**Table S1.** Comparison between experimental density from litterature () of PEG (1) + water (2) with calculated density values () by using a nonlinear regression for the testing dataset at 298.15K.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **PEG molecular weight [Reference]** |  | **(g/cm3)** | **ρ cal(g/cm3)** | **AAD (%)** |
| PEG 300[ 24] | 0.0000 | 0.9970 | 0.9970 | 0.0030 |
| 0.0066 | 1.0126 | 1.0125 | 0.0140 |
| 0.0148 | 1.0289 | 1.0292 | 0.0319 |
| 0.0251 | 1.0460 | 1.0469 | 0.0903 |
| 0.0385 | 1.0633 | 1.0653 | 0.1843 |
| 0.0566 | 1.0794 | 1.0833 | 0.3609 |
| 0.0826 | 1.0942 | 1.0997 | 0.5050 |
| 0.1229 | 1.1067 | 1.1124 | 0.5156 |
| 0.1937 | 1.1150 | 1.1194 | 0.3943 |
| 0.3508 | 1.1209 | 1.1212 | 0.0225 |
| 1.0000 | 1.1233 | 1.1212 | 0.1864 |
| PEG 400[26] | 0.0000 | 0.9970 | 0.9970 | 0.0035 |
| 0.0050 | 1.0126 | 1.0126 | 0.0036 |
| 0.0190 | 1.0468 | 1.0474 | 0.0606 |
| 0.0291 | 1.0645 | 1.0658 | 0.1242 |
| 0.0431 | 1.0814 | 1.0843 | 0.2693 |
| 0.0634 | 1.0965 | 1.1011 | 0.4159 |
| 0.0951 | 1.1082 | 1.1137 | 0.4972 |
| 0.1504 | 1.1158 | 1.1203 | 0.4054 |
| 0.2719 | 1.1200 | 1.1219 | 0.1668 |
| 0.3403 | 1.1207 | 1.1219 | 0.1076 |
| 0.4330 | 1.1213 | 1.1219 | 0.0545 |
| 0.5199 | 1.1215 | 1.1219 | 0.0366 |
| 0.6873 | 1.1217 | 1.1219 | 0.0188 |
| 0.7996 | 1.1217 | 1.1219 | 0.0188 |
| 0.8923 | 1.1218 | 1.1219 | 0.0099 |
| 1.0000 | 1.1218 | 1.1219 | 0.0099 |
| PEG 400[30] | 0.0000 | 0.9970 | 0.9970 | 0.0035 |
| 0.0050 | 1.0131 | 1.0126 | 0.0457 |
| 0.0111 | 1.0298 | 1.0293 | 0.0486 |
| 0.0189 | 1.0471 | 1.0472 | 0.0121 |
| 0.0292 | 1.0650 | 1.0660 | 0.0921 |
| 0.0431 | 1.0821 | 1.0843 | 0.2045 |
| 0.0633 | 1.0971 | 1.1010 | 0.3554 |
| 0.0951 | 1.1090 | 1.1137 | 0.4247 |
| 0.1527 | 1.1164 | 1.1204 | 0.3608 |
| 0.2885 | 1.1204 | 1.1219 | 0.1325 |
| 1.0000 | 1.1224 | 1.1219 | 0.0436 |
| PEG 600[35] | 0.0000 | 0.9970 | 0.9971 | 0.0072 |
| 0.0075 | 1.0309 | 1.0297 | 0.1116 |
| 0.0196 | 1.0662 | 1.0665 | 0.0324 |
| 0.0431 | 1.0995 | 1.1025 | 0.2700 |
| 0.1001 | 1.1156 | 1.1214 | 0.5219 |
| 0.1998 | 1.1217 | 1.1231 | 0.1231 |
| 0.3001 | 1.1225 | 1.1231 | 0.0535 |
| 0.3994 | 1.1226 | 1.1231 | 0.0446 |
| 0.4983 | 1.1228 | 1.1231 | 0.0268 |
| 0.6977 | 1.1230 | 1.1231 | 0.0090 |
| 0.8849 | 1.1232 | 1.1231 | 0.0088 |
| 1.0000 | 1.1233 | 1.1231 | 0.0177 |