SUPPLEMENTARY MATERIAL TO

**Quantitative structure-property relationship studies for prediction vapor pressure of volatile organic compounds**

MOUNIA ZINEand DJELLOUL MESSADI

*Environmental and Food Safety Laboratory, Badji Mokhtar-Annaba University, BP.12, 23000 Annaba, Algeria*

THE PREDICTIVE QSPR MODEL

Table S.The data set and the corresponding Experimental and predicted values of log *p*/kpa for the training and validation sets

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ID | Name | log *p*v/Pa (Exp) | log *p*v/Pa (Pred) | *X*0*sol* | *SpPosA\_H*2 | *GATS*2*e* | *Hy* | *Hat* (*h*ii) | eistd. |
| 1 | 1,1,2-Trichloro-ethane | 3.48 | 3.3841 | 5.784 | 0.541 | 1.078 | -0.359 | 0.105 | -0.4647 |
| 2 | Iodomethane | 4.72 | 4.7638 | 3.5 | 0.5 | 0.97 | -0.315 | 0.101 | 0.211 |
| 3 | Iodoethane | 4.12 | 4.631 | 4.207 | 0.515 | 1.071 | -0.528 | 0.072 | 2.3469 |
| 4 | 1-Bromobutane | 3.72 | 3.63 | 5.121 | 0.57 | 0.95 | -0.719 | 0.03 | -0.3867 |
| 5 | Hexan-2-one | 2.71 | 3.1166 | 5.699 | 0.56 | 0.534 | -0.802 | 0.118 | 2.014 |
| 6 | 2-Methylheptane | 3.41 | 3.662 | 6.406 | 0.576 | 1.317 | -0.946 | 0.108 | 1.2283 |
| 7 | 2,3,4-Trimethylpentane | 3.53 | 3.6423 | 6.732 | 0.548 | 1.128 | -0.946 | 0.145 | 0.5827 |
| 8 | 1,1-Dichloroethane | 4.47 | 4.1496 | 4.577 | 0.5 | 0.74 | -0.431 | 0.1 | -1.5394 |
| 9 | éthylcyclohexane | 3.12 | 3.264 | 5.82 | 0.633 | 1.348 | -0.946 | 0.136 | 0.7362 |
| 10 | 1-Propoxypropane | 3.95 | 4.1052 | 5.536 | 0.588 | 1.641 | -0.802 | 0.163 | 0.8319 |
| 11 | 1,2-Dichloroethene | 4.63 | 4.188 | 4.414 | 0.55 | 1.25 | -0.431 | 0.054 | -1.9698 |
| 12 | 2-Bromopropane | 4.42 | 4.4842 | 4.577 | 0.5 | 0.801 | -0.646 | 0.12 | 0.3188 |
| 13 | 3,3-Dimethylpentane | 4.02 | 3.9226 | 5.914 | 0.55 | 1.076 | -0.936 | 0.073 | -0.4478 |
| 14 | toluène | 3.42 | 3.2118 | 5.113 | 0.632 | 1.016 | -0.936 | 0.132 | -1.0569 |
| 15 | 1,4-Xylene | 3.12 | 2.9552 | 5.983 | 0.61 | 0.893 | -0.946 | 0.085 | -0.7732 |
| 16 | Ethylbenzène | 3.12 | 2.9638 | 5.82 | 0.633 | 1.084 | -0.946 | 0.118 | -0.7736 |

Table S.Continued

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ID | Name | log *p*v/Pa (Exp) | log *p*v/Pa (Pred) | *X*0*sol* | *SpPosA\_H*2 | *GATS*2*e* | *Hy* | *Hat* (*h*ii) | eistd. |
| 17 | 1,2-Xylene | 2.42 | 2.9182 | 5.983 | 0.613 | 0.893 | -0.946 | 0.09 | 2.3562 |
| 18 | Ethanol | 3.87 | 3.8322 | 2.707 | 0.515 | 1.026 | 0.638 | 0.261 | -0.2442 |
| 19 | Methylcyclopentane | 4.25 | 4.2475 | 4.406 | 0.599 | 1.299 | -0.921 | 0.109 | -0.0122 |
| 20 | 2-Methyl-2-propanol | 3.7 | 3.6991 | 4.5 | 0.482 | 0.728 | 0.132 | 0.173 | -0.0051 |
| 21 | 2-Propylènenitrile | 4.15 | 4.0264 | 3.414 | 0.55 | 0.47 | -0.646 | 0.23 | -0.751 |
| 22 | Pent-1-ene | 4.96 | 4.7238 | 4.121 | 0.57 | 1.313 | -0.898 | 0.111 | -1.1554 |
| 23 | Dichloromethane | 4.75 | 4.7186 | 3.707 | 0.515 | 1.232 | -0.264 | 0.094 | -0.1493 |
| 24 | Butyronitrile | 3.12 | 3.4784 | 4.121 | 0.57 | 0.412 | -0.719 | 0.211 | 2.099 |
| 25 | Propan-1-ol | 3.41 | 3.384 | 3.414 | 0.55 | 0.956 | 0.323 | 0.182 | -0.144 |
| 26 | Butan-1-ol | 2.82 | 3.0135 | 4.121 | 0.57 | 0.926 | 0.132 | 0.158 | 1.0282 |
| 27 | 2-Methylpropan-1-ol | 3.12 | 3.2801 | 4.284 | 0.541 | 0.912 | 0.132 | 0.118 | 0.7935 |
| 28 | 1,2-Dichlorobenzene | 2.13 | 1.8814 | 6.983 | 0.613 | 0.642 | -0.71 | 0.232 | -1.5148 |
| 29 | 2,2,4-Trimethylpentane | 3.79 | 3.7334 | 6.784 | 0.53 | 1.034 | -0.946 | 0.185 | -0.3156 |
| 30 | Pentan-2-one | 3.31 | 3.4448 | 4.992 | 0.556 | 0.531 | -0.767 | 0.115 | 0.6638 |
| 31 | 2,4-Dimethylpentane | 4.1 | 4.1299 | 5.862 | 0.545 | 1.183 | -0.936 | 0.089 | 0.141 |
| 32 | (1-Methylethyl)benzene | 2.82 | 2.6799 | 6.69 | 0.619 | 1.026 | -0.954 | 0.124 | -0.7011 |
| 33 | Propan-2-ol | 3.75 | 3.8153 | 3.577 | 0.5 | 0.859 | 0.323 | 0.15 | 0.3419 |
| 34 | 1-Chloropropane | 4.66 | 4.324 | 3.914 | 0.55 | 0.934 | -0.646 | 0.069 | -1.5356 |
| 35 | 2,2-Dimethylbutane | 4.63 | 4.4817 | 5.207 | 0.523 | 1.005 | -0.921 | 0.104 | -0.717 |
| 36 | pentaméthylène | 4.63 | 4.907 | 3.536 | 0.585 | 1.4 | -0.898 | 0.195 | 1.5733 |
| 37 | 2-Methyl-2-butene | 4.72 | 4.6084 | 4.284 | 0.541 | 0.963 | -0.898 | 0.097 | -0.5337 |
| 38 | propyl formate | 4.02 | 3.5854 | 4.828 | 0.57 | 0.906 | -0.614 | 0.034 | -1.8789 |
| 39 | Diethyl ether | 4.87 | 4.9728 | 4.121 | 0.57 | 1.726 | -0.719 | 0.211 | 0.6022 |
| 40\* | Dibromomethan | 3.76 | 4.3039 | 4.707 | 0.515 | 1.272 | -0.264 | 0.107 | 2.3622 |
| 41\* | 1,3-Dichlorobenzene | 2.12 | 1.8198 | 6.983 | 0.618 | 0.642 | -0.71 | 0.237 | -1.4105 |

Table S.Continued

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ID | Name | log *p*v/Pa (Exp) | log *p*v/Pa (Pred) | *X*0*sol* | *SpPosA\_H*2 | *GATS*2*e* | *Hy* | *Hat* (*h*ii) | eistd. |
| 42\* | 3-Pentanone | 3.33 | 3.3708 | 4.992 | 0.562 | 0.531 | -0.767 | 0.113 | 0.1776 |
| 43\* | Ethyl acetate | 4.12 | 3.5608 | 4.992 | 0.556 | 0.799 | -0.614 | 0.04 | -2.342 |
| 44\* | 2-Butanone | 4.11 | 3.8998 | 4.284 | 0.541 | 0.534 | -0.719 | 0.136 | -0.9284 |
| 45\* | Hexane | 4.29 | 4.5053 | 4.828 | 0.57 | 1.382 | -0.921 | 0.085 | 0.9237 |
| 46\* | Pentane | 4.85 | 4.7773 | 4.121 | 0.57 | 1.36 | -0.898 | 0.116 | -0.3174 |
| 47\* | 1,2-Dichloropropane | 3.83 | 3.7066 | 5.284 | 0.541 | 0.964 | -0.539 | 0.042 | -0.5175 |
| 48\* | Heptane | 3.76 | 3.9942 | 5.536 | 0.588 | 1.398 | -0.936 | 0.082 | 1.0032 |
| 49\* | 1,2-dichloroethane | 4.03 | 4.0937 | 4.414 | 0.55 | 1.167 | -0.431 | 0.041 | 0.2668 |
| 50\* | 1-Bromopropane | 4.12 | 4.1189 | 4.414 | 0.55 | 0.956 | -0.646 | 0.039 | -0.0048 |
| 51\* | Ethyl acetate | 2.42 | 2.8565 | 5.983 | 0.618 | 0.893 | -0.946 | 0.098 | 1.886 |

\* Test compounds