Table S8: compilation of QSPRs for hydrolysis

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| --- | --- | --- | --- | --- | --- |
| **Symbol** | **Endpoint** | **Equation, method and/or algorithm** | **R2** | **Compound class(es)** | **References** |
| log(Khy) | - | log khy (pH 4, 22°C) = - 0.65 ELUMO - 0.62 | 0.776 | 6 Sulfonylurea herbicides | Berger and Wolfe (1996), Mamy (2014) |
| log(Khy) | - | log khy (pH 4, 40°C) = - 11.04 ELUMO - 10.36 | 0.702 | 6 Sulfonylurea herbicides | Berger and Wolfe (1996), Mamy (2014) |
| log(Khy) | - | log khy (buffer pH7, 40°C, MNDO) = 1690 ALPCO + 59.7 ALPHeterocycle atom, 4 - 1116 | 0.724 | 11 Sulfonylurea herbicides | Berger et al. (2002), Mamy (2014) |
| log(Khy) | - | log khy (buffer pH10, 40°C, MNDO) = 427 ALPCO + 26.5 ALPHeterocycle atom, 4 - 289 | 0.797 | 11 Sulfonylurea herbicides | Berger et al. (2002), Mamy (2014) |
| log(Khy) | - | log khy (buffer pH7, 40°C, PM3) = - 227 SE(CO) - 123 SE(4) - 96.3 | 0.814 | 11 Sulfonylurea herbicides | Berger et al. (2002), Mamy (2014) |
| log(Khy) | - | log khy (buffer pH10, 40°C, PM3) = 82.2 SE(CO) - 55.6 SE(4) + 8.4 | 0.476 | 11 Sulfonylurea herbicides | Berger et al. (2002), Mamy (2014) |
| log(Khy) | - | log khy (Sterile soil, MNDO) = 13978 ALPCO + 205 ALPHeterocycle atom, 4 - 9027 | 0.909 | 11 Sulfonylurea herbicides | Berger et al. (2002), Mamy (2014) |
| log(Khy) | - | log khy (Sterile sediment, MNDO) = 1108 ALPCO + 35.9 ALPHeterocycle atom, 4 - 731 | 0.824 | 11 Sulfonylurea herbicides | Berger et al. (2002), Mamy (2014) |
| log(Khy) | - | log khy (Sterile soil, PM3) = - 461 SE(CO) - 307 SE(4) - 189 | 0.021 | 11 Sulfonylurea herbicides | Berger et al. (2002), Mamy (2014) |
| log(Khy) | - | log khy (Sterile sediment, PM3) = - 136 SE(CO) - 70.6 SE(4) - 58.2 | 0.836 | 11 Sulfonylurea herbicides | Berger et al. (2002), Mamy (2014) |
| log(k) | First-order rate constant for neutral and pseudo first-order for base-promoted hydrolysis | log k = 1.64 (±0.42) σ(para) –1.37 (±0.17) | 0.858 | 14 p-substituted benzonitriles | European Commission (2003) |
| log(KOH) | 2nd-order alkaline hydrolysis rate constant | log kOH = 1.17 σ + 2.26 | 0.992 | 18 Benzoic esters | Harris (1990) |
| log(KOH) | 2nd-order alkaline hydrolysis rate constant | log kOH = 1.4 Σ σ - 0.47 | 0.99 | 4 Phosphoric acid esters | Harris (1990) |
| log(KOH) | 2nd-order hydrolysis rate constant | log kOH = - 9.65 q(P) + 2.85 ES(alcohol) + 4.89 | 0.896 | 19(?) Phosphoric acid esters | Johnson (1985) |
| log(KOH) | 2nd-order alkaline hydrolysis rate constant | log kOH = 4.59 σ\* + 1.52 ES - 1.02 | 0.975 | 5 Phthalate esters | Wolfe (1980) |
| log(Khy) | 2nd-order alkaline hydrolysis rate constant | log khyd. = - 0.26 (±0.001) pKa(alcohol) - 1.3 (±0.1) | 1 | 3 N-Methyl-N-phenylcarbamates | Wolfe (1978) |
| log(Khy) | 2nd-order alkaline hydrolysis rate constant | log khyd. = - 1.15 (±0.02) pKa(alcohol) + 13.6 (±0.2) | 0.99 | 20 N-phenylcarbamates | Wolfe (1978) |
| log(Khy) | 2nd-order alkaline hydrolysis rate constant | log khyd. = - 0.91 (±0.03) pKa(alcohol) + 9.3 (±0.4) | 0.99 | 6 N-Methylcarbamates | Wolfe (1978) |
| log(Khy) | 2nd-order alkaline hydrolysis rate constant | log khyd. = - 0.17 (±0.04) pKa(alcohol) - 2.6 (±0.4) | 0.8 | 7 N,N-Dimethylcarbamates | Wolfe (1978) |
| log(KOH) | 2nd-order alkaline hydrolysis rate constant | log kOH = 2.39 σ\*(R1, R2) + 0.96 σ(X1) + 7.97 σ\* (R3) + 2.81 σ(X2) + 0.275 | 0.973 | 62 Carbamates, X1R1N(R2)C(O)OR3X2, where R2=hydrogen, R1=alkyl or phenyl and R3=alkyl or phenyl with X1 and X2 their respective substituents | European Commission. (2003) |
| log(KOH) | 2nd-order alkaline hydrolysis rate constant | log kOH = 7.99 σ\*(R3) + 0.31 σ(X2) + 3.14 ES(R1, R2) + 0.442 | 0.903 | 18 Carbamates, X1R1N(R2)C(O)OR3X2, where R2=alkyl or phenyl NOT hydrogen, R1=alkyl or phenyl and R3=alkyl or phenyl with X1 and X2 their respective substituents | European Commission. (2003) |
| log(KOH) | 2nd-order alkaline hydrolysis rate constant | log kOH = 0.98 ES(R) + 0.25 ES(R’) + 2.24 σ\*(R) + 2.24 σ\*(R’) + 2.09 σ (X) + 1.21 σ(X’) + 2.69 | 0.974 | 103 Any chemical that contains an ester bond –C(=O)-O-; developed with alkyl/aryl - alkyl/aryl esters X-R-C(=O)-O-R’-X’, where R, R’ can be alkyl or aryl substituents and X, X’ any other substituents | European Commission. (2003) |
| log(Kcorr) | pseudo first-order reaction rate constant of reductive hydrolysis, corrected for the fraction of compound sorbed to sediment | log kcorr. = 0.54 log Kow + 0.57 σ - 5.28 | 0.925 | 17 Meta- and para-substituted benzonitriles | Peijnenburg (1993) |
| log(Kcorr) | pseudo first-order reaction rate constant of reductive hydrolysis, corrected for the fraction of compound sorbed to sediment | log kcorr. = - 0.46 log Kow + 1.26 σ - 4.56 | 0.981 | 7 Ortho-substituted benzonitriles | Peijnenburg (1993) |
| log(Ki/Ko) | k(i) is the pseudo first-order alkaline hydrolysis rate constant, and k(o) is the corresponding constant for CH3-Br hydrolysis | log k(i)/k(o) = -11.9 (±3.5) σ(I) | 0.77 | 16 Saturated linear and branched bromoalkanes with phenyl, chloro and bromo substituents | European Commission. (2003) |
| log(k) | second order base-catalyzed hydrolysis rate constant | log k = 101.812 - 60.4041 (RCC) - 10.1978 (ZCN) | 0.912 | 17 Imides | Buss (2001) |
| log(k) | second order base-catalyzed hydrolysis rate constant | log k = 1.15776 + 2.5015 (LUMO2) - 23.6256 (ZCO) | 0.864 | 17 Imides | Buss (2001) |
| KOH | Alkaline Hydrolysis Rate Constants | Quantum topological molecular similarity method. Semiempirical model AM1 (HF/ 3-21G(d), HF/6-31G(d), B3LYP/6-311+G(2d,p)) | 0.93 | 40 Esters | Chaudry (2003) |
| log(Khy) (log(kh)) | hydrolysis rate constant (kH) | Log(kH)=-4.21Es+4.58 s-23.64 | - | 5/2 Haloacetic acids | Chen (2011) |
| log(Khy) (log(kh)) | hydrolysis rate constant (kH) | Log(kH)=-1.32Es-6.23 s-2.61 | - | 12/6(?) Halomethanes | Chen (2011) |
| log(Khy) (log(kh)) | hydrolysis rate constant (kH) | Log(kH)=-4.45Es-4.04 s-10.52 | - | 4/1 Haloacetaldehydes | Chen (2011) |
| log(Khy) (log(kh)) | hydrolysis rate constant (kH) | Log(kH)=-3.79Es-8.44 s-1.07 | - | 5/5 Haloketones | Chen (2011) |
| log(Khy) (log(kh)) | hydrolysis rate constant (kH) | Log(kH)=0.38Es+3.59 s-5.03 | - | 7/5(?) Haloacetonitriles | Chen (2011) |
| log(KOH) | Alkaline Hydrolysis rate constants | log (kOH)cal1 = c1x1,1 + c2x1,2 + … + c38x1,38 | 0.887 | 41Carboxylic acid esters | Collette (1990) |
| log(Kb) | base-catalyzed rate constant | log Kb  =  0.92Es{R1} + 0.31Es{R2} + 2.16 sigma\*{R1} + 2.30 sigma\*{R2} + 2.10 sigmaX{R1} + 1.25 sigmaX{R2} + 2.67 | 0.982(R); 0.965(R2) | 124 Esters  R1-C(=O)-O-R2 | HYDROWIN (EPISUITE) Mill et al (1987) |
| log(Kb) | base-catalyzed rate constant | log Kb = 7.99 sigma\*{R3} + 0.316 Sum[sigmaX{R1+R2}] + 3.14 Sum[Es{R1+R2}] + 0.442 | ? | Di-N-substituted carbamates R1-N(-R2)-C(=O)-O-R3 | HYDROWIN (EPISUITE) |
| log(Kb) | base-catalyzed rate constant | log Kb = 2.3 Sum[sigma\*{R1+R2}] + 0.96 Sum[sigmaX{R1+R2}] + 7.97 sigma\*{R3} + 2.81 sigmaX{R3} - 0.275 | ? | Carbamates R1-N(-R2)-C(=O)-O-R3 | HYDROWIN (EPISUITE) |
| log(Ka) | acid-catalyzed rate constant for epoxides | log Ka  =  0.359 Summation[Es{R}]  -  2.15 Summation[sigma\*{R}]  +  1.015 Co  -  1.765 | 0.89 (R); 0.8 (R2) | 14 aliphatic epoxide | Mill et al (1987)HYDROWIN (EPISUITE) |
| log(Ka) | acid-catalyzed rate constant for epoxides | log Ka  =  -0.88 Summation[Es{R}]  -  4.18 Summation[sigma\*{R}]  +  0.63CT  +  0.47Do  - 1.36 Co  -  0.98 | 0.97(R); 0.94(R2) | 20 Vinylic-aromatic epoxides | Mill et al (1987)HYDROWIN (EPISUITE) |
| log(Kb) | base-catalyzed rate constant | log Kb  =  2.99 simga\*{Y2}  +  2.83 Summation [Es{Y1+Y2+Y3}]  + 0.995 fx  -  0.633 | 0.998(R); 0.996(R2) | 12 Halomethanes X-C(Y1)(Y2)Y3 | Mill et al (1987)  HYDROWIN (EPISUITE) |
| log(Kb) | base-catalyzed rate constant | log Kb  =  2.09 Summation[sigma\*{R1+R2+R3}]  +  0.491 Summation [Es{R1+R2+R3}]  +  3.20 fx  -  15.49 | 0.99(R); 0.98(R2) | 7 Alkyl halides | Mill et al (1987)HYDROWIN (EPISUITE) |
| DT50 | The half-life for base-catalyzed rate constants at pH 8 | Half-life  =  0.6931 / (Kb)(1.0E-6) | - | - | HYDROWIN (EPISUITE) |
| log(k) | Total calculated hydrolysis rate constant for hydrolysis in water | log k Hydrolysis = logkc +δIPlogkc +δEPlogkc  The hydrolysis rate constant contributions from these three sub-models are then summed to give the total calculated hydrolysis rate constant. | - | 576 Carboxylic acid esters | Whiteside (2006) (SPARC) |
| k1 | base-catalyzed hydrolysis rate constants (k1) | k1 = −17.118 (±0.130) + 0.137 (±0.021) δCβ | 0.933 | 5 Methacrylates | Fujisawa (2012) |
| k1 | base-catalyzed hydrolysis rate constants (k1) | k1 = 0.2288 (±0.015) + 0.0026 (±0.001) Hf | 0.891 | 5 Acrylates and methacrylates | Fujisawa (2012) |
| k1 | base-catalyzed hydrolysis rate constants (k1) | k1 = 0.211(±0.006) + 0.00044(8.1 × 10−5) ΔHf° | 0.907 | 5 Acrylates and methacrylates | Fujisawa (2012) |
| k2 | base-catalyzed hydrolysis rate constants (k2) | k2 = 0.085 (±0.016) + 0.0013 (±0.000) Hf | 0.941 | 4 MA, EA, MMA and EMA | Fujisawa (2012) |
| log(k) | hydrolytic rate constant | log k = 1.081(+-0.346) + 6.577(+-0.993)AN + 0.094(+-0.019)log P - 2.542(+-1.237)NUFD | 0.823 | 37 Benzoglycolamide Ester Prodrugs | Narasimhan (2006) |
| log(k) | hydrolytic rate constant | log k = 0.844(+-0.341) + 7.280(+-0.976)AN + 0.099(+-0.020)log P | 0.799 | 37 Benzoglycolamide Ester Prodrugs | Narasimhan (2006) |
| log(k) | hydrolytic rate constant | log k = 1.723(+-0.377) + 9.358(+-1.139)AN | 0.657 | 37 Benzoglycolamide Ester Prodrugs | Narasimhan (2006) |
| log(k) | reaction rate constants | log k = 37.5 + 78.2 O1 - 22.6 C1 - 0.481 LUMO | 0.93 | 35/41 Esters | Zhang (2005) |
| log(k) | reaction rate constants | log k - 34.1 - 91.0 O1 - 7.56 C1 - 2.42 LUMO | 0.922 | 35/41 Esters | Zhang (2005) |
| log(k) | reaction rate constants | log k = 26.3+ 67.8 O1 + 2.81 C1 - 14.2 LUMO | 0.929 | 35/41 Esters | Zhang (2005) |
| log(k) | reaction rate constants | log k = 33.8 + 83.6 O1 - 0.33 C1 - 13.9 LUMO | 0.915 | 34/41 Esters | Zhang (2005) |
| ln(k) | decomposition rate constant | lnk = -9.684Es - 36.76, where Es(THAA) = SIGMA(Es(Xi)); Xi = F; Cl; Br; or I: | 0.9987 | 5 (BDCAA, DBCAA, TBAA, TCAA and TFAA) | Zhang (2002) |
| ln(k) | hydrolysis rate constants | ln k = 1.6865 - 0.58608 1XVP | 0.943 | 11 Organophosphorus pesticides | Tanji (1995) |
| ln(k) | hydrolysis rate constants | ln k = -3.0238 + 2.0233 1XVP | 0.876 | 8 Ethyl alkanoates (with e- withdrawing groups) | Tanji (1995) |
| ln(k) | hydrolysis rate constants | ln k = 5.1685 - 4.1185 1XVP | 0.714 | 9 Ethyl alkanoates (e- donating groups) | Tanji (1995) |
| ln(k) | hydrolysis rate constants | ln k = 0.13073 + 0.71001 1ST ORDER CHI | 0.914 | 10 Alkyl Halides | Tanji (1995) |
| ? | hydrolysis rates | Partial Least Squares Regression (PLSR) | - | 103 (of which 32 stable against hydrolysis)Various kinds of chemicals including Carbamates, Triazines, Chloroacetanilides, Organophosphates | Tsuyuri et al. |
| log(DT50) | Hydrolysis half-life (Abiotic degradation in water) | log T(0.5) = 4.189 +0.104\*Kier&Hall index (order 0) -2.974\*ZX Shadow / ZX Rectangle (AM1) + 105.902\*HACA-2/TMSA (Zefirov) (all) -1.918\*Polarity parameter (Zefirov) / distance -0.662\*Square root of Charged (Zefirov) Surface Area of O atoms + 0.999\*Min net atomic charge (AM1) for N atoms | 0.715 | 166/83Structurally heterogeneous and highly structurally heterogeneous and highly representative of many classes of already defined problematic chemicals | Karelson |
| Dlog | the dependence of the meta, para polar, ortho inductive and resonance substituent effects on the solvent electrophilicity, DE, calculated using log k values for various solvents | Dlog km,p = log kX – log kH = (0.010 ± 0.023) + (1.77 ± 0.04)s – (0.0683 ± 0.0055)DEs | 0.990025 | 55 Substituted benzoic acids, X-C6H4CO2C6H5 | Nummert (2013) |
| Km,p | the contribution of the meta and para polar effects to the rates in the alkaline hydrolysis of phenyl esters of substituted benzoic acids | log km,p = (–1.620 ± 0.042) + (2.09 ± 0.10)s | 0.984064 | 8 substituted benzoic acids, X-C6H4CO2C6H5 | Nummert (2013) |
| Kortho | log k values for phenyl esters of ortho-substituted benzoic acids | log kortho = (–1.549 ± 0.051) + (2.42 ± 0.08)sI + (0.55 ± 0.09)s°R + (2.93 ± 0.11)EsB | 0.994009 | 10 substituted benzoic acids, X-C6H4CO2C6H5 | Nummert (2013) |
| T | Transformation | T (water, 60°C) = a ALPij + b | 0.77 | 10 Phenylurea herbicides | Berger et al. (2001), Mamy (2014) |
| T | Transformation | T (soil, 60°C) = a ALPij + b | 0.745 | 10 Phenylurea herbicides | Berger et al. (2001). Mamy (2014) |