 | 315.0 | 0.5 |
| 0.0994 | 313.6 | 313.0 | −0.6 |
| 0.1264 | 311.6 | 311.6 | 0.0 |
| 0.1989 | 306.4 | 306.7 | 0.3 |
| 0.2995 | 297.9 | 297.8 | −0.1 |
| 0.4006 | 286.7 | 286.7 | 0.0 |
| 0.4349 | 282.9 | 282.8 | −0.1 |
| 0.4707 | 279.2 | 279.2 | 0.0 |
| 0.4986 | 276.7 | 276.9 | 0.2 |
| 0.5158[c] | 276.0 | 275.9 | −0.1 |
| 0.5503 | 279.6 | 279.3 | −0.3 |
| 0.5961 | 283.1 | 283.0 | −0.1 |
| 0.6979 | 290.0 | 290.4 | 0.4 |
| 0.7628 | 294.3 | 294.4 | 0.1 |
| 0.7987 | 297.0 | 296.5 | −0.5 |
| 0.8983 | 301.4 | 301.4 | 0.0 |
| 0.9682 | 304.0 | 304.3 | 0.3 |
| 1.0000 | 305.5 | 305.5 | 0.0 |
| | | AAD (K)[d] | 0.2 |

[a] By the Ott and Goates' empirical equation.

[b] $\Delta T_m = T_m^{cal} - T_m^{exp}$.

[c] Eutectic point.

[d] $\mathrm{AAD} = (1/n_p)\sum_{k=1}^{n_p}|T_m^{cal,k} - T_m^{exp,k}|$.

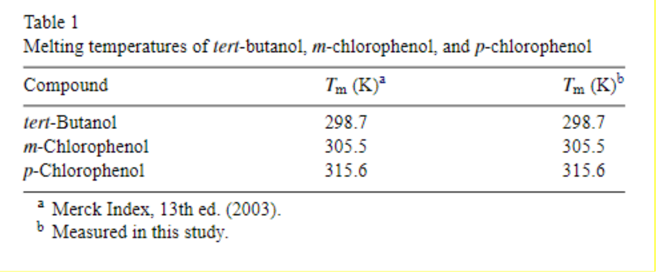


Table 1
Melting temperatures of *tert*-butanol, *m*-chlorophenol, and *p*-chlorophenol

| Compound | $T_m$ (K)[a] | $T_m$ (K)[b] |
|---|---|---|
| *tert*-Butanol | 298.7 | 298.7 |
| *m*-Chlorophenol | 305.5 | 305.5 |
| *p*-Chlorophenol | 315.6 | 315.6 |

[a] Merck Index, 13th ed. (2003).

[b] Measured in this study.

*tert*-butanol + *m*-chlorophenol

Tze-Min Her, Liang-Sun Lee, Shih-Chieh Hsu, Solid–liquid equilibria of mixtures containingtert-butanol,m-chlorophenol, andp-chlorophenol and development ofadductive crystallization processes, Fluid Phase Equilibria 237 (2005) 152–161

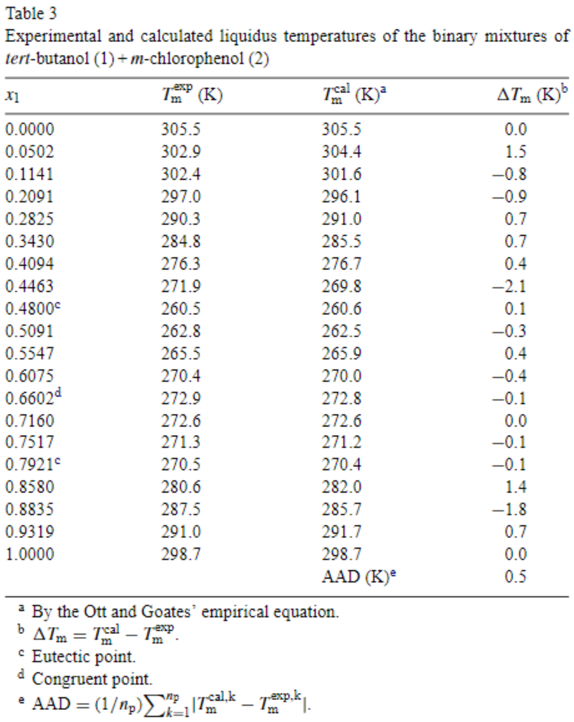


Table 3
Experimental and calculated liquidus temperatures of the binary mixtures of *tert*-butanol (1) + *m*-chlorophenol (2)

| $x_1$ | $T_m^{exp}$ (K) | $T_m^{cal}$ (K)[a] | $\Delta T_m$ (K)[b] |
|---|---|---|---|
| 0.0000 | 305.5 | 305.5 | 0.0 |
| 0.0502 | 302.9 | 304.4 | 1.5 |
| 0.1141 | 302.4 | 301.6 | −0.8 |
| 0.2091 | 297.0 | 296.1 | −0.9 |
| 0.2825 | 290.3 | 291.0 | 0.7 |
| 0.3430 | 284.8 | 285.5 | 0.7 |
| 0.4094 | 276.3 | 276.7 | 0.4 |
| 0.4463 | 271.9 | 269.8 | −2.1 |
| 0.4800[c] | 260.5 | 260.6 | 0.1 |
| 0.5091 | 262.8 | 262.5 | −0.3 |
| 0.5547 | 265.5 | 265.9 | 0.4 |
| 0.6075 | 270.4 | 270.0 | −0.4 |
| 0.6602[d] | 272.9 | 272.8 | −0.1 |
| 0.7160 | 272.6 | 272.6 | 0.0 |
| 0.7517 | 271.3 | 271.2 | −0.1 |
| 0.7921[c] | 270.5 | 270.4 | −0.1 |
| 0.8580 | 280.6 | 282.0 | 1.4 |
| 0.8835 | 287.5 | 285.7 | −1.8 |
| 0.9319 | 291.0 | 291.7 | 0.7 |
| 1.0000 | 298.7 | 298.7 | 0.0 |
| | | AAD (K)[e] | 0.5 |

[a] By the Ott and Goates' empirical equation.

[b] $\Delta T_m = T_m^{cal} - T_m^{exp}$.

[c] Eutectic point.

[d] Congruent point.

[e] $AAD = (1/n_p)\sum_{k=1}^{np}|T_m^{cal,k} - T_m^{exp,k}|$.

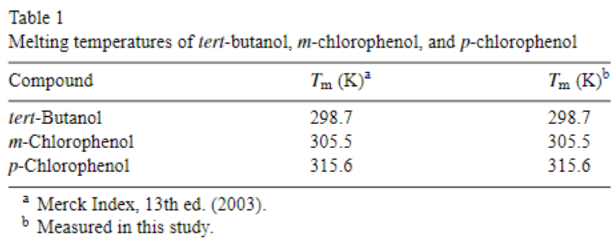


Table 1
Melting temperatures of *tert*-butanol, *m*-chlorophenol, and *p*-chlorophenol

| Compound | $T_m$ (K)[a] | $T_m$ (K)[b] |
|---|---|---|
| *tert*-Butanol | 298.7 | 298.7 |
| *m*-Chlorophenol | 305.5 | 305.5 |
| *p*-Chlorophenol | 315.6 | 315.6 |

[a] Merck Index, 13th ed. (2003).

[b] Measured in this study.

*tert*-butanol + *p*-chlorophenol
Tze-Min Her, Liang-Sun Lee, Shih-Chieh Hsu, Solid–liquid equilibria of mixtures containingtert-butanol,m-chlorophenol, andp-chlorophenol and development ofadductive crystallization processes, Fluid Phase Equilibria 237 (2005) 152–161

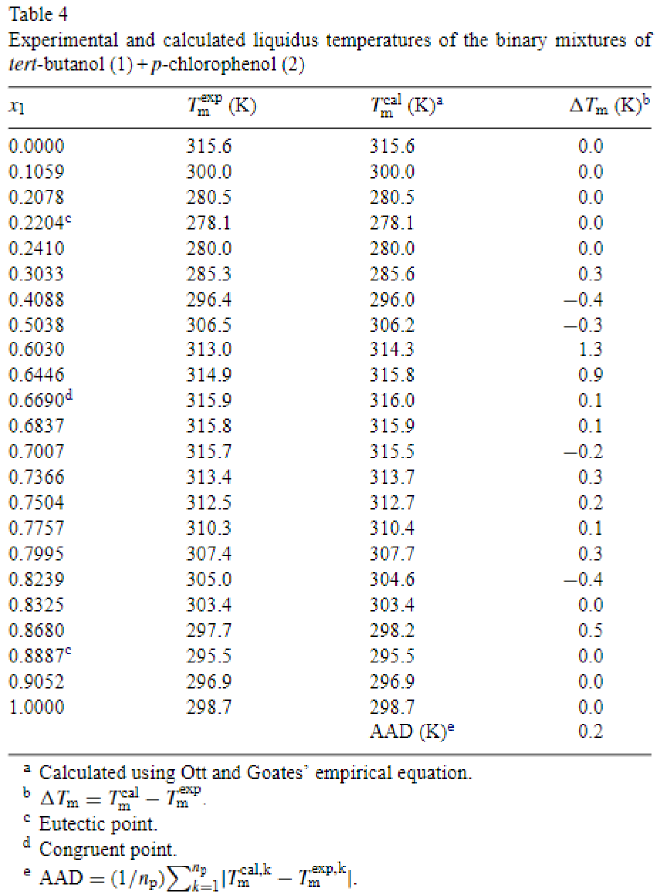


Table 4
Experimental and calculated liquidus temperatures of the binary mixtures of *tert*-butanol (1) + *p*-chlorophenol (2)

| $x_1$ | $T_m^{exp}$ (K) | $T_m^{cal}$ (K)[a] | $\Delta T_m$ (K)[b] |
|---|---|---|---|
| 0.0000 | 315.6 | 315.6 | 0.0 |
| 0.1059 | 300.0 | 300.0 | 0.0 |
| 0.2078 | 280.5 | 280.5 | 0.0 |
| 0.2204[c] | 278.1 | 278.1 | 0.0 |
| 0.2410 | 280.0 | 280.0 | 0.0 |
| 0.3033 | 285.3 | 285.6 | 0.3 |
| 0.4088 | 296.4 | 296.0 | −0.4 |
| 0.5038 | 306.5 | 306.2 | −0.3 |
| 0.6030 | 313.0 | 314.3 | 1.3 |
| 0.6446 | 314.9 | 315.8 | 0.9 |
| 0.6690[d] | 315.9 | 316.0 | 0.1 |
| 0.6837 | 315.8 | 315.9 | 0.1 |
| 0.7007 | 315.7 | 315.5 | −0.2 |
| 0.7366 | 313.4 | 313.7 | 0.3 |
| 0.7504 | 312.5 | 312.7 | 0.2 |
| 0.7757 | 310.3 | 310.4 | 0.1 |
| 0.7995 | 307.4 | 307.7 | 0.3 |
| 0.8239 | 305.0 | 304.6 | −0.4 |
| 0.8325 | 303.4 | 303.4 | 0.0 |
| 0.8680 | 297.7 | 298.2 | 0.5 |
| 0.8887[c] | 295.5 | 295.5 | 0.0 |
| 0.9052 | 296.9 | 296.9 | 0.0 |
| 1.0000 | 298.7 | 298.7 | 0.0 |
|  |  | AAD (K)[e] | 0.2 |

[a] Calculated using Ott and Goates' empirical equation.
[b] $\Delta T_m = T_m^{cal} - T_m^{exp}$.
[c] Eutectic point.
[d] Congruent point.
[e] $\mathrm{AAD} = (1/n_p)\sum_{k=1}^{n_p} |T_m^{cal,k} - T_m^{exp,k}|$.

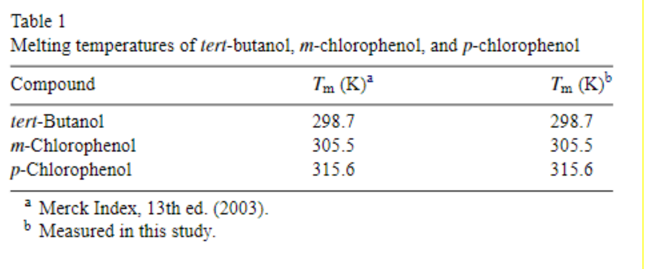


Table 1
Melting temperatures of *tert*-butanol, *m*-chlorophenol, and *p*-chlorophenol

| Compound | $T_m$ (K)[a] | $T_m$ (K)[b] |
|---|---|---|
| *tert*-Butanol | 298.7 | 298.7 |
| *m*-Chlorophenol | 305.5 | 305.5 |
| *p*-Chlorophenol | 315.6 | 315.6 |

[a] Merck Index, 13th ed. (2003).
[b] Measured in this study.

diphenyl ether + biphenyl

D. Cabaleiro, C. Gracia-Fernández, L. Lugo, (Solid + liquid) phase equilibria and heat capacity of (diphenyl ether + biphenyl) mixtures used as thermal energy storage materials, The Journal of Chemical Thermodynamics, Volume 74, July 2014, Pages 43-50

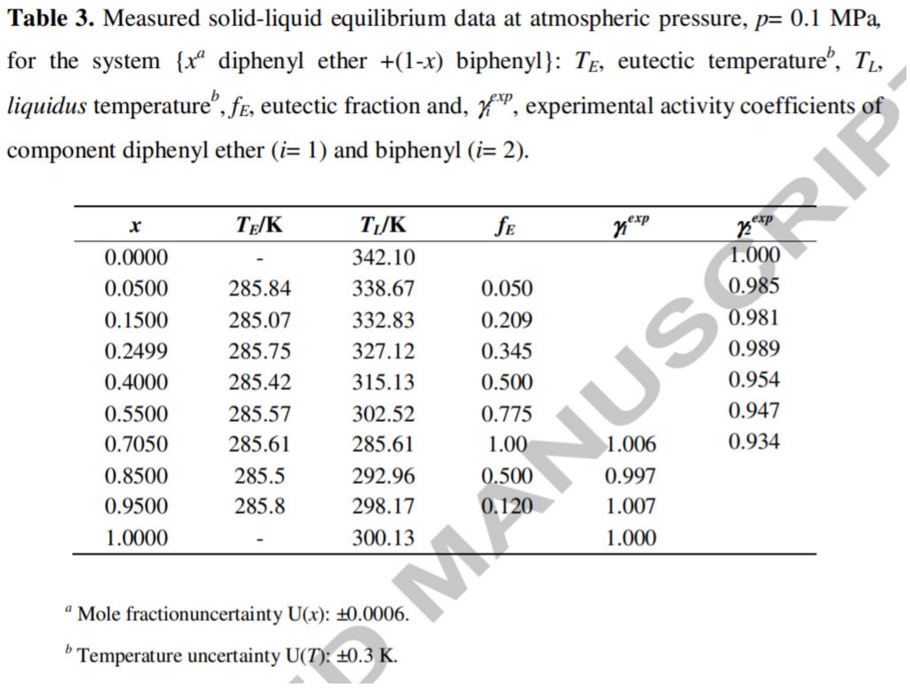


**Table 3.** Measured solid-liquid equilibrium data at atmospheric pressure, $p$= 0.1 MPa, for the system {$x^a$ diphenyl ether +(1-$x$) biphenyl}: $T_E$, eutectic temperature[b], $T_L$, *liquidus* temperature[b], $f_E$, eutectic fraction and, $\gamma_i^{exp}$, experimental activity coefficients of component diphenyl ether ($i$= 1) and biphenyl ($i$= 2).

| $x$ | $T_E$/K | $T_L$/K | $f_E$ | $\gamma_1^{exp}$ | $\gamma_2^{exp}$ |
|---|---|---|---|---|---|
| 0.0000 | - | 342.10 | | | 1.000 |
| 0.0500 | 285.84 | 338.67 | 0.050 | | 0.985 |
| 0.1500 | 285.07 | 332.83 | 0.209 | | 0.981 |
| 0.2499 | 285.75 | 327.12 | 0.345 | | 0.989 |
| 0.4000 | 285.42 | 315.13 | 0.500 | | 0.954 |
| 0.5500 | 285.57 | 302.52 | 0.775 | | 0.947 |
| 0.7050 | 285.61 | 285.61 | 1.00 | 1.006 | 0.934 |
| 0.8500 | 285.5 | 292.96 | 0.500 | 0.997 | |
| 0.9500 | 285.8 | 298.17 | 0.120 | 1.007 | |
| 1.0000 | - | 300.13 | | 1.000 | |

[a] Mole fractionuncertainty U($x$): ±0.0006.

[b] Temperature uncertainty U($T$): ±0.3 K.

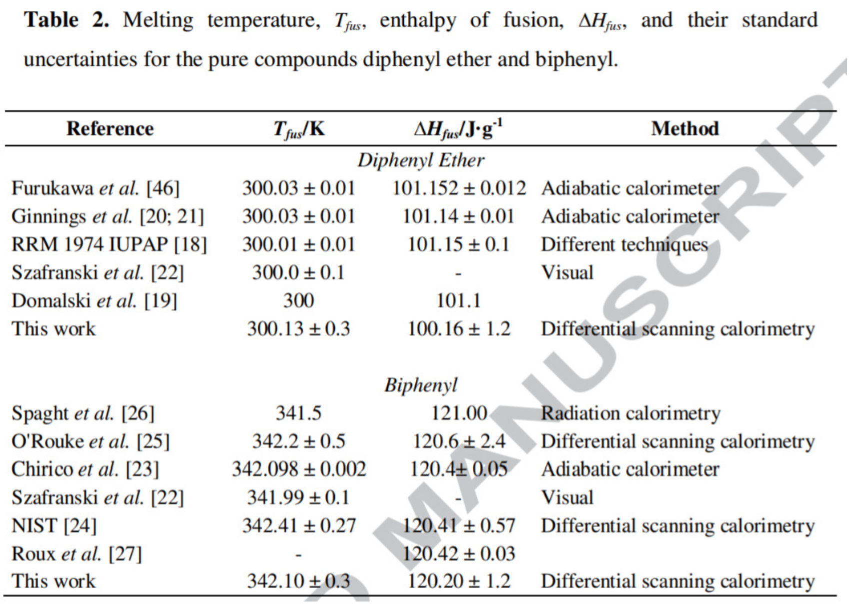


**Table 2.** Melting temperature, $T_{fus}$, enthalpy of fusion, $\Delta H_{fus}$, and their standard uncertainties for the pure compounds diphenyl ether and biphenyl.

| Reference | $T_{fus}$/K | $\Delta H_{fus}$/J·g$^{-1}$ | Method |
|---|---|---|---|
| | | *Diphenyl Ether* | |
| Furukawa *et al.* [46] | 300.03 ± 0.01 | 101.152 ± 0.012 | Adiabatic calorimeter |
| Ginnings *et al.* [20; 21] | 300.03 ± 0.01 | 101.14 ± 0.01 | Adiabatic calorimeter |
| RRM 1974 IUPAP [18] | 300.01 ± 0.01 | 101.15 ± 0.1 | Different techniques |
| Szafranski *et al.* [22] | 300.0 ± 0.1 | - | Visual |
| Domalski *et al.* [19] | 300 | 101.1 | |
| This work | 300.13 ± 0.3 | 100.16 ± 1.2 | Differential scanning calorimetry |
| | | *Biphenyl* | |
| Spaght *et al.* [26] | 341.5 | 121.00 | Radiation calorimetry |
| O'Rouke *et al.* [25] | 342.2 ± 0.5 | 120.6 ± 2.4 | Differential scanning calorimetry |
| Chirico *et al.* [23] | 342.098 ± 0.002 | 120.4± 0.05 | Adiabatic calorimeter |
| Szafranski *et al.* [22] | 341.99 ± 0.1 | - | Visual |
| NIST [24] | 342.41 ± 0.27 | 120.41 ± 0.57 | Differential scanning calorimetry |
| Roux *et al.* [27] | - | 120.42 ± 0.03 | |
| This work | 342.10 ± 0.3 | 120.20 ± 1.2 | Differential scanning calorimetry |

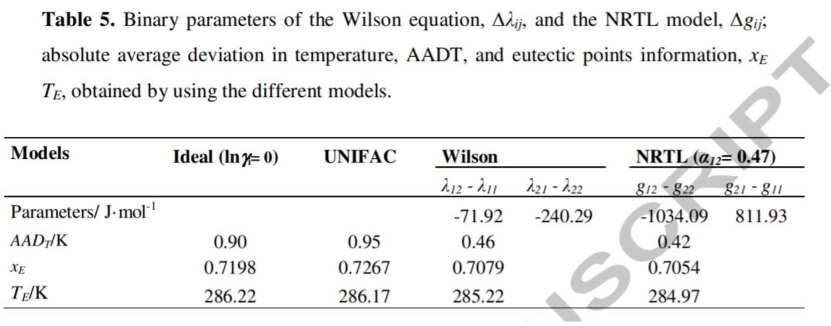


**Table 5.** Binary parameters of the Wilson equation, $\Delta\lambda_{ij}$, and the NRTL model, $\Delta g_{ij}$; absolute average deviation in temperature, AADT, and eutectic points information, $x_E$ $T_E$, obtained by using the different models.

| Models | Ideal ($\ln\gamma_i$= 0) | UNIFAC | Wilson | | NRTL ($\alpha_{12}$= 0.47) | |
|---|---|---|---|---|---|---|
| | | | $\lambda_{12}$ - $\lambda_{11}$ | $\lambda_{21}$ - $\lambda_{22}$ | $g_{12}$ - $g_{22}$ | $g_{21}$ - $g_{11}$ |
| Parameters/ J·mol$^{-1}$ | | | -71.92 | -240.29 | -1034.09 | 811.93 |
| $AAD_T$/K | 0.90 | 0.95 | 0.46 | | 0.42 | |
| $x_E$ | 0.7198 | 0.7267 | 0.7079 | | 0.7054 | |
| $T_E$/K | 286.22 | 286.17 | 285.22 | | 284.97 | |

ODABRATI JEDAN MODEL

*n*-octan-1-ol + *n*-hexadecane

Zofia Plesnar, Pawel Gierycz, Andrzej Bylicki, (Solid + liquid) equilibria in (*n*-octan-1-ol + *n*-hexadecane or *n*-dodecane or *n*-undecane), J. Chem. Thermodynamics 1990, 22, 393-398

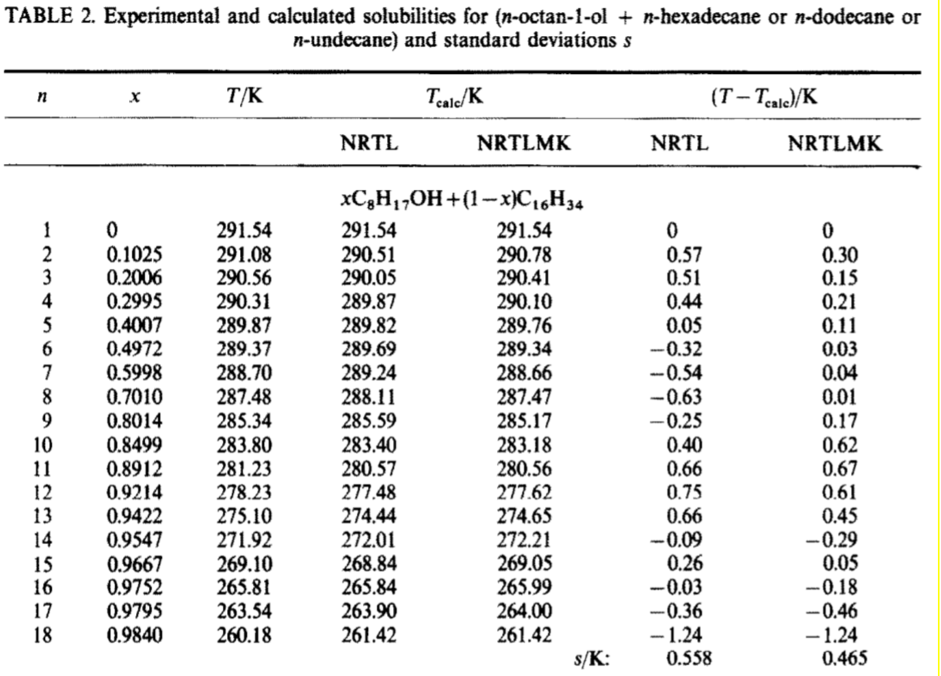


TABLE 2. Experimental and calculated solubilities for (*n*-octan-1-ol + *n*-hexadecane or *n*-dodecane or *n*-undecane) and standard deviations *s*

| $n$ | $x$ | $T$/K | $T_{calc}$/K |  | $(T-T_{calc})$/K |  |
|---|---|---|---|---|---|---|
|  |  |  | NRTL | NRTLMK | NRTL | NRTLMK |
|  |  |  | $xC_8H_{17}OH+(1-x)C_{16}H_{34}$ |  |  |  |
| 1 | 0 | 291.54 | 291.54 | 291.54 | 0 | 0 |
| 2 | 0.1025 | 291.08 | 290.51 | 290.78 | 0.57 | 0.30 |
| 3 | 0.2006 | 290.56 | 290.05 | 290.41 | 0.51 | 0.15 |
| 4 | 0.2995 | 290.31 | 289.87 | 290.10 | 0.44 | 0.21 |
| 5 | 0.4007 | 289.87 | 289.82 | 289.76 | 0.05 | 0.11 |
| 6 | 0.4972 | 289.37 | 289.69 | 289.34 | −0.32 | 0.03 |
| 7 | 0.5998 | 288.70 | 289.24 | 288.66 | −0.54 | 0.04 |
| 8 | 0.7010 | 287.48 | 288.11 | 287.47 | −0.63 | 0.01 |
| 9 | 0.8014 | 285.34 | 285.59 | 285.17 | −0.25 | 0.17 |
| 10 | 0.8499 | 283.80 | 283.40 | 283.18 | 0.40 | 0.62 |
| 11 | 0.8912 | 281.23 | 280.57 | 280.56 | 0.66 | 0.67 |
| 12 | 0.9214 | 278.23 | 277.48 | 277.62 | 0.75 | 0.61 |
| 13 | 0.9422 | 275.10 | 274.44 | 274.65 | 0.66 | 0.45 |
| 14 | 0.9547 | 271.92 | 272.01 | 272.21 | −0.09 | −0.29 |
| 15 | 0.9667 | 269.10 | 268.84 | 269.05 | 0.26 | 0.05 |
| 16 | 0.9752 | 265.81 | 265.84 | 265.99 | −0.03 | −0.18 |
| 17 | 0.9795 | 263.54 | 263.90 | 264.00 | −0.36 | −0.46 |
| 18 | 0.9840 | 260.18 | 261.42 | 261.42 | −1.24 | −1.24 |
|  |  |  |  | $s$/K: | 0.558 | 0.465 |

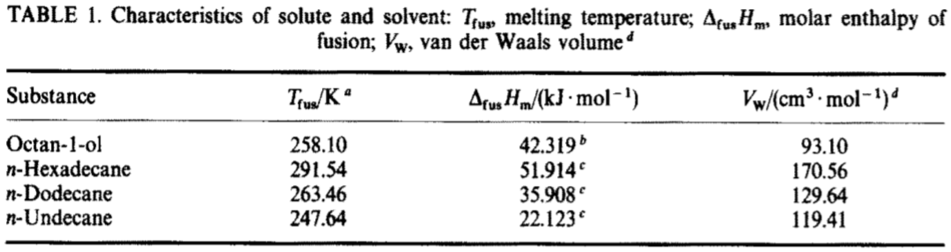


TABLE 1. Characteristics of solute and solvent: $T_{fus}$, melting temperature; $\Delta_{fus}H_m$, molar enthalpy of fusion; $V_W$, van der Waals volume[d]

| Substance | $T_{fus}$/K[a] | $\Delta_{fus}H_m$/(kJ · mol$^{-1}$) | $V_W$/(cm$^3$ · mol$^{-1}$)[d] |
|---|---|---|---|
| Octan-1-ol | 258.10 | 42.319[b] | 93.10 |
| *n*-Hexadecane | 291.54 | 51.914[c] | 170.56 |
| *n*-Dodecane | 263.46 | 35.908[c] | 129.64 |
| *n*-Undecane | 247.64 | 22.123[c] | 119.41 |

*n*-octan-1-ol + *n*-dodecane

Zofia Plesnar, Pawel Gierycz, Andrzej Bylicki, (Solid + liquid) equilibria in (*n*-octan-1-ol + *n*-hexadecane or *n*-dodecane or *n*-undecane), J. Chem. Thermodynamics 1990, 22, 393-398

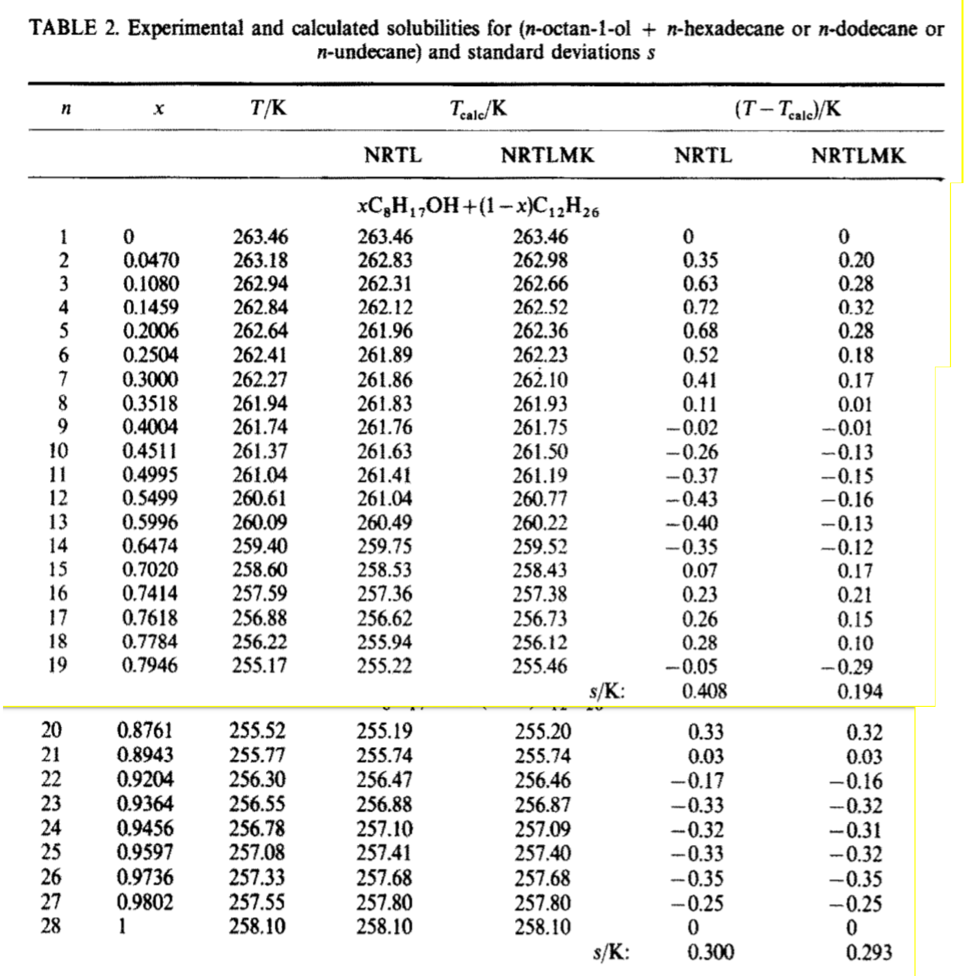


TABLE 2. Experimental and calculated solubilities for (*n*-octan-1-ol + *n*-hexadecane or *n*-dodecane or *n*-undecane) and standard deviations *s*

| *n* | *x* | $T$/K | $T_{calc}$/K |  | $(T - T_{calc})$/K |  |
|---|---|---|---|---|---|---|
|  |  |  | NRTL | NRTLMK | NRTL | NRTLMK |
|  |  |  | $xC_8H_{17}OH+(1-x)C_{12}H_{26}$ |  |  |  |
| 1 | 0 | 263.46 | 263.46 | 263.46 | 0 | 0 |
| 2 | 0.0470 | 263.18 | 262.83 | 262.98 | 0.35 | 0.20 |
| 3 | 0.1080 | 262.94 | 262.31 | 262.66 | 0.63 | 0.28 |
| 4 | 0.1459 | 262.84 | 262.12 | 262.52 | 0.72 | 0.32 |
| 5 | 0.2006 | 262.64 | 261.96 | 262.36 | 0.68 | 0.28 |
| 6 | 0.2504 | 262.41 | 261.89 | 262.23 | 0.52 | 0.18 |
| 7 | 0.3000 | 262.27 | 261.86 | 262.10 | 0.41 | 0.17 |
| 8 | 0.3518 | 261.94 | 261.83 | 261.93 | 0.11 | 0.01 |
| 9 | 0.4004 | 261.74 | 261.76 | 261.75 | −0.02 | −0.01 |
| 10 | 0.4511 | 261.37 | 261.63 | 261.50 | −0.26 | −0.13 |
| 11 | 0.4995 | 261.04 | 261.41 | 261.19 | −0.37 | −0.15 |
| 12 | 0.5499 | 260.61 | 261.04 | 260.77 | −0.43 | −0.16 |
| 13 | 0.5996 | 260.09 | 260.49 | 260.22 | −0.40 | −0.13 |
| 14 | 0.6474 | 259.40 | 259.75 | 259.52 | −0.35 | −0.12 |
| 15 | 0.7020 | 258.60 | 258.53 | 258.43 | 0.07 | 0.17 |
| 16 | 0.7414 | 257.59 | 257.36 | 257.38 | 0.23 | 0.21 |
| 17 | 0.7618 | 256.88 | 256.62 | 256.73 | 0.26 | 0.15 |
| 18 | 0.7784 | 256.22 | 255.94 | 256.12 | 0.28 | 0.10 |
| 19 | 0.7946 | 255.17 | 255.22 | 255.46 | −0.05 | −0.29 |
|  |  |  |  | *s*/K: | 0.408 | 0.194 |
| 20 | 0.8761 | 255.52 | 255.19 | 255.20 | 0.33 | 0.32 |
| 21 | 0.8943 | 255.77 | 255.74 | 255.74 | 0.03 | 0.03 |
| 22 | 0.9204 | 256.30 | 256.47 | 256.46 | −0.17 | −0.16 |
| 23 | 0.9364 | 256.55 | 256.88 | 256.87 | −0.33 | −0.32 |
| 24 | 0.9456 | 256.78 | 257.10 | 257.09 | −0.32 | −0.31 |
| 25 | 0.9597 | 257.08 | 257.41 | 257.40 | −0.33 | −0.32 |
| 26 | 0.9736 | 257.33 | 257.68 | 257.68 | −0.35 | −0.35 |
| 27 | 0.9802 | 257.55 | 257.80 | 257.80 | −0.25 | −0.25 |
| 28 | 1 | 258.10 | 258.10 | 258.10 | 0 | 0 |
|  |  |  |  | *s*/K: | 0.300 | 0.293 |

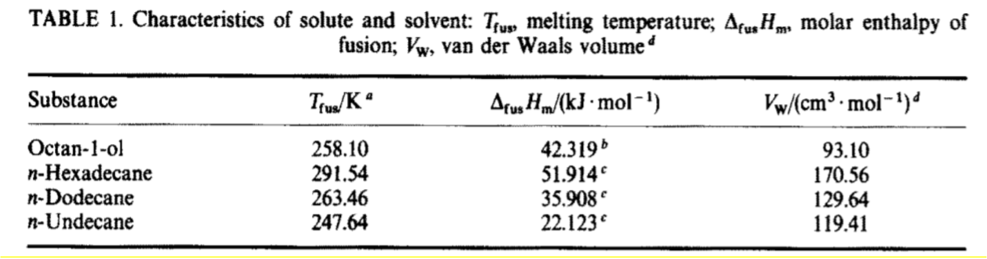


TABLE 1. Characteristics of solute and solvent: $T_{fus}$, melting temperature; $\Delta_{fus}H_m$, molar enthalpy of fusion; $V_W$, van der Waals volume[d]

| Substance | $T_{fus}$/K[a] | $\Delta_{fus}H_m$/(kJ · mol$^{-1}$) | $V_W$/(cm$^3$ · mol$^{-1}$)[d] |
|---|---|---|---|
| Octan-1-ol | 258.10 | 42.319[b] | 93.10 |
| *n*-Hexadecane | 291.54 | 51.914[c] | 170.56 |
| *n*-Dodecane | 263.46 | 35.908[c] | 129.64 |
| *n*-Undecane | 247.64 | 22.123[c] | 119.41 |

*n*-octan-1-ol + *n*-undecane

Zofia Plesnar, Pawel Gierycz, Andrzej Bylicki, (Solid + liquid) equilibria in (*n*-octan-1-ol + *n*-hexadecane or *n*-dodecane or *n*-undecane), J. Chem. Thermodynamics 1990, 22, 393-398

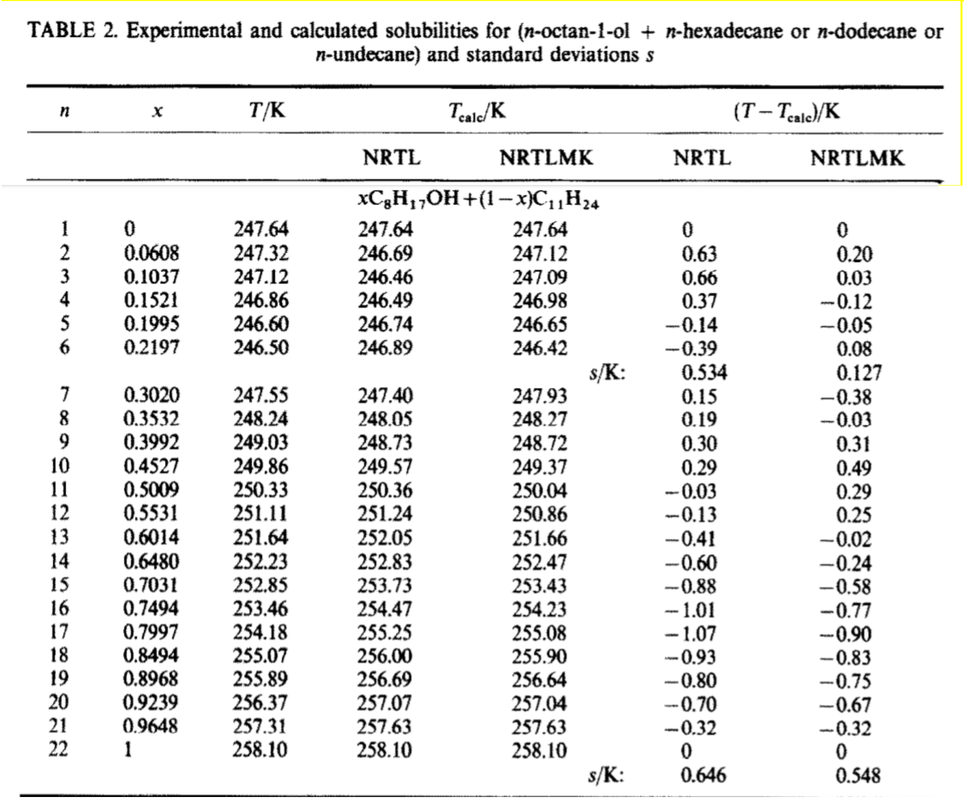


TABLE 2. Experimental and calculated solubilities for (*n*-octan-1-ol + *n*-hexadecane or *n*-dodecane or *n*-undecane) and standard deviations *s*

| $n$ | $x$ | $T$/K | $T_{calc}$/K | | $(T-T_{calc})$/K | |
|---|---|---|---|---|---|---|
| | | | NRTL | NRTLMK | NRTL | NRTLMK |
| | | | $xC_8H_{17}OH+(1-x)C_{11}H_{24}$ | | | |
| 1 | 0 | 247.64 | 247.64 | 247.64 | 0 | 0 |
| 2 | 0.0608 | 247.32 | 246.69 | 247.12 | 0.63 | 0.20 |
| 3 | 0.1037 | 247.12 | 246.46 | 247.09 | 0.66 | 0.03 |
| 4 | 0.1521 | 246.86 | 246.49 | 246.98 | 0.37 | −0.12 |
| 5 | 0.1995 | 246.60 | 246.74 | 246.65 | −0.14 | −0.05 |
| 6 | 0.2197 | 246.50 | 246.89 | 246.42 | −0.39 | 0.08 |
| | | | | $s$/K: | 0.534 | 0.127 |
| 7 | 0.3020 | 247.55 | 247.40 | 247.93 | 0.15 | −0.38 |
| 8 | 0.3532 | 248.24 | 248.05 | 248.27 | 0.19 | −0.03 |
| 9 | 0.3992 | 249.03 | 248.73 | 248.72 | 0.30 | 0.31 |
| 10 | 0.4527 | 249.86 | 249.57 | 249.37 | 0.29 | 0.49 |
| 11 | 0.5009 | 250.33 | 250.36 | 250.04 | −0.03 | 0.29 |
| 12 | 0.5531 | 251.11 | 251.24 | 250.86 | −0.13 | 0.25 |
| 13 | 0.6014 | 251.64 | 252.05 | 251.66 | −0.41 | −0.02 |
| 14 | 0.6480 | 252.23 | 252.83 | 252.47 | −0.60 | −0.24 |
| 15 | 0.7031 | 252.85 | 253.73 | 253.43 | −0.88 | −0.58 |
| 16 | 0.7494 | 253.46 | 254.47 | 254.23 | −1.01 | −0.77 |
| 17 | 0.7997 | 254.18 | 255.25 | 255.08 | −1.07 | −0.90 |
| 18 | 0.8494 | 255.07 | 256.00 | 255.90 | −0.93 | −0.83 |
| 19 | 0.8968 | 255.89 | 256.69 | 256.64 | −0.80 | −0.75 |
| 20 | 0.9239 | 256.37 | 257.07 | 257.04 | −0.70 | −0.67 |
| 21 | 0.9648 | 257.31 | 257.63 | 257.63 | −0.32 | −0.32 |
| 22 | 1 | 258.10 | 258.10 | 258.10 | 0 | 0 |
| | | | | $s$/K: | 0.646 | 0.548 |

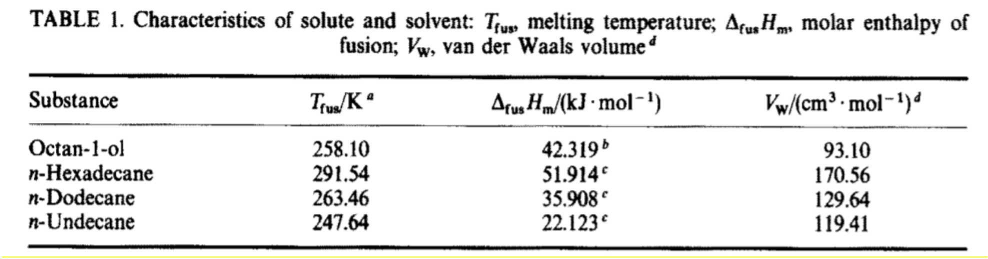


TABLE 1. Characteristics of solute and solvent: $T_{fus}$, melting temperature; $\Delta_{fus}H_m$, molar enthalpy of fusion; $V_W$, van der Waals volume[d]

| Substance | $T_{fus}$/K[a] | $\Delta_{fus}H_m$/(kJ · mol$^{-1}$) | $V_W$/(cm$^3$ · mol$^{-1}$)[d] |
|---|---|---|---|
| Octan-1-ol | 258.10 | 42.319[b] | 93.10 |
| *n*-Hexadecane | 291.54 | 51.914[c] | 170.56 |
| *n*-Dodecane | 263.46 | 35.908[c] | 129.64 |
| *n*-Undecane | 247.64 | 22.123[c] | 119.41 |

1-ethyl-1-methylmorpholinium bromide + diethylene glycol

Marek Królikowski, Marta Królikowska, Aleksandra Lipińska, Phase equilibria study on bromide-based ionic liquids with glycols and sulfolane. Experimental data and correlation, The Journal of Chemical Thermodynamics, Volume 122, July 2018, Pages 142-153

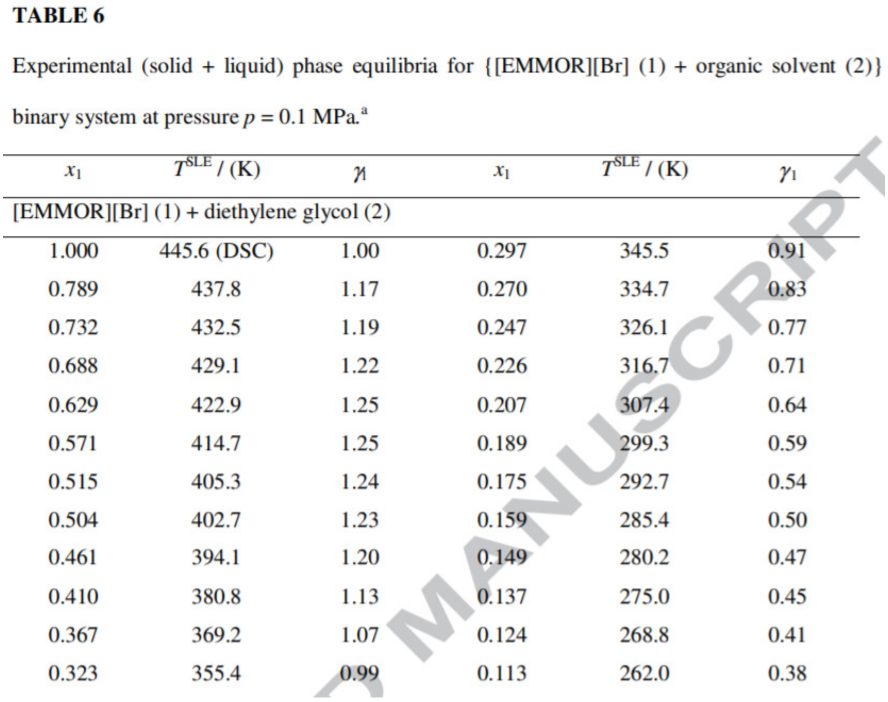


**TABLE 6**

Experimental (solid + liquid) phase equilibria for {[EMMOR][Br] (1) + organic solvent (2)} binary system at pressure $p$ = 0.1 MPa.[a]

| $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| [EMMOR][Br] (1) + diethylene glycol (2) | | | | | |
| 1.000 | 445.6 (DSC) | 1.00 | 0.297 | 345.5 | 0.91 |
| 0.789 | 437.8 | 1.17 | 0.270 | 334.7 | 0.83 |
| 0.732 | 432.5 | 1.19 | 0.247 | 326.1 | 0.77 |
| 0.688 | 429.1 | 1.22 | 0.226 | 316.7 | 0.71 |
| 0.629 | 422.9 | 1.25 | 0.207 | 307.4 | 0.64 |
| 0.571 | 414.7 | 1.25 | 0.189 | 299.3 | 0.59 |
| 0.515 | 405.3 | 1.24 | 0.175 | 292.7 | 0.54 |
| 0.504 | 402.7 | 1.23 | 0.159 | 285.4 | 0.50 |
| 0.461 | 394.1 | 1.20 | 0.149 | 280.2 | 0.47 |
| 0.410 | 380.8 | 1.13 | 0.137 | 275.0 | 0.45 |
| 0.367 | 369.2 | 1.07 | 0.124 | 268.8 | 0.41 |
| 0.323 | 355.4 | 0.99 | 0.113 | 262.0 | 0.38 |

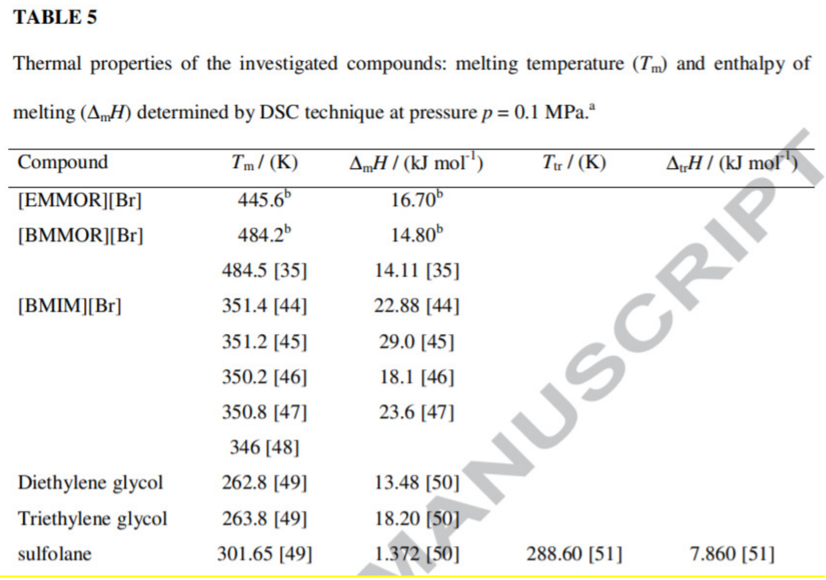


**TABLE 5**

Thermal properties of the investigated compounds: melting temperature ($T_m$) and enthalpy of melting ($\Delta_m H$) determined by DSC technique at pressure $p$ = 0.1 MPa.[a]

| Compound | $T_m$ / (K) | $\Delta_m H$ / (kJ mol$^{-1}$) | $T_{tr}$ / (K) | $\Delta_{tr} H$ / (kJ mol$^{-1}$) |
|---|---|---|---|---|
| [EMMOR][Br] | 445.6[b] | 16.70[b] | | |
| [BMMOR][Br] | 484.2[b] | 14.80[b] | | |
| | 484.5 [35] | 14.11 [35] | | |
| [BMIM][Br] | 351.4 [44] | 22.88 [44] | | |
| | 351.2 [45] | 29.0 [45] | | |
| | 350.2 [46] | 18.1 [46] | | |
| | 350.8 [47] | 23.6 [47] | | |
| | 346 [48] | | | |
| Diethylene glycol | 262.8 [49] | 13.48 [50] | | |
| Triethylene glycol | 263.8 [49] | 18.20 [50] | | |
| sulfolane | 301.65 [49] | 1.372 [50] | 288.60 [51] | 7.860 [51] |

1-ethyl-1-methylmorpholinium bromide + triethylene glycol
Marek Królikowski, Marta Królikowska, Aleksandra Lipińska, Phase equilibria study on bromide-based ionic liquids with glycols and sulfolane. Experimental data and correlation, The Journal of Chemical Thermodynamics, Volume 122, July 2018, Pages 142-153

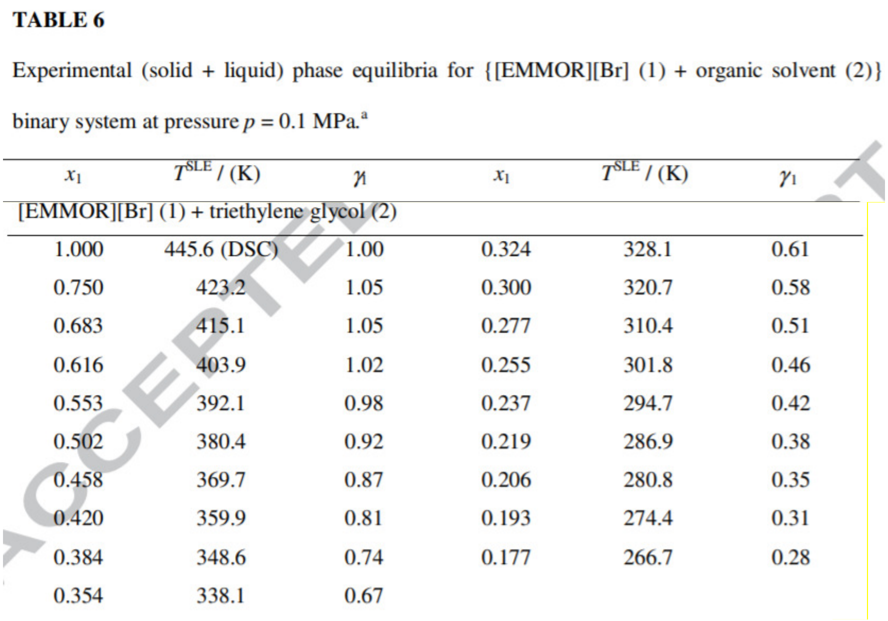


**TABLE 6**

Experimental (solid + liquid) phase equilibria for {[EMMOR][Br] (1) + organic solvent (2)} binary system at pressure $p$ = 0.1 MPa.[a]

| $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| [EMMOR][Br] (1) + triethylene glycol (2) | | | | | |
| 1.000 | 445.6 (DSC) | 1.00 | 0.324 | 328.1 | 0.61 |
| 0.750 | 423.2 | 1.05 | 0.300 | 320.7 | 0.58 |
| 0.683 | 415.1 | 1.05 | 0.277 | 310.4 | 0.51 |
| 0.616 | 403.9 | 1.02 | 0.255 | 301.8 | 0.46 |
| 0.553 | 392.1 | 0.98 | 0.237 | 294.7 | 0.42 |
| 0.502 | 380.4 | 0.92 | 0.219 | 286.9 | 0.38 |
| 0.458 | 369.7 | 0.87 | 0.206 | 280.8 | 0.35 |
| 0.420 | 359.9 | 0.81 | 0.193 | 274.4 | 0.31 |
| 0.384 | 348.6 | 0.74 | 0.177 | 266.7 | 0.28 |
| 0.354 | 338.1 | 0.67 | | | |

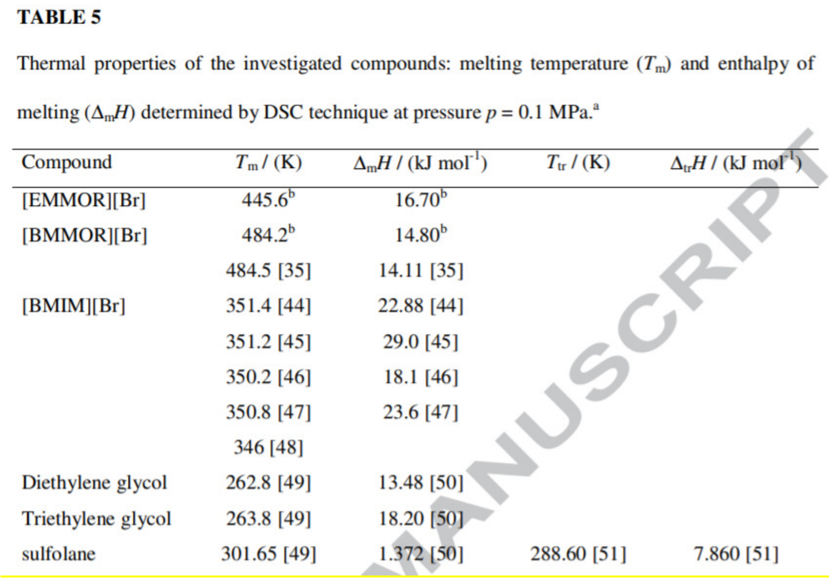


**TABLE 5**

Thermal properties of the investigated compounds: melting temperature ($T_m$) and enthalpy of melting ($\Delta_m H$) determined by DSC technique at pressure $p$ = 0.1 MPa.[a]

| Compound | $T_m$ / (K) | $\Delta_m H$ / (kJ mol$^{-1}$) | $T_{tr}$ / (K) | $\Delta_{tr} H$ / (kJ mol$^{-1}$) |
|---|---|---|---|---|
| [EMMOR][Br] | 445.6[b] | 16.70[b] | | |
| [BMMOR][Br] | 484.2[b] | 14.80[b] | | |
| | 484.5 [35] | 14.11 [35] | | |
| [BMIM][Br] | 351.4 [44] | 22.88 [44] | | |
| | 351.2 [45] | 29.0 [45] | | |
| | 350.2 [46] | 18.1 [46] | | |
| | 350.8 [47] | 23.6 [47] | | |
| | 346 [48] | | | |
| Diethylene glycol | 262.8 [49] | 13.48 [50] | | |
| Triethylene glycol | 263.8 [49] | 18.20 [50] | | |
| sulfolane | 301.65 [49] | 1.372 [50] | 288.60 [51] | 7.860 [51] |

1-ethyl-1-methylmorpholinium bromide + sulfolane

Marek Królikowski, Marta Królikowska, Aleksandra Lipińska, Phase equilibria study on bromide-based ionic liquids with glycols and sulfolane. Experimental data and correlation, The Journal of Chemical Thermodynamics, Volume 122, July 2018, Pages 142-153

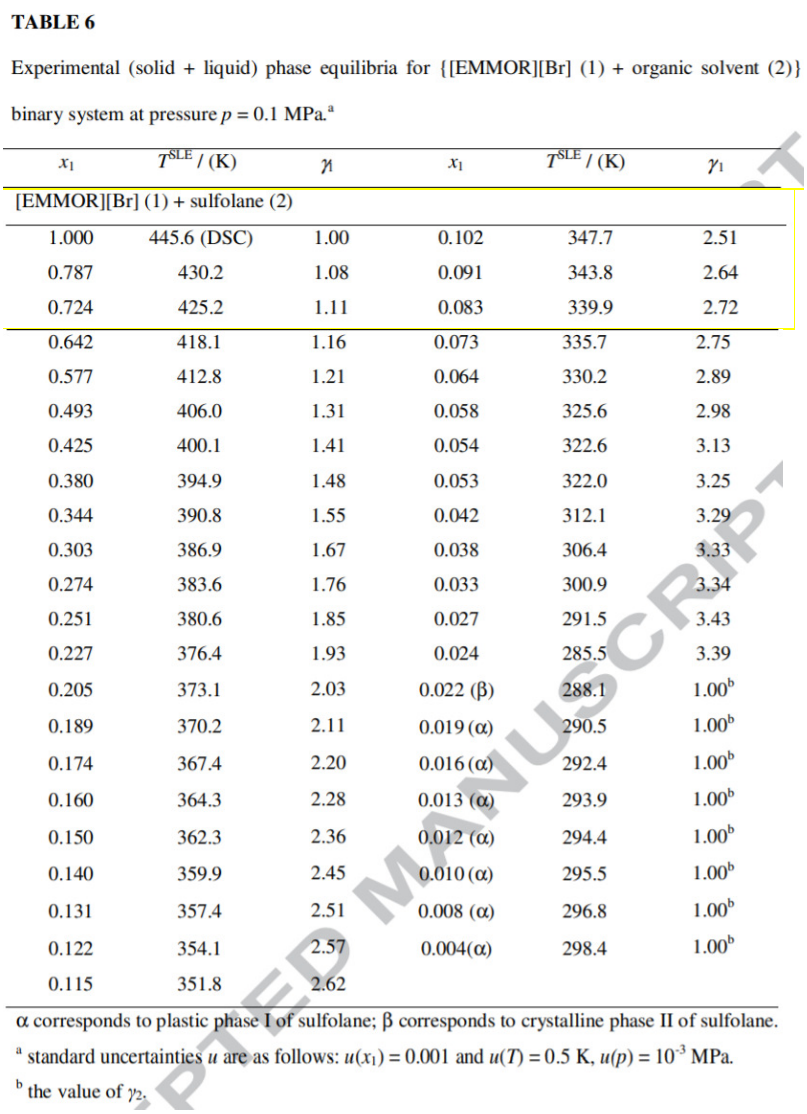


**TABLE 6**

Experimental (solid + liquid) phase equilibria for {[EMMOR][Br] (1) + organic solvent (2)} binary system at pressure $p$ = 0.1 MPa.[a]

| $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| [EMMOR][Br] (1) + sulfolane (2) | | | | | |
| 1.000 | 445.6 (DSC) | 1.00 | 0.102 | 347.7 | 2.51 |
| 0.787 | 430.2 | 1.08 | 0.091 | 343.8 | 2.64 |
| 0.724 | 425.2 | 1.11 | 0.083 | 339.9 | 2.72 |
| 0.642 | 418.1 | 1.16 | 0.073 | 335.7 | 2.75 |
| 0.577 | 412.8 | 1.21 | 0.064 | 330.2 | 2.89 |
| 0.493 | 406.0 | 1.31 | 0.058 | 325.6 | 2.98 |
| 0.425 | 400.1 | 1.41 | 0.054 | 322.6 | 3.13 |
| 0.380 | 394.9 | 1.48 | 0.053 | 322.0 | 3.25 |
| 0.344 | 390.8 | 1.55 | 0.042 | 312.1 | 3.29 |
| 0.303 | 386.9 | 1.67 | 0.038 | 306.4 | 3.33 |
| 0.274 | 383.6 | 1.76 | 0.033 | 300.9 | 3.34 |
| 0.251 | 380.6 | 1.85 | 0.027 | 291.5 | 3.43 |
| 0.227 | 376.4 | 1.93 | 0.024 | 285.5 | 3.39 |
| 0.205 | 373.1 | 2.03 | 0.022 (β) | 288.1 | 1.00[b] |
| 0.189 | 370.2 | 2.11 | 0.019 (α) | 290.5 | 1.00[b] |
| 0.174 | 367.4 | 2.20 | 0.016 (α) | 292.4 | 1.00[b] |
| 0.160 | 364.3 | 2.28 | 0.013 (α) | 293.9 | 1.00[b] |
| 0.150 | 362.3 | 2.36 | 0.012 (α) | 294.4 | 1.00[b] |
| 0.140 | 359.9 | 2.45 | 0.010 (α) | 295.5 | 1.00[b] |
| 0.131 | 357.4 | 2.51 | 0.008 (α) | 296.8 | 1.00[b] |
| 0.122 | 354.1 | 2.57 | 0.004(α) | 298.4 | 1.00[b] |
| 0.115 | 351.8 | 2.62 | | | |

α corresponds to plastic phase I of sulfolane; β corresponds to crystalline phase II of sulfolane.

[a] standard uncertainties $u$ are as follows: $u(x_1)$ = 0.001 and $u(T)$ = 0.5 K, $u(p)$ = $10^{-3}$ MPa.

[b] the value of $\gamma_2$.

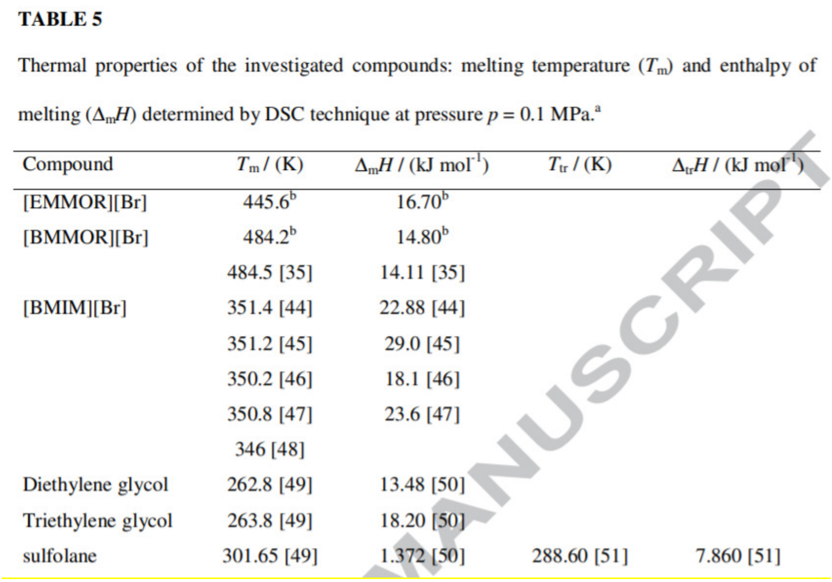


**TABLE 5**

Thermal properties of the investigated compounds: melting temperature ($T_m$) and enthalpy of melting ($\Delta_m H$) determined by DSC technique at pressure $p$ = 0.1 MPa.[a]

| Compound | $T_m$ / (K) | $\Delta_m H$ / (kJ mol$^{-1}$) | $T_{tr}$ / (K) | $\Delta_{tr} H$ / (kJ mol$^{-1}$) |
|---|---|---|---|---|
| [EMMOR][Br] | 445.6[b] | 16.70[b] | | |
| [BMMOR][Br] | 484.2[b] | 14.80[b] | | |
| | 484.5 [35] | 14.11 [35] | | |
| [BMIM][Br] | 351.4 [44] | 22.88 [44] | | |
| | 351.2 [45] | 29.0 [45] | | |
| | 350.2 [46] | 18.1 [46] | | |
| | 350.8 [47] | 23.6 [47] | | |
| | 346 [48] | | | |
| Diethylene glycol | 262.8 [49] | 13.48 [50] | | |
| Triethylene glycol | 263.8 [49] | 18.20 [50] | | |
| sulfolane | 301.65 [49] | 1.372 [50] | 288.60 [51] | 7.860 [51] |

1-butyl-1-methylmorpholinium bromide + diethylene glycol

Marek Królikowski, Marta Królikowska, Aleksandra Lipińska, Phase equilibria study on bromide-based ionic liquids with glycols and sulfolane. Experimental data and correlation, The Journal of Chemical Thermodynamics, Volume 122, July 2018, Pages 142-153

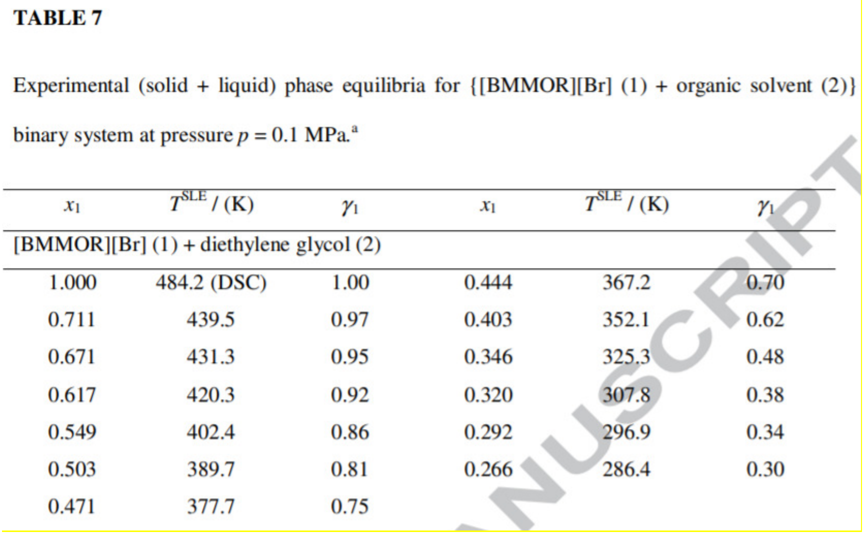


**TABLE 7**

Experimental (solid + liquid) phase equilibria for {[BMMOR][Br] (1) + organic solvent (2)} binary system at pressure $p = 0.1$ MPa.[a]

| $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| [BMMOR][Br] (1) + diethylene glycol (2) | | | | | |
| 1.000 | 484.2 (DSC) | 1.00 | 0.444 | 367.2 | 0.70 |
| 0.711 | 439.5 | 0.97 | 0.403 | 352.1 | 0.62 |
| 0.671 | 431.3 | 0.95 | 0.346 | 325.3 | 0.48 |
| 0.617 | 420.3 | 0.92 | 0.320 | 307.8 | 0.38 |
| 0.549 | 402.4 | 0.86 | 0.292 | 296.9 | 0.34 |
| 0.503 | 389.7 | 0.81 | 0.266 | 286.4 | 0.30 |
| 0.471 | 377.7 | 0.75 | | | |

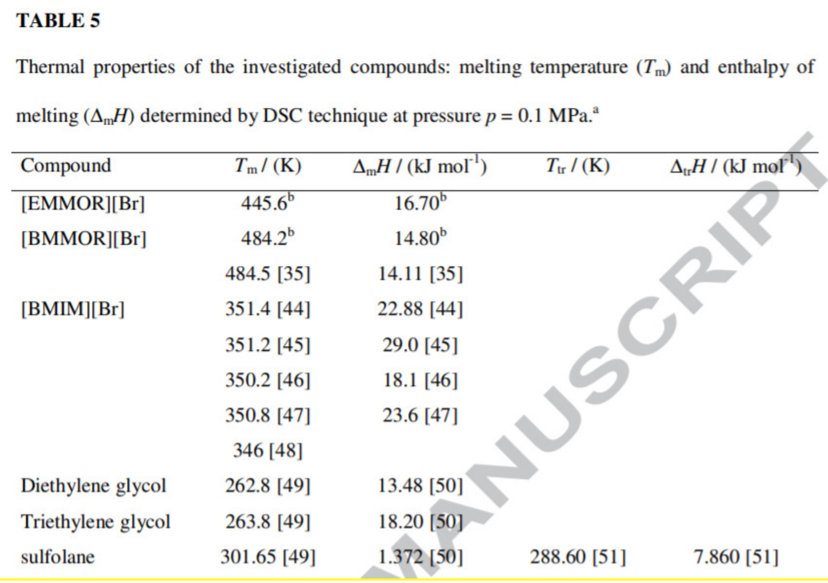


**TABLE 5**

Thermal properties of the investigated compounds: melting temperature ($T_m$) and enthalpy of melting ($\Delta_m H$) determined by DSC technique at pressure $p = 0.1$ MPa.[a]

| Compound | $T_m$ / (K) | $\Delta_m H$ / (kJ mol$^{-1}$) | $T_{tr}$ / (K) | $\Delta_{tr}H$ / (kJ mol$^{-1}$) |
|---|---|---|---|---|
| [EMMOR][Br] | 445.6[b] | 16.70[b] | | |
| [BMMOR][Br] | 484.2[b] | 14.80[b] | | |
| | 484.5 [35] | 14.11 [35] | | |
| [BMIM][Br] | 351.4 [44] | 22.88 [44] | | |
| | 351.2 [45] | 29.0 [45] | | |
| | 350.2 [46] | 18.1 [46] | | |
| | 350.8 [47] | 23.6 [47] | | |
| | 346 [48] | | | |
| Diethylene glycol | 262.8 [49] | 13.48 [50] | | |
| Triethylene glycol | 263.8 [49] | 18.20 [50] | | |
| sulfolane | 301.65 [49] | 1.372 [50] | 288.60 [51] | 7.860 [51] |

1-butyl-1-methylmorpholinium bromide + triethylene glycol
Marek Królikowski, Marta Królikowska, Aleksandra Lipińska, Phase equilibria study on bromide-based ionic liquids with glycols and sulfolane. Experimental data and correlation, The Journal of Chemical Thermodynamics, Volume 122, July 2018, Pages 142-153

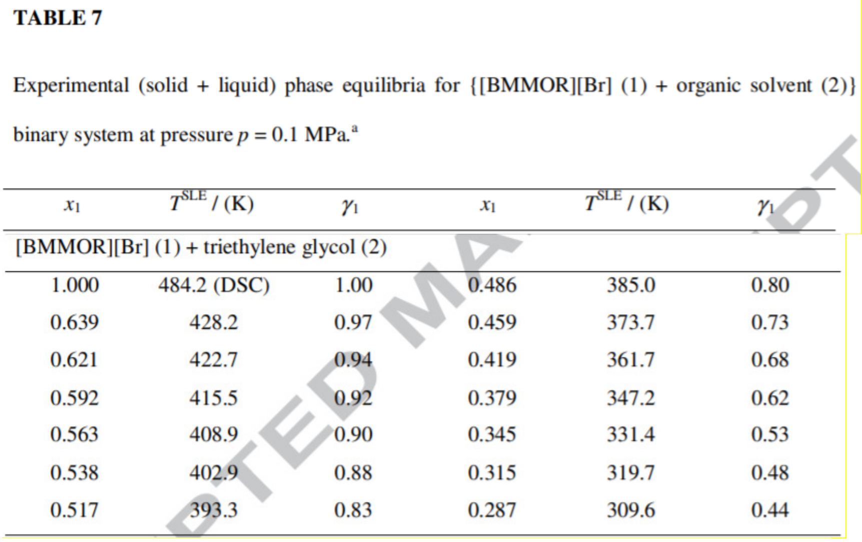


**TABLE 7**

Experimental (solid + liquid) phase equilibria for {[BMMOR][Br] (1) + organic solvent (2)} binary system at pressure $p = 0.1$ MPa.[a]

| $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| [BMMOR][Br] (1) + triethylene glycol (2) | | | | | |
| 1.000 | 484.2 (DSC) | 1.00 | 0.486 | 385.0 | 0.80 |
| 0.639 | 428.2 | 0.97 | 0.459 | 373.7 | 0.73 |
| 0.621 | 422.7 | 0.94 | 0.419 | 361.7 | 0.68 |
| 0.592 | 415.5 | 0.92 | 0.379 | 347.2 | 0.62 |
| 0.563 | 408.9 | 0.90 | 0.345 | 331.4 | 0.53 |
| 0.538 | 402.9 | 0.88 | 0.315 | 319.7 | 0.48 |
| 0.517 | 393.3 | 0.83 | 0.287 | 309.6 | 0.44 |

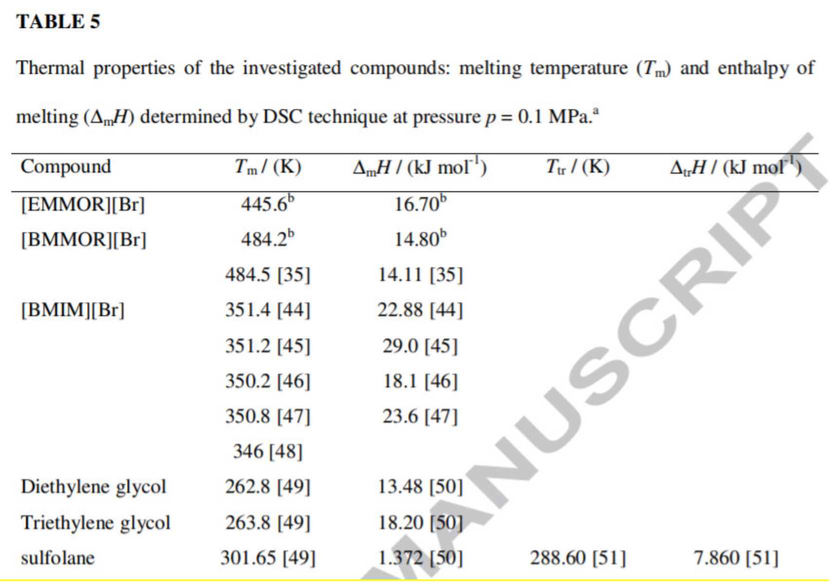


**TABLE 5**

Thermal properties of the investigated compounds: melting temperature ($T_m$) and enthalpy of melting ($\Delta_m H$) determined by DSC technique at pressure $p = 0.1$ MPa.[a]

| Compound | $T_m$ / (K) | $\Delta_m H$ / (kJ mol$^{-1}$) | $T_{tr}$ / (K) | $\Delta_{tr} H$ / (kJ mol$^{-1}$) |
|---|---|---|---|---|
| [EMMOR][Br] | 445.6[b] | 16.70[b] | | |
| [BMMOR][Br] | 484.2[b] | 14.80[b] | | |
| | 484.5 [35] | 14.11 [35] | | |
| [BMIM][Br] | 351.4 [44] | 22.88 [44] | | |
| | 351.2 [45] | 29.0 [45] | | |
| | 350.2 [46] | 18.1 [46] | | |
| | 350.8 [47] | 23.6 [47] | | |
| | 346 [48] | | | |
| Diethylene glycol | 262.8 [49] | 13.48 [50] | | |
| Triethylene glycol | 263.8 [49] | 18.20 [50] | | |
| sulfolane | 301.65 [49] | 1.372 [50] | 288.60 [51] | 7.860 [51] |

1-butyl-1-methylmorpholinium bromide + sulfolane

Marek Królikowski, Marta Królikowska, Aleksandra Lipińska, Phase equilibria study on bromide-based ionic liquids with glycols and sulfolane. Experimental data and correlation, The Journal of Chemical Thermodynamics, Volume 122, July 2018, Pages 142-153

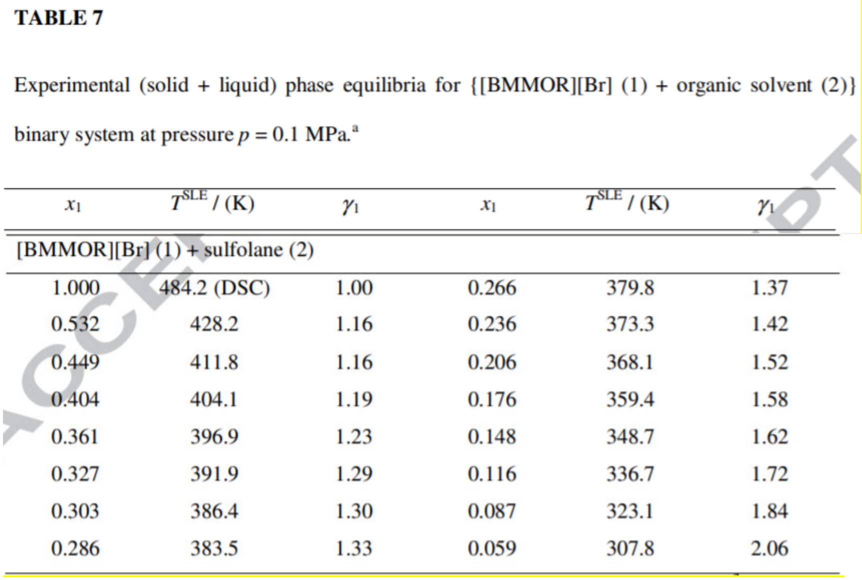


**TABLE 7**

Experimental (solid + liquid) phase equilibria for {[BMMOR][Br] (1) + organic solvent (2)} binary system at pressure $p = 0.1$ MPa.[a]

| $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| [BMMOR][Br] (1) + sulfolane (2) | | | | | |
| 1.000 | 484.2 (DSC) | 1.00 | 0.266 | 379.8 | 1.37 |
| 0.532 | 428.2 | 1.16 | 0.236 | 373.3 | 1.42 |
| 0.449 | 411.8 | 1.16 | 0.206 | 368.1 | 1.52 |
| 0.404 | 404.1 | 1.19 | 0.176 | 359.4 | 1.58 |
| 0.361 | 396.9 | 1.23 | 0.148 | 348.7 | 1.62 |
| 0.327 | 391.9 | 1.29 | 0.116 | 336.7 | 1.72 |
| 0.303 | 386.4 | 1.30 | 0.087 | 323.1 | 1.84 |
| 0.286 | 383.5 | 1.33 | 0.059 | 307.8 | 2.06 |

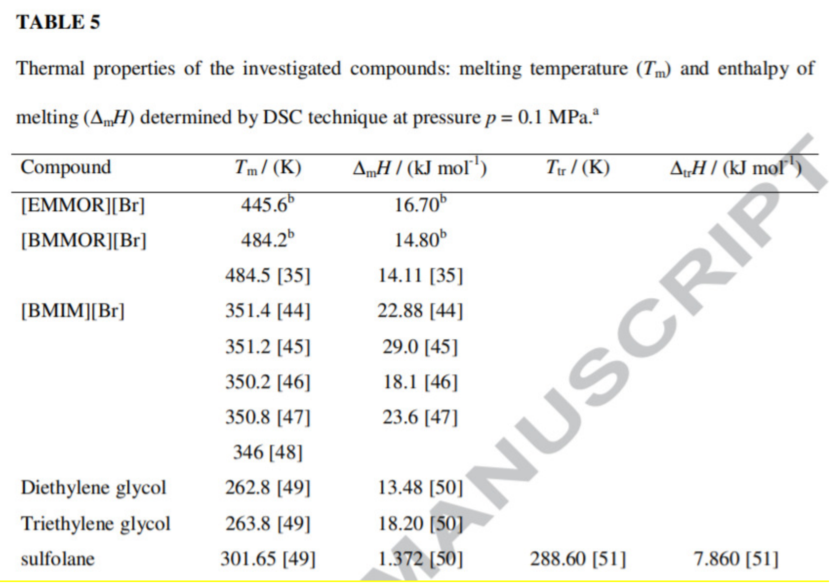


**TABLE 5**

Thermal properties of the investigated compounds: melting temperature ($T_m$) and enthalpy of melting ($\Delta_m H$) determined by DSC technique at pressure $p = 0.1$ MPa.[a]

| Compound | $T_m$ / (K) | $\Delta_m H$ / (kJ mol$^{-1}$) | $T_{tr}$ / (K) | $\Delta_{tr} H$ / (kJ mol$^{-1}$) |
|---|---|---|---|---|
| [EMMOR][Br] | $445.6^{b}$ | $16.70^{b}$ | | |
| [BMMOR][Br] | $484.2^{b}$ | $14.80^{b}$ | | |
| | 484.5 [35] | 14.11 [35] | | |
| [BMIM][Br] | 351.4 [44] | 22.88 [44] | | |
| | 351.2 [45] | 29.0 [45] | | |
| | 350.2 [46] | 18.1 [46] | | |
| | 350.8 [47] | 23.6 [47] | | |
| | 346 [48] | | | |
| Diethylene glycol | 262.8 [49] | 13.48 [50] | | |
| Triethylene glycol | 263.8 [49] | 18.20 [50] | | |
| sulfolane | 301.65 [49] | 1.372 [50] | 288.60 [51] | 7.860 [51] |

1-butyl-1-methylimidazolium bromide + diethylene glycol
Marek Królikowski, Marta Królikowska, Aleksandra Lipińska, Phase equilibria study on bromide-based ionic liquids with glycols and sulfolane. Experimental data and correlation, The Journal of Chemical Thermodynamics, Volume 122, July 2018, Pages 142-153

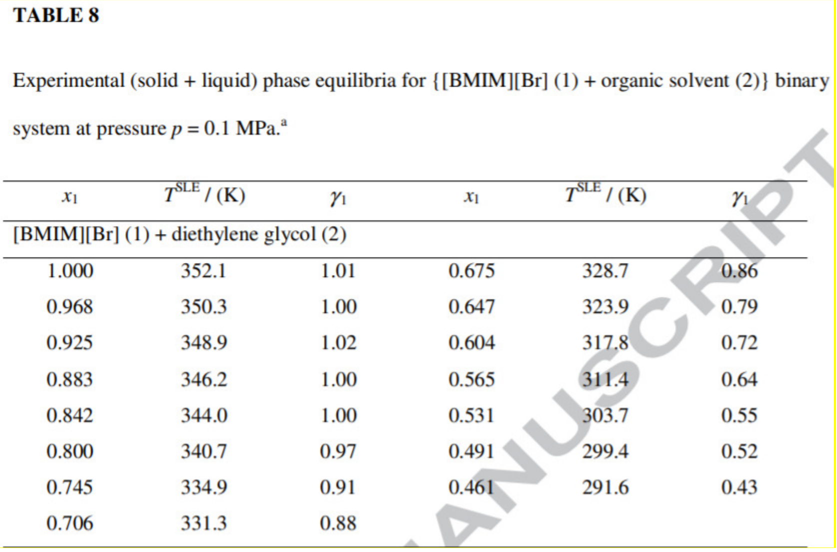


**TABLE 8**

Experimental (solid + liquid) phase equilibria for {[BMIM][Br] (1) + organic solvent (2)} binary system at pressure $p = 0.1$ MPa.[a]

| $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| [BMIM][Br] (1) + diethylene glycol (2) | | | | | |
| 1.000 | 352.1 | 1.01 | 0.675 | 328.7 | 0.86 |
| 0.968 | 350.3 | 1.00 | 0.647 | 323.9 | 0.79 |
| 0.925 | 348.9 | 1.02 | 0.604 | 317.8 | 0.72 |
| 0.883 | 346.2 | 1.00 | 0.565 | 311.4 | 0.64 |
| 0.842 | 344.0 | 1.00 | 0.531 | 303.7 | 0.55 |
| 0.800 | 340.7 | 0.97 | 0.491 | 299.4 | 0.52 |
| 0.745 | 334.9 | 0.91 | 0.461 | 291.6 | 0.43 |
| 0.706 | 331.3 | 0.88 | | | |

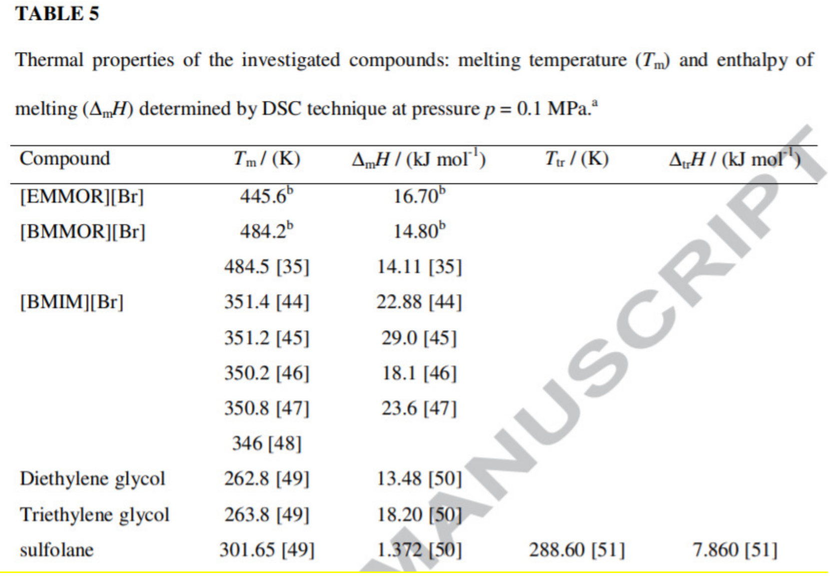


**TABLE 5**

Thermal properties of the investigated compounds: melting temperature ($T_m$) and enthalpy of melting ($\Delta_m H$) determined by DSC technique at pressure $p = 0.1$ MPa.[a]

| Compound | $T_m$ / (K) | $\Delta_m H$ / (kJ mol$^{-1}$) | $T_{tr}$ / (K) | $\Delta_{tr} H$ / (kJ mol$^{-1}$) |
|---|---|---|---|---|
| [EMMOR][Br] | 445.6[b] | 16.70[b] | | |
| [BMMOR][Br] | 484.2[b] | 14.80[b] | | |
| | 484.5 [35] | 14.11 [35] | | |
| [BMIM][Br] | 351.4 [44] | 22.88 [44] | | |
| | 351.2 [45] | 29.0 [45] | | |
| | 350.2 [46] | 18.1 [46] | | |
| | 350.8 [47] | 23.6 [47] | | |
| | 346 [48] | | | |
| Diethylene glycol | 262.8 [49] | 13.48 [50] | | |
| Triethylene glycol | 263.8 [49] | 18.20 [50] | | |
| sulfolane | 301.65 [49] | 1.372 [50] | 288.60 [51] | 7.860 [51] |

1-butyl-1-methylimidazolium bromide + triethylene glycol
Marek Królikowski, Marta Królikowska, Aleksandra Lipińska, Phase equilibria study on bromide-based ionic liquids with glycols and sulfolane. Experimental data and correlation, The Journal of Chemical Thermodynamics, Volume 122, July 2018, Pages 142-153

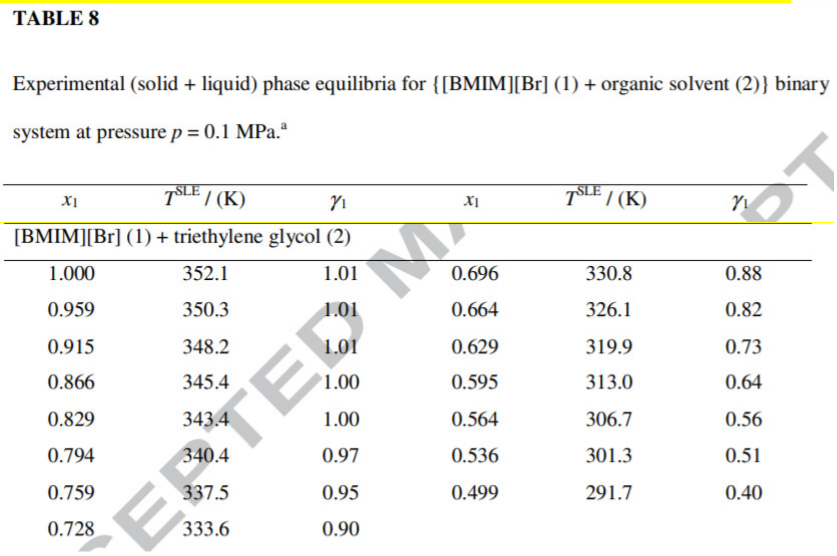


**TABLE 8**

Experimental (solid + liquid) phase equilibria for {[BMIM][Br] (1) + organic solvent (2)} binary system at pressure $p = 0.1$ MPa.[a]

| $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| [BMIM][Br] (1) + triethylene glycol (2) | | | | | |
| 1.000 | 352.1 | 1.01 | 0.696 | 330.8 | 0.88 |
| 0.959 | 350.3 | 1.01 | 0.664 | 326.1 | 0.82 |
| 0.915 | 348.2 | 1.01 | 0.629 | 319.9 | 0.73 |
| 0.866 | 345.4 | 1.00 | 0.595 | 313.0 | 0.64 |
| 0.829 | 343.4 | 1.00 | 0.564 | 306.7 | 0.56 |
| 0.794 | 340.4 | 0.97 | 0.536 | 301.3 | 0.51 |
| 0.759 | 337.5 | 0.95 | 0.499 | 291.7 | 0.40 |
| 0.728 | 333.6 | 0.90 | | | |

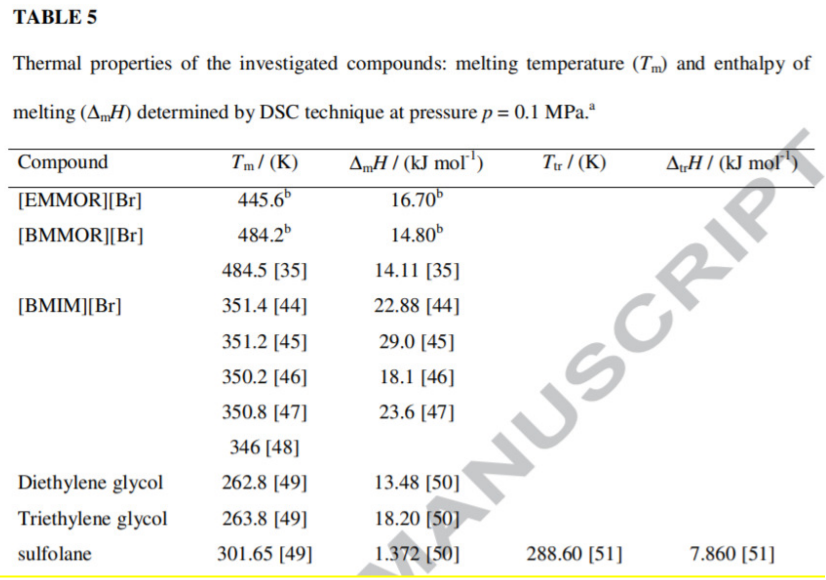


**TABLE 5**

Thermal properties of the investigated compounds: melting temperature ($T_m$) and enthalpy of melting ($\Delta_m H$) determined by DSC technique at pressure $p = 0.1$ MPa.[a]

| Compound | $T_m$ / (K) | $\Delta_m H$ / (kJ mol$^{-1}$) | $T_{tr}$ / (K) | $\Delta_{tr}H$ / (kJ mol$^{-1}$) |
|---|---|---|---|---|
| [EMMOR][Br] | 445.6[b] | 16.70[b] | | |
| [BMMOR][Br] | 484.2[b] | 14.80[b] | | |
| | 484.5 [35] | 14.11 [35] | | |
| [BMIM][Br] | 351.4 [44] | 22.88 [44] | | |
| | 351.2 [45] | 29.0 [45] | | |
| | 350.2 [46] | 18.1 [46] | | |
| | 350.8 [47] | 23.6 [47] | | |
| | 346 [48] | | | |
| Diethylene glycol | 262.8 [49] | 13.48 [50] | | |
| Triethylene glycol | 263.8 [49] | 18.20 [50] | | |
| sulfolane | 301.65 [49] | 1.372 [50] | 288.60 [51] | 7.860 [51] |

1-butyl-1-methylimidazolium bromide + sulfolane
Marek Królikowski, Marta Królikowska, Aleksandra Lipińska, Phase equilibria study on bromide-based ionic liquids with glycols and sulfolane. Experimental data and correlation, The Journal of Chemical Thermodynamics, Volume 122, July 2018, Pages 142-153

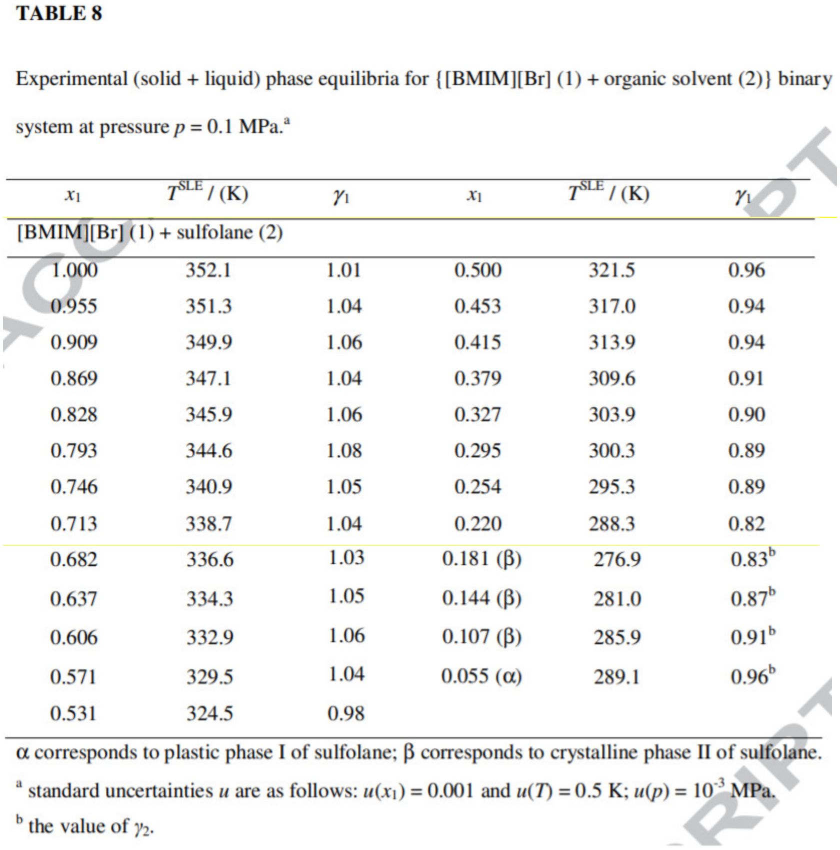


**TABLE 8**

Experimental (solid + liquid) phase equilibria for {[BMIM][Br] (1) + organic solvent (2)} binary system at pressure $p$ = 0.1 MPa.[a]

| $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ | $x_1$ | $T^{SLE}$ / (K) | $\gamma_1$ |
|---|---|---|---|---|---|
| [BMIM][Br] (1) + sulfolane (2) | | | | | |
| 1.000 | 352.1 | 1.01 | 0.500 | 321.5 | 0.96 |
| 0.955 | 351.3 | 1.04 | 0.453 | 317.0 | 0.94 |
| 0.909 | 349.9 | 1.06 | 0.415 | 313.9 | 0.94 |
| 0.869 | 347.1 | 1.04 | 0.379 | 309.6 | 0.91 |
| 0.828 | 345.9 | 1.06 | 0.327 | 303.9 | 0.90 |
| 0.793 | 344.6 | 1.08 | 0.295 | 300.3 | 0.89 |
| 0.746 | 340.9 | 1.05 | 0.254 | 295.3 | 0.89 |
| 0.713 | 338.7 | 1.04 | 0.220 | 288.3 | 0.82 |
| 0.682 | 336.6 | 1.03 | 0.181 (β) | 276.9 | 0.83[b] |
| 0.637 | 334.3 | 1.05 | 0.144 (β) | 281.0 | 0.87[b] |
| 0.606 | 332.9 | 1.06 | 0.107 (β) | 285.9 | 0.91[b] |
| 0.571 | 329.5 | 1.04 | 0.055 (α) | 289.1 | 0.96[b] |
| 0.531 | 324.5 | 0.98 | | | |

α corresponds to plastic phase I of sulfolane; β corresponds to crystalline phase II of sulfolane.

[a] standard uncertainties $u$ are as follows: $u(x_1)$ = 0.001 and $u(T)$ = 0.5 K; $u(p)$ = $10^{-3}$ MPa.

[b] the value of $\gamma_2$.

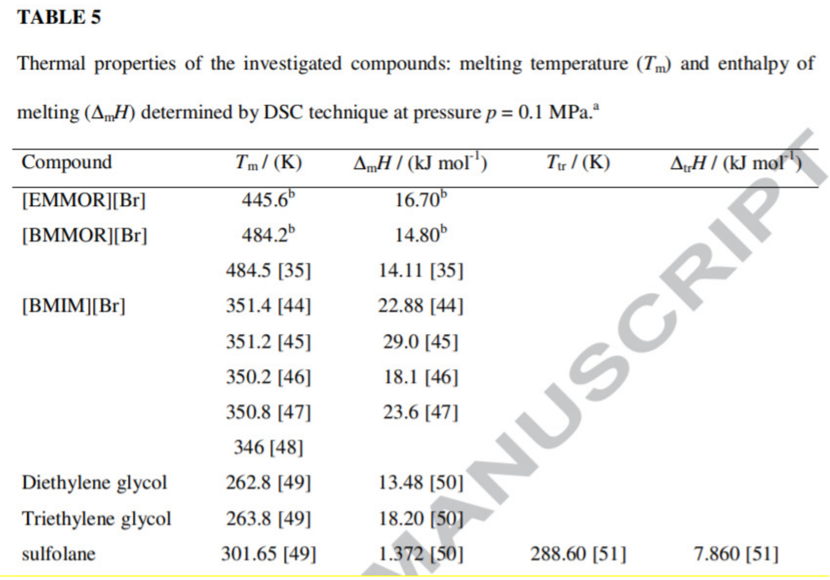


**TABLE 5**

Thermal properties of the investigated compounds: melting temperature ($T_m$) and enthalpy of melting ($\Delta_m H$) determined by DSC technique at pressure $p$ = 0.1 MPa.[a]

| Compound | $T_m$ / (K) | $\Delta_m H$ / (kJ mol$^{-1}$) | $T_{tr}$ / (K) | $\Delta_{tr} H$ / (kJ mol$^{-1}$) |
|---|---|---|---|---|
| [EMMOR][Br] | 445.6[b] | 16.70[b] | | |
| [BMMOR][Br] | 484.2[b] | 14.80[b] | | |
| | 484.5 [35] | 14.11 [35] | | |
| [BMIM][Br] | 351.4 [44] | 22.88 [44] | | |
| | 351.2 [45] | 29.0 [45] | | |
| | 350.2 [46] | 18.1 [46] | | |
| | 350.8 [47] | 23.6 [47] | | |
| | 346 [48] | | | |
| Diethylene glycol | 262.8 [49] | 13.48 [50] | | |
| Triethylene glycol | 263.8 [49] | 18.20 [50] | | |
| sulfolane | 301.65 [49] | 1.372 [50] | 288.60 [51] | 7.860 [51] |