# Solvation parameters for the 209 PCBs: calculation of physicochemical properties

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## Supplimentary material: Tables S1 to S5.

**Table S1.** Observed [25] and predicted values of the water to hexane partition coefficient, as log P6

| PCB | Obs | Pred |
|---|---|---|
| 1 | 4.76 [a] | 4.71 |
| 29 | 5.76 | 5.72 |
| 52 | 6.28 | 6.08 |
| 155 | 6.50 | 7.01 |
| 209 | 7.14 | 9.02 |

[a] Observed value for water-to-heptane partition (3)

**Table S2.** Comparison of observed and predicted values of water solubility, as log Sw ( mol $dm^{-3}$) at 298 K

| | Log Sw [a] | | | |
|---|---|---|---|---|
| PCB | HM [7] | LDV [5] | FAV [5] | Pred |
| 3 | -5.16 | -4.76 | -4.69 | -4.93 |
| 8 | -5.28 | -5.13 | -5.19 | -5.41 |
| 15 | -6.56 | -5.30 | -5.37 | -5.50 |
| 28 | -5.98 | -6.00 | -6.05 | -6.00 |
| 29 | -6.20 | -5.74 | -5.82 | -6.01 |
| 31 | -6.41 | -6.07 | -6.12 | -6.01 |
| 52 | -7.04 | -6.17 | -6.32 | -6.50 |
| 61 | -7.32 | -6.44 | -6.46 | -6.59 |
| 101 | -7.51 | -6.98 | -6.99 | -7.06 |
| 105 | -7.98 | -6.95 | -7.13 | -7.13 |
| 118 | -7.39 | -7.05 | -7.17 | -7.15 |
| 138 | -7.69 | -7.68 | -7.73 | -7.63 |
| 153 | -8.57 | -7.42 | -7.51 | -7.63 |
| 155 | -8.20 | -7.41 | -7.42 | -7.57 |
| 180 | -8.01 | -8.10 | -7.88 | -8.16 |
| 194 | -9.20 | -8.05 | -8.25 | -8.81 |
| 206 | -10.27 | -9.62 (8) | -9.77 (30) | -9.36 |
| 207 | | | | -9.33 |
| 208 | -10.41 (10) | | | -9.34 |
| 209 | -10.83 (10) | -9.00 (8) | -10.37 (30) | -9.90 |

[a] Columns 2-4 list observed values from the quoted references, and in column 5 are given our predicted values on eqn. (9).

**Table S3.** Comparison of observed and predicted values of the gas to water partition coefficient, as log Kw, at 298 K

| PCB | (7) | (4) | LDV (5) | FAV (5) | LogP16 | **L** | Pred eqn. (10) |
|---|---|---|---|---|---|---|---|
| 3 | 1.24 | 2.06 | 1.84 | 2.02 | 4.93 | 6.718 | 1.79 |
| 8 | 1.67 | 1.98 | 1.98 | 2.04 | 5.31 | 7.197 | 1.89 |
| 15 | 0.99 | 2.09 | 2.24 | 2.27 | 5.45 | 7.580 | 2.13 |
| 28 | 2.00 | 1.83 | 1.87 | 1.91 | 5.88 | 7.904 | 2.03 |
| 29 | 1.08 | 1.83 | 1.88 | 1.91 | 5.88 | 7.722 | 1.84 |
| 31 | 1.26 | 1.91 | 1.83 | 1.86 | 5.88 | 7.862 | 1.98 |
| 52 | | 1.90 | 1.94 | 1.99 | 6.27 | 8.144 | 1.87 |
| 61 | 1.38 | 1.85 | 2.08 | 2.09 | 6.41 | 8.687 | 2.27 |
| 101 | 1.35 | 1.76 | 1.90 | 2.01 | 6.79 | 8.868 | 2.07 |
| 105 | 1.47 | 1.86 | 1.87 | 2.25 | 6.92 | 9.594 | 2.67 |
| 118 | 1.93 | 1.83 | 1.89 | 2.23 | 6.94 | 9.396 | 2.46 |
| 138 | 2.00 | 1.74 | 1.80 | 1.92 | 7.32 | 9.772 | 2.45 |
| 153 | 1.16 | 1.66 | 2.00 | 2.10 | 7.32 | 9.587 | 2.27 |
| 155 | 0.99 | 1.48 | 1.51 | 1.43 | 7.28 | 8.715 | 1.44 |
| 180 | 2.27 | 1.82 | 2.63 | 2.48 | 7.82 | 10.415 | 2.59 |
| 194 | | 2.36 | 2.56 | 2.75 | 8.43 | 11.186 | 2.76 |
| | | | ` | | | | |
| 206 | | 2.22 | 4.09 [a] | | 8.94 | 11.450 | 2.51 |
| 207 | | 1.41 | 2.23 [a] | | 8.92 | 10.904 | 1.99 |
| 208 | | 1.41 | 2.46 [a] | | 8.92 | 10.922 | 2.00 |
| 209 | 0.42 | 1.41 | 4.28 [a] | | 9.45 | 11.703 | 2.26 |

[a] Calculated values, ref. (32)

**Table S4.** Comparison of observed and predicted values of the gas to dry octanol partition coefficient, as log Koct, at 298 K

| PCB | 34, 38 | 35 | 36 [a] | 37 | 39 [a] | LDV (5) | FAV (5) | Pred |
|---|---|---|---|---|---|---|---|---|
| 3 | 6.82 | | 6.79 | 6.93 | 6.92 | 6.82 | 6.78 | 6.60 |
| 8 | | | 7.39 | | 7.05 | 7.40 | 7.34 | 7.11 |
| 15 | 7.67 | | 7.65 | 7.77 | 7.89 | 7.65 | 7.85 | 7.44 |
| 18 | | 7.60 | 7.58 | | 7.29 | | | 7.42 |
| 28 | | | 8.16 | | 7.94 | 7.93 | 7.85 | 7.79 |
| 29 | 7.82 | | 7.80 | 8.03 | 8.06 | 7.80 | 7.78 | 7.62 |
| 31 | | | 8.16 | | 7.98 | 7.93 | 7.94 | 7.75 |
| 44 | | 8.36 | 8.49 | | 8.48 | | | 8.23 |
| 49 | 8.39 | | 8.43 | | 8.12 | | | 8.12 |
| 52 | | 8.22 | 8.27 | 8.44 | 8.01 | 8.22 | 8.22 | 8.08 |
| 53 | 8.03 | | 7.95 | | 7.75 | | | 7.90 |
| 61 | 8.73 | | 8.64 | | 8.77 | 8.64 | 8.55 | 8.56 |
| 64 | | 8.41 | 8.40 | 8.75 | 8.41 | | | 8.27 |
| 66 | 9.01 | | 9.05 | | 9.13 | | | 8.59 |
| 77 | 9.70 | | 9.69 | | 9.47 | | | 9.01 |
| 95 | 8.80 | 8.71 | 8.83 | | 8.82 | | | 8.57 |
| 96 | 8.53 | | 8.54 | | 8.54 | | | 8.39 |
| 101 | 9.06 | | 9.06 | 9.05 | 9.11 | 8.90 | 8.79 | 8.79 |
| 105 | 10.01 | | 9.92 | | 9.94 | 10.01 | 9.45 | 9.44 |
| 110 | | 9.06 | 9.34 | | 9.02 | | | 9.06 |
| 118 | 9.81 | | 9.79 | | 9.66 | 9.82 | 9.36 | 9.25 |
| 126 | 10.35 | | 10.42 | | 10.38 | | | 9.68 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 138 | 9.81 | | 9.94 | | 9.83 | 9.76 | 9.66 | 9.66 |
| 149 | | 9.27 | 9.49 | | 9.50 | | | 9.27 |
| 153 | 9.73 | 9.37 | 9.75 | 9.65 | 9.77 | 9.52 | 9.44 | 9.49 |
| 155 | 8.99 | | 8.89 | | 9.04 | 8.89 | 9.14 | 8.68 |
| 171 | 10.25 | | 10.22 | | 10.40 | | | 9.94 |
| 180 | 10.52 | 9.88 | 10.44 | | 10.75 | 10.14 | 10.16 | 10.31 |
| 187 | | 9.87 | 9.95 | | 10.30 | | | 9.78 |
| 194 | | | 11.31 | | 11.07 | 11.30 | 11.13 | 11.04 |
| | | | | | | | | |
| 206 | | | 11.49 | 11.51 [b] | 11.62 | | | 11.32 |
| 207 | | | 10.95 | 11.61 [b] | 11.55 | | | 10.82 |
| 208 | | | 10.96 | 11.40 [b] | 11.44 | | | 10.83 |
| 209 | | | 11.64 | 11.96 [b] | 12.12 | | | 11.60 |

[a] Most of these values are predicted, including those for PCB206-PCB209. [b] Predicted values.[38]

**Table S5.** Comparison of log Koct for gas to dry octanol partition, with log Koct(wet) for gas to wet octanol partition, calculated from log Kw and log Poct, and through eqn. (11), at 298 K.

| | LDV | | FAV | | Predictions | | Eq (11) |
|---|---|---|---|---|---|---|---|
| PCB | Wet | Dry | Wet | Dry | Wet [a] | Dry | Wet [b] |
| 3 | 6.33 | 6.82 | 6.67 | 6.78 | 6.50 | 6.60 | 6.51 |
| 8 | 7.07 | 7.40 | 7.16 | 7.34 | 6.99 | 7.11 | 7.02 |
| 15 | 7.64 | 7.65 | 7.63 | 7.85 | 7.33 | 7.44 | 7.30 |
| 28 | 7.42 | 7.93 | 7.57 | 7.85 | 7.63 | 7.79 | 7.66 |
| 29 | 7.62 | 7.80 | 7.51 | 7.78 | 7.45 | 7.62 | 7.51 |
| 31 | 7.62 | 7.93 | 7.64 | 7.94 | 7.59 | 7.75 | 7.63 |
| 52 | 7.96 | 8.22 | 7.90 | 8.22 | 7.87 | 8.08 | 7.98 |
| 61 | 8.25 | 8.64 | 8.20 | 8.55 | 8.37 | 8.56 | 8.38 |
| 101 | 8.05 | 8.90 | 8.34 | 8.79 | 8.55 | 8.79 | 8.65 |
| 105 | 8.48 | 10.01 | 9.07 | 9.45 | 9.23 | 9.44 | 9.21 |
| 118 | 8.38 | 9.82 | 8.92 | 9.36 | 9.03 | 9.25 | 9.04 |
| 138 | 8.80 | 9.76 | 9.13 | 9.66 | 9.40 | 9.66 | 9.47 |
| 153 | 8.71 | 9.52 | 8.97 | 9.44 | 9.22 | 9.49 | 9.32 |
| 155 | 8.87 | 8.89 | 8.61 | 9.14 | 8.35 | 8.68 | 8.59 |
| 180 | 9.83 | 10.14 | 9.64 | 10.13 | 10.01 | 10.31 | 10.07 |
| 194 | 10.23 | 11.30 | 10.51 | 11.13 | 10.71 | 11.04 | 10.77 |
| | | | | | | | |
| 206 | | | | | 10.93 | 11.32 | 11.06 |
| 207 | | | | | 10.39 | 10.82 | 10.60 |
| 208 | | | | | 10.41 | 10.83 | 10.62 |
| 209 | | | | | 11.14 | 11.60 | 11.34 |

[a] Indirect predictions, see text. [b] Direct predictions through eq 11.