Table S9: compilation of QSPRs for reaction with 1O2

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| --- | --- | --- | --- | --- | --- |
| **Symbol** | **Endpoint** | **Equation** | **R2** | **Compound class(es)** | **References** |
| log(K1O2) | reaction rate constant with singlet oxygen | log k = -4.36E1/2+ 10.92 | 0.81 | 21 phenols | Rorije (1996) |
| log(K1O2) | reaction rate constant with singlet oxygen | log k = - 1.49EHOMO + 21.84 | 0.8 | 21 phenols | Rorije (1996) |
| log(K1O2) | reaction rate constant with singlet oxygen | 15 descriptors, namely electronic properties from molecular orbital calculations and physicochernical properties. PLS analysis and MLR | 0.871 | 14/7 Phenols | Rorije (1996) |
| log(K1O2) | oxidation rate constants by singlet oxygen (1O2) | log kArO- = 9.61 +- 0.10 - 2.04 +- 0.15E1/2 | 0.935089 | 14 anionic phenols | Tratnyek (1991) |
| log(K1O2) | oxidation rate constants by singlet oxygen (1O2) | log kArO- = 8.9 +- 0.4 - 3.5 +- 0.5E1/2 | 0.7225 | 19 phenols | Tratnyek (1991) |
| log(K1O2) | oxidation rate constants by singlet oxygen (1O2) | log kArO- = 8.49 +- 0.08 - 1.38 +- 0.14SIGMA(s-m,p) | 0.917764 | 11 anionic phenols | Tratnyek (1991) |
| log(K1O2) | oxidation rate constants by singlet oxygen (1O2) | log kArOH = 7.0 +- 0.1 - 1.2 +- 0.2SIGMA(s-m,p) | 0.8281 | 12 phenols | Tratnyek (1991) |
| log(K1O2) | oxidation rate constants by singlet oxygen (1O2) | log kArO- = 8.33 +- 0.10 - 1.16 +- 0.12SIGMA(s-o,m,p) + 2.31 +- 0.55SIGMA(F) + 0.41 +- 0.18SIGMA(Es) | 0.913936 | 21 anionic phenols | Tratnyek (1991) |
| log(K1O2) | oxidation rate constants by singlet oxygen (1O2) | log kArOH = 7 .1 +- 0.1 - 1.0 +- 0.2SIGMA(s-o,m,p) | 0.7056 | 19 phenols | Tratnyek (1991) |
| log(K1O2) | second order rate constant for reaction with singlet oxygen | log k(1O2) = 5.5(+-0.5) + 0.36(+-0.07)log k(ClO2) cross-correlation with ClO2 reaction rate constants | 0.95 | 10 phenols and polychlorophenols | Canonica (2003) |
| ? | oxidation reactions in surface waters | HOMO R3e+ descriptors. Linear regression | 0.935 | 19 phenols | Gramatica (2005) |