**Supplementary file**

**Development and validation of a unified graphical sorption model: application to sorption of organic liquids into low density polyethylene (LDPE) polymeric membrane**

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**Table S1**. Results obtained for *α*, *β* and *γ*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Compound Name** | **T (K)** | *n* | *α* | *β* | *γ* |
| 1-HEPTANOL | 288.15 | # 1 | 0.6126 | 1.7868 | 1.9895 |
|  |  | # 2 | 0.7357 | 1.7733 | 1.8529 |
|  |  | # 3 | 0.7913 | 1.7748 | 1.8048 |
| **Average** | | | **0.7132** | **1.7783** | **1.8824** |
|  | 298.15 | # 1 | 1.1066 | 1.4024 | 0.9234 |
|  |  | # 2 | 0.5315 | 1.4249 | 1.5676 |
|  |  | # 3 | 1.1321 | 1.8288 | 1.5060 |
| **Average** | | | **0.9234** | **1.5520** | **1.3323** |
|  | 308.15 | # 1 | 0.5180 | 1.4745 | 1.6366 |
|  |  | # 2 | 0.6036 | 1.6156 | 1.7613 |
|  |  | # 3 | 0.6892 | 1.7568 | 1.8859 |
| **Average** | | | **0.6036** | **1.6156** | **1.7613** |
| 1-HEXANOL | 288.15 | # 1 | 0.7132 | 1.5871 | 1.6231 |
|  |  | # 2 | 0.9084 | 1.6997 | 1.6096 |
|  |  | # 3 | 1.0180 | 1.6712 | 1.4715 |
| **Average** | | | **0.8799** | **1.6527** | **1.5681** |
|  | 298.15 | # 1 | 1.2132 | 1.7838 | 1.4580 |
|  |  | # 2 | 1.7132 | 1.9805 | 1.2928 |
|  |  | # 3 | 0.6156 | 1.5991 | 1.7372 |
| **Average** | | | **1.1807** | **1.7878** | **1.4960** |
|  | 308.15 | # 1 | 0.9084 | 1.8964 | 1.8889 |
|  |  | # 2 | 0.5661 | 1.7087 | 1.9640 |
|  |  | # 3 | 1.4339 | 1.5961 | 1.0000 |
| **Average** | | | **0.9695** | **1.7337** | **1.6176** |
| 1-OCTANOL | 288.15 | # 1 | 1.8183 | 1.9384 | 1.2898 |
|  |  | # 2 | 1.2883 | 1.9174 | 1.4159 |
|  |  | # 3 | 0.5225 | 1.7102 | 1.9715 |
| **Average** | | | **1.2097** | **1.8553** | **1.5591** |
|  | 298.15 | # 1 | 0.5691 | 1.7087 | 1.9309 |
|  |  | # 2 | 0.6156 | 1.7072 | 1.8904 |
|  |  | # 3 | 0.6622 | 1.7057 | 1.8498 |
| **Average** | | | **0.6288.156** | **1.7072** | **1.8904** |
|  | 308.15 | # 1 | 0.7087 | 1.7042 | 1.8093 |
|  |  | # 2 | 0.7553 | 1.7027 | 1.7688 |
|  |  | # 3 | 0.7868 | 1.3258 | 1.2132 |
| **Average** | | | **0.7503** | **1.5776** | **1.5971** |
| 1-PENTANOL | 288.15 | # 1 | 1.9625 | 1.8874 | 1.0315 |
|  |  | # 2 | 1.1622 | 1.9715 | 1.7973 |
|  |  | # 3 | 0.8649 | 1.7823 | 1.7913 |
| **Average** | | | **1.3299** | **1.8804** | **1.5400** |
|  | 298.15 | # 1 | 0.6066 | 1.7628 | 1.9955 |
|  |  | # 2 | 0.6141 | 1.6381 | 1.8198 |
|  |  | # 3 | 0.6411 | 1.7538 | 1.9595 |
| **Average** | | | **0.6206** | **1.7182** | **1.9249** |
|  | 308.15 | # 1 | 0.7402 | 1.7958 | 1.9489 |
|  |  | # 2 | 0.7477 | 1.6712 | 1.7733 |
|  |  | # 3 | 0.7748 | 1.7868 | 1.9129 |
| **Average** | | | **0.7542** | **1.7513** | **1.8784** |
| 1-PROPANOL | 288.15 | # 1 | 0.8814 | 1.7042 | 1.7267 |
|  |  | # 2 | 0.9084 | 1.8198 | 1.8664 |
|  |  | # 3 | 0.9880 | 1.6216 | 1.5405 |
| **Average** | | | **0.9298.159** | **1.7152** | **1.7112** |
|  | 298.15 | # 1 | 1.0345 | 1.9775 | 1.9955 |
|  |  | # 2 | 1.0691 | 1.9685 | 1.9595 |
|  |  | # 3 | 1.4084 | 1.9610 | 1.7162 |
| **Average** | | | **1.1707** | **1.9690** | **1.8904** |
|  | 308.15 | # 1 | 1.5420 | 1.9940 | 1.6697 |
|  |  | # 2 | 1.9159 | 1.9775 | 1.3904 |
|  |  | # 3 | 0.5165 | 1.0330 | 1.2643 |
| **Average** | | | **1.3248** | **1.6682** | **1.4415** |
| BENZENE | 288.15 | # 1 | 0.7357 | 1.7733 | 1.8529 |
|  |  | # 2 | 0.5225 | 1.7102 | 1.9715 |
|  |  | # 3 | 1.1622 | 1.9715 | 1.7973 |
| **Average** | | | **0.8068** | **1.8183** | **1.8739** |
|  | 298.15 | # 1 | 0.9084 | 1.8198 | 1.8664 |
|  |  | # 2 | 1.4084 | 1.9610 | 1.7162 |
|  |  | # 3 | 1.9159 | 1.9775 | 1.3904 |
| **Average** | | | **1.4109** | **1.9194** | **1.6577** |
|  | 308.15 | # 1 | 0.6141 | 1.6381 | 1.8198 |
|  |  | # 2 | 0.8814 | 1.7042 | 1.7267 |
|  |  | # 3 | 1.0180 | 1.6712 | 1.4715 |
| **Average** | | | **0.8378** | **1.6712** | **1.6727** |
| BENZOYL-CHLORIDE | 298.15 | # 1 | 1.8183 | 1.9384 | 1.2898 |
|  |  | # 2 | 0.9880 | 1.6216 | 1.5405 |
|  |  | # 3 | 0.5661 | 1.7087 | 1.9640 |
| **Average** | | | **1.1241** | **1.7562** | **1.5981** |
| CHLOROBENZENE | 298.15 | # 1 | 0.7402 | 1.7958 | 1.9489 |
|  |  | # 2 | 0.9084 | 1.6997 | 1.6096 |
|  |  | # 3 | 0.6126 | 1.7868 | 1.9895 |
| **Average** | | | **0.7537** | **1.7608** | **1.8493** |
| CYCLOHEXANE | 288.15 | # 1 | 0.7357 | 1.7733 | 1.8529 |
|  |  | # 2 | 0.7913 | 1.7748 | 1.8048 |
|  |  | # 3 | 1.1066 | 1.4024 | 0.9234 |
| **Average** | | | **0.8779** | **1.6502** | **1.5270** |
|  | 298.15 | # 1 | 0.5315 | 1.4249 | 1.5676 |
|  |  | # 2 | 1.1321 | 1.8288 | 1.5060 |
|  |  | # 3 | 0.5180 | 1.4745 | 1.6366 |
| **Average** | | | **0.7272** | **1.5761** | **1.5701** |
|  | 308.15 | # 1 | 0.6036 | 1.6156 | 1.7613 |
|  |  | # 2 | 0.6892 | 1.7568 | 1.8859 |
|  |  | # 3 | 0.7132 | 1.5871 | 1.6231 |
| **Average** | | | **0.6687** | **1.6532** | **1.7568** |
| ETHANOL | 288.15 | # 1 | 0.9084 | 1.6997 | 1.6096 |
|  |  | # 2 | 1.0180 | 1.6712 | 1.4715 |
|  |  | # 3 | 1.2132 | 1.7838 | 1.4580 |
| **Average** | | | **1.0465** | **1.7182** | **1.5130** |
|  | 298.15 | # 1 | 1.7132 | 1.9805 | 1.2928 |
|  |  | # 2 | 0.6156 | 1.5991 | 1.7372 |
|  |  | # 3 | 0.9084 | 1.8964 | 1.8889 |
| **Average** | | | **1.0791** | **1.8253** | **1.6396** |
|  | 308.15 | # 1 | 0.5661 | 1.7087 | 1.9640 |
|  |  | # 2 | 1.4339 | 1.5961 | 1.0000 |
|  |  | # 3 | 1.8183 | 1.9384 | 1.2898 |
| **Average** | | | **1.2728** | **1.7477** | **1.4179** |
| ETHYLBENZENE | 288.15 | # 1 | 1.2883 | 1.9174 | 1.4159 |
|  |  | # 2 | 0.5225 | 1.7102 | 1.9715 |
|  |  | # 3 | 0.5691 | 1.7087 | 1.9309 |
| **Average** | | | **0.7933** | **1.7788** | **1.7728** |
|  | 298.15 | # 1 | 0.6156 | 1.7072 | 1.8904 |
|  |  | # 2 | 0.6622 | 1.7057 | 1.8498 |
|  |  | # 3 | 0.7087 | 1.7042 | 1.8093 |
| **Average** | | | **0.6622** | **1.7057** | **1.8498** |
|  | 308.15 | # 1 | 0.7553 | 1.7027 | 1.7688 |
|  |  | # 2 | 0.7868 | 1.3258 | 1.2132 |
|  |  | # 3 | 1.9625 | 1.8874 | 1.0315 |
| **Average** | | | **1.1682** | **1.6386** | **1.3378** |
| ETHYLCYCLOHEXANE | 288.15 | # 1 | 1.1622 | 1.9715 | 1.7973 |
|  |  | # 2 | 0.8649 | 1.7823 | 1.7913 |
|  |  | # 3 | 0.6066 | 1.7628 | 1.9955 |
| **Average** | | | **0.8779** | **1.8389** | **1.8614** |
|  | 298.15 | # 1 | 0.6141 | 1.6381 | 1.8198 |
|  |  | # 2 | 0.6411 | 1.7538 | 1.9595 |
|  |  | # 3 | 0.7402 | 1.7958 | 1.9489 |
| **Average** | | | **0.6651** | **1.7292** | **1.9094** |
|  | 308.15 | # 1 | 0.7477 | 1.6712 | 1.7733 |
|  |  | # 2 | 0.7748 | 1.7868 | 1.9129 |
|  |  | # 3 | 0.8814 | 1.7042 | 1.7267 |
| **Average** | | | **0.8013** | **1.7207** | **1.8043** |
| METHANOL | 288.15 | # 1 | 0.9084 | 1.8198 | 1.8664 |
|  |  | # 2 | 0.9880 | 1.6216 | 1.5405 |
|  |  | # 3 | 1.0345 | 1.9775 | 1.9955 |
| **Average** | | | **0.9770** | **1.8063** | **1.8008** |
|  | 298.15 | # 1 | 1.0691 | 1.9685 | 1.9595 |
|  |  | # 2 | 1.4084 | 1.9610 | 1.7162 |
|  |  | # 3 | 1.5420 | 1.9940 | 1.6697 |
| **Average** | | | **1.3398** | **1.9745** | **1.7818** |
|  | 308.15 | # 1 | 1.9159 | 1.9775 | 1.3904 |
|  |  | # 2 | 0.5165 | 1.0330 | 1.2643 |
|  |  | # 3 | 0.7357 | 1.7733 | 1.8529 |
| **Average** | | | **1.0560** | **1.5946** | **1.5025** |
| METHYLCYCLOHEXANE | 288.15 | # 1 | 0.5225 | 1.7102 | 1.9715 |
|  |  | # 2 | 1.1622 | 1.9715 | 1.7973 |
|  |  | # 3 | 0.9084 | 1.8198 | 1.8664 |
| **Average** | | | **0.8644** | **1.8338** | **1.8784** |
|  | 298.15 | # 1 | 1.4084 | 1.9610 | 1.7162 |
|  |  | # 2 | 1.9159 | 1.9775 | 1.3904 |
|  |  | # 3 | 0.6141 | 1.6381 | 1.8198 |
| **Average** | | | **1.3128** | **1.8589** | **1.6421** |
|  | 308.15 | # 1 | 0.8814 | 1.7042 | 1.7267 |
|  |  | # 2 | 1.0180 | 1.6712 | 1.4715 |
|  |  | # 3 | 1.8183 | 1.9384 | 1.2898 |
| **Average** | | | **1.2392** | **1.7713** | **1.4960** |
| N-BUTANOL | 288.15 | # 1 | 0.9880 | 1.6216 | 1.5405 |
|  |  | # 2 | 0.5661 | 1.7087 | 1.9640 |
|  |  | # 3 | 0.7402 | 1.7958 | 1.9489 |
| **Average** | | | **0.7648** | **1.7087** | **1.8178** |
|  | 298.15 | # 1 | 0.9084 | 1.6997 | 1.6096 |
|  |  | # 2 | 0.6126 | 1.7868 | 1.9895 |
|  |  | # 3 | 0.7357 | 1.7733 | 1.8529 |
| **Average** | | | **0.7522** | **1.7533** | **1.8173** |
|  | 308.15 | # 1 | 0.7913 | 1.7748 | 1.8048 |
|  |  | # 2 | 1.1066 | 1.4024 | 0.9234 |
|  |  | # 3 | 0.5315 | 1.4249 | 1.5676 |
| **Average** | | | **0.8098** | **1.5340** | **1.4319** |
| N-HEPTANE | 288.15 | # 1 | 1.1321 | 1.8288 | 1.5060 |
|  |  | # 2 | 0.5180 | 1.4745 | 1.6366 |
|  |  | # 3 | 0.6036 | 1.6156 | 1.7613 |
| **Average** | | | **0.7512** | **1.6396** | **1.6346** |
|  | 298.15 | # 1 | 0.6892 | 1.7568 | 1.8859 |
|  |  | # 2 | 0.7132 | 1.5871 | 1.6231 |
|  |  | # 3 | 0.9084 | 1.6997 | 1.6096 |
| **Average** | | | **0.7703** | **1.6812** | **1.7062** |
|  | 308.15 | # 1 | 1.0180 | 1.6712 | 1.4715 |
|  |  | # 2 | 1.2132 | 1.7838 | 1.4580 |
|  |  | # 3 | 1.7132 | 1.9805 | 1.2928 |
| **Average** | | | **1.3148** | **1.8118** | **1.4074** |
| N-HEXANE | 288.15 | # 1 | 0.6156 | 1.5991 | 1.7372 |
|  |  | # 2 | 0.9084 | 1.8964 | 1.8889 |
|  |  | # 3 | 0.5661 | 1.7087 | 1.9640 |
| **Average** | | | **0.6967** | **1.7347** | **1.8634** |
|  | 298.15 | # 1 | 1.4339 | 1.5961 | 1.0000 |
|  |  | # 2 | 1.8183 | 1.9384 | 1.2898 |
|  |  | # 3 | 1.2883 | 1.9174 | 1.4159 |
| **Average** | | | **1.51308.15** | **1.8173** | **1.2352** |
|  | 308.15 | # 1 | 0.5225 | 1.7102 | 1.9715 |
|  |  | # 2 | 0.5691 | 1.7087 | 1.9309 |
|  |  | # 3 | 0.6156 | 1.7072 | 1.8904 |
| **Average** | | | **0.5691** | **1.7087** | **1.9309** |
| NITROBENZENE | 298.15 | # 1 | 0.6622 | 1.7057 | 1.8498 |
|  |  | # 2 | 0.7087 | 1.7042 | 1.8093 |
|  |  | # 3 | 0.7553 | 1.7027 | 1.7688 |
| **Average** | | | **0.7087** | **1.7042** | **1.8093** |
| N-OCTANE | 288.15 | # 1 | 0.7868 | 1.3258 | 1.2132 |
|  |  | # 2 | 1.9625 | 1.8874 | 1.0315 |
|  |  | # 3 | 1.1622 | 1.9715 | 1.7973 |
| **Average** | | | **1.3038** | **1.7282** | **1.3473** |
|  | 298.15 | # 1 | 0.8649 | 1.7823 | 1.7913 |
|  |  | # 2 | 0.6066 | 1.7628 | 1.9955 |
|  |  | # 3 | 0.6141 | 1.6381 | 1.8198 |
| **Average** | | | **0.6952** | **1.7277** | **1.8689** |
|  | 308.15 | # 1 | 0.6411 | 1.7538 | 1.9595 |
|  |  | # 2 | 0.7402 | 1.7958 | 1.9489 |
|  |  | # 3 | 0.7477 | 1.6712 | 1.7733 |
| **Average** | | | **0.7097** | **1.7403** | **1.8939** |
| N-PENTANE | 288.15 | # 1 | 0.7748 | 1.7868 | 1.9129 |
|  |  | # 2 | 0.8814 | 1.7042 | 1.7267 |
|  |  | # 3 | 0.9084 | 1.8198 | 1.8664 |
| **Average** | | | **0.8549** | **1.7703** | **1.8353** |
|  | 298.15 | # 1 | 0.9880 | 1.6216 | 1.5405 |
|  |  | # 2 | 1.0345 | 1.9775 | 1.9955 |
|  |  | # 3 | 1.0691 | 1.9685 | 1.9595 |
| **Average** | | | **1.0305** | **1.8559** | **1.8318** |
| TOLUENE | 288.15 | # 1 | 1.4084 | 1.9610 | 1.7162 |
|  |  | # 2 | 1.5420 | 1.9940 | 1.6697 |
|  |  | # 3 | 1.9159 | 1.9775 | 1.3904 |
| **Average** | | | **1.6221** | **1.9775** | **1.5921** |
|  | 298.15 | # 1 | 0.5165 | 1.0330 | 1.2643 |
|  |  | # 2 | 0.7357 | 1.7733 | 1.8529 |
|  |  | # 3 | 0.5225 | 1.7102 | 1.9715 |
| **Average** | | | **0.5916** | **1.5055** | **1.6962** |
|  | 308.15 | # 1 | 1.1622 | 1.9715 | 1.7973 |
|  |  | # 2 | 0.9084 | 1.8198 | 1.8664 |
|  |  | # 3 | 1.4084 | 1.9610 | 1.7162 |
| **Average** | | | **1.288.1597** | **1.9174** | **1.7933** |
| WATER | 288.15 | # 1 | 1.9159 | 1.9775 | 1.3904 |
|  |  | # 2 | 0.6141 | 1.6381 | 1.8198 |
|  |  | # 3 | 0.8814 | 1.7042 | 1.7267 |
| **Average** | | | **1.1371** | **1.7733** | **1.6456** |
|  | 298.15 | # 1 | 1.0180 | 1.6712 | 1.4715 |
|  |  | # 2 | 1.8183 | 1.9384 | 1.2898 |
|  |  | # 3 | 0.9880 | 1.6216 | 1.5405 |
| **Average** | | | **1.2748** | **1.7437** | **1.4339** |
|  | 308.15 | # 1 | 0.5661 | 1.7087 | 1.9640 |
|  |  | # 2 | 0.7402 | 1.7958 | 1.9489 |
|  |  | # 3 | 0.9084 | 1.6997 | 1.6096 |
| **Average** | | | **0.7382** | **1.7347** | **1.8408** |