Journal of the Serbian Chemical Society
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*J. Serb. Chem. Soc. 80* (5) S176–S178 (2015) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

# Quantitative relationships for the prediction of the vapor pressure of some hydrocarbons from the van der Waals molecular surface

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*J. Serb. Chem. Soc.* 80 (5) (2015) 659–671

TABLE S-I. Vapor pressure data sets for: a) alkanes; b) cycloalkanes. The experimental data, $A_e$, are the values of vapor pressure, log (*VP* / Pa) at 298.15 K;[18] the substituents: M – methyl, E – ethyl, IPR – isopropyl, PR – propyl, BU – butyl

| No | C*n* or CyC*n* | $A_{exp}$ = log (*VP* / Pa) | $S^W$ / Å$^2$ | $A_{calc\ or\ pred}$ = = log (*VP* / Pa)$_{calc}$[a] | $\Delta A$ = = $A_{exp}$–$A_{calc}$ |
|---|---|---|---|---|---|
| a) C*n*, where n represents the number of carbon atoms in an alkane molecule | | | | | |
| 1 | C2 | 6.62 | 70.896 | 6.522 | 0.098 |
| 2 | C3 | 5.97 | 92.848 | 5.992 | –0.02 |
| 3 | C4 | 5.38 | 114.83 | 5.46 | –0.08 |
| 4 | 2M-C3 | 5.54 | 114.11 | 5.478 | 0.062 |
| 5 | C5 | 4.83 | 136.62 | 4.933 | –0.1 |
| 6 | 2M-C4 | 4.96 | 134.18 | 4.992 | –0.03 |
| 7 | 22MM-C3 | 5.23 | 134.48 | 4.985 | 0.245 |
| 8 | C6 | 4.3 | 158.59 | 4.402 | –0.1 |
| 9 | 3M-C5 | 4.4 | 153.57 | 4.523 | –0.12 |
| 10 | 2M-C5 | 4.44 | 155.89 | 4.467 | –0.03 |
| 11 | 23MM-C4 | 4.49 | 151.86 | 4.565 | –0.08 |
| 12 | 22MM-C4 | 4.82 | 152.20 | 4.556 | 0.264 |
| 13 | C7 | 3.78 | 180.46 | 3.873 | –0.09 |
| 14 | 3M-C6 | 3.91 | 175.30 | 3.998 | –0.09 |
| 15 | 2M-C6 | 3.94 | 177.74 | 3.939 | 0.001 |
| 16 | 23MM-C5 | 3.96 | 170.73 | 4.109 | –0.15 |
| 17 | 33MM-C5 | 4.04 | 168.74 | 4.157 | –0.12 |
| 18 | 223MMM-C4 | 4.135 | 167.74 | 4.181 | –0.05 |

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TABLE S-I. Continued

| No | C*n* or CyC*n* | $A_{exp}$ = log (*VP* / Pa) | $S^W$ / Å$^2$ | $A_{calc\ or\ pred}$ = = log (*VP* / Pa)$_{calc}$[a] | $\Delta A$ = = $A_{exp}$–$A_{calc}$ |
|---|---|---|---|---|---|
| a) C*n*, where n represents the number of carbon atoms in an alkane molecule | | | | | |
| 19 | 24MM-C5 | 4.02 | 174.47 | 4.018 | 0.002 |
| 20 | 22MM-C5 | 4.14 | 173.79 | 4.034 | 0.106 |
| 21 | C8 | 3.27 | 202.23 | 3.347 | –0.08 |
| 22 | 3E-C6 | 3.428 | 195.35 | 3.513 | –0.09 |
| 23 | 3M-C7 | 3.417 | 197.04 | 3.472 | –0.06 |
| 24 | 34MM-C6 | 3.481 | 189.82 | 3.647 | –0.17 |
| 25 | 3E3M-C5 | 3.486 | 185.25 | 3.757 | –0.27 |
| 26 | 4M-C7 | 3.436 | 196.97 | 3.474 | –0.04 |
| 27 | 2M-C7 | 3.439 | 199.68 | 3.409 | 0.03 |
| 28 | 3E2M-C5 | 3.503 | 192.53 | 3.582 | –0.08 |
| 29 | 23MM-C6 | 3.495 | 193.49 | 3.558 | –0.06 |
| 30 | 233MMM-C5 | 3.556 | 184.91 | 3.766 | –0.21 |
| 31 | 234MMM-C5 | 3.55 | 185.75 | 3.745 | –0.2 |
| 32 | 33MM-C6 | 3.581 | 190.4 | 3.633 | –0.05 |
| 33 | 223MMM-C5 | 3.631 | 186.76 | 3.721 | –0.09 |
| 34 | 24MM-C6 | 3.607 | 194.69 | 3.529 | 0.078 |
| 35 | 25MM-C6 | 3.606 | 197.02 | 3.473 | 0.133 |
| 36 | 22MM-C6 | 3.657 | 195.69 | 3.505 | 0.152 |
| 37 | 224MMM-C5 | 3.818 | 190.77 | 3.624 | 0.194 |
| 38 | C9 | 2.77 | 224.1 | 2.818 | –0.05 |
| 39 | 3M-C8 | 2.921 | 219.05 | 2.94 | –0.02 |
| 40 | 4M-C8 | 2.959 | 218.84 | 2.945 | 0.014 |
| 41 | 2M-C8 | 2.927 | 221.45 | 2.882 | 0.045 |
| 42 | 2233MMMM-C5 | 3.103 | 196.87 | 3.476 | –0.37 |
| 43 | 3E24MM-C5 | 3.126 | 207.95 | 3.209 | –0.08 |
| 44 | 26MM-C7 | 3.094 | 218.95 | 2.943 | 0.151 |
| 45 | 3E22MM-C5 | 3.177 | 204.41 | 3.294 | –0.12 |
| 46 | 225MMM-C6 | 3.347 | 215.04 | 3.037 | 0.31 |
| 47 | 2244MMMM-C5 | 3.427 | 207.63 | 3.216 | 0.211 |
| 48 | 2233MMMM-C6 | 2.73 | 218.45 | 2.955 | –0.23 |
| 49 | 22MM-C8 | 2.686 | 239.68 | 2.441 | 0.245 |
| 50 | 2M-C9 | 2.4 | 243.38 | 2.352 | 0.048 |
| 51 | 335-MMMC7 | 2.746 | 226.57 | 2.758 | –0.01 |
| 52 | 33EE-C5 | 2.988 | 198.61 | 3.434 | –0.45 |
| 53 | 3M-C9 | 2.421 | 240.97 | 2.41 | 0.011 |
| 54 | 4M-C9 | 2.49 | 240.81 | 2.414 | 0.076 |
| 55 | 5M-C9 | 2.468 | 240.83 | 2.414 | 0.054 |
| 56 | C1 | 7.79 | 48.541 | 7.063 | 0.727 |
| 57 | C10 | 2.27 | 246.02 | 2.288 | –0.02 |
| 58 | C11 | 1.745 | 267.74 | 1.763 | –0.02 |
| 59 | C12 | 1.252 | 289.89 | 1.227 | 0.025 |

TABLE S-I. Continued

| No | C*n* or CyC*n* | $A_{exp}$ = log (*VP* / Pa) | $S^W$ / Å$^2$ | $A_{calc\ or\ pred}$ = = log (*VP* / Pa)$_{calc}$[a] | $\Delta A$ = = $A_{exp}$–$A_{calc}$ |
|---|---|---|---|---|---|
| | a) C*n*, where n represents the number of carbon atoms in an alkane molecule | | | | |
| 60 | C13 | 0.755 | 311.47 | 0.705 | 0.05 |
| 61 | C14 | 0.27 | 333.61 | 0.17 | 0.1 |
| 62 | C15 | –0.183 | 355.38 | –0.36 | 0.173 |
| 63 | C16 | –0.7 | 377.38 | –0.89 | 0.188 |
| | b) CyC*n*, where *n* represents the number of carbon atoms in the cycle (Cy) of a cycloalkane molecule | | | | |
| 1 | CyC3 | 5.85 | 80.531 | 6.289 | –0.439 |
| 2 | CyC4 | 5.195 | 98.905 | 5.845 | –0.65 |
| 3 | CyC5 | 4.62 | 117.025 | 5.407 | –0.787 |
| 4 | CyC6 | 4.11 | 135.333 | 4.964 | –0.854 |
| 5 | CyC7 | 3.45 | 150.489 | 4.598 | –1.148 |
| 6 | CyC8 | 2.876 | 167.417 | 4.189 | –1.313 |
| 7 | E-CyC5 | 3.727 | 155.334 | 4.481 | –0.754 |
| 8 | E-CyC6 | 3.23 | 176.719 | 3.964 | –0.734 |
| 9 | IPR-CyC5 | 3.332 | 176.106 | 3.978 | –0.646 |
| 10 | IPR-CycloC6 | 2.747 | 198.422 | 3.439 | –0.692 |
| 11 | 1,1MM-CyC5 | 4.006 | 157.207 | 4.435 | –0.429 |
| 12 | 1,1MM-CyC6 | 3.48 | 173.535 | 4.041 | –0.561 |
| 13 | BU-CyloC6 | 2.243 | 220.344 | 2.909 | –0.666 |
| 14 | *cis*-1,2MM-CyC5 | 3.799 | 156.622 | 4.450 | –0.651 |
| 15 | *trans*-1,2MM-CyC5 | 3.931 | 158.805 | 4.397 | –0.466 |
| 16 | *cis*-1,3MM-CyC6 | 3.457 | 177.856 | 3.936 | –0.479 |
| 17 | *trans*-1,3MM-CyC6 | 3.371 | 175.33 | 3.997 | –0.626 |
| 18 | cis-1,3MM-Cy5 | 3.945 | 158.861 | 4.395 | –0.45 |
| 19 | *trans*-1,3MM-CyC5 | 3.934 | 158.507 | 4.404 | –0.47 |
| 20 | *cis*-1,4MM-CyC6 | 3.379 | 175.575 | 3.991 | –0.612 |
| 21 | *trans*-1,4MM-CyC6 | 3.481 | 173.064 | 4.052 | –0.571 |

[a]Calculated ($A_{calc}$) values of log *VP* with Eq. (7) for the training set; predicted values ($A_{pred}$) of log *VP* with Eq. (7), developed for training set composed of alkanes in part a)