Table S4: compilation of QSPRs for chlorination ClO2

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| --- | --- | --- | --- | --- | --- | --- | --- |
| **Symbol** | **Endpoint** | **Equation** | **R2** | **Q2** | **Compound class(es)** | **N** | **Reference** |
| log(KClO2) | Second order rate constant | log k(1O) = 5.5(+-0.5) + 0.36(+-0.07)log k(ClO2) | 0.95 |  | substitutred phenols | 10 | Canonica (2003) |
| log(KClO2) | Second-order rate constants (kClO2) | log (kPhOH) = 0.41 (+-0.50) - 4.69 (+-1.13) SIGMA(s+ o,m,p) | 0.86 | - | Non-dissociated phenols | 15 | Lee and von Gunten (2012) |
| log(KClO2) | Second-order rate constants (kClO2) | log (kPhO-) = 8.03 (+-0.13) - 3.24 (+-0.28) SIGMA(s- o,m,p) | 0.95 | - | Dissociated phenols | 32 | Lee and von Gunten (2012) |
| log(KClO2) | Second-order rate constants (kClO2) | log (kArNH2) = 5.34 (+-0.67) - 2.47 (+-0.94) SIGMA(s+ o,m,p) | 0.99 | - | Anilines | 4 | Lee and von Gunten (2012) |
| log(KClO2) | Second-order rate constants (kClO2) | log (k3amine) = 4.82 (+-0.13) - 1.72 (+-0.40) SIGMA(s\*) | 0.86 | - | Tertiary amines | 16 | Lee and von Gunten (2012) |
| log(KClO2) | Second-order rate constants (kClO2) | log (k1&2amine) = 4.53 (+-1.23) - 4.51 (+-1.64) SIGMA(s\*) | 0.79 | - | Primary & secondary amines | 12 | Lee and von Gunten (2012) |
| log(KClO2) | Second-order rate constants (kClO2) | logkaromatic (O3) = 3.19 (+-0.57) + 0.76 (+-0.11) logkaromatic (ClO2) | 0.94 | - | Aromatics | 16 | Lee and von Gunten (2012) |
| log(KClO2) | Kinetic rate constant | logk = 0.466E[2] - 0.174E[4] - 2.998 | 0.854515 | - | anilines | 10 | Fan (2005) |
| log(KClO2) (log(kArO-)) | Kinetic rate constant for phenolic anions | log kAr O- = 8.2(+-0.2) - 3.2(+-0.4) SIGMA(s o,m, p) | 0.9409 |  | phenolic anions | 23 | Tratnyek (1994) |
| log(KClO2) (log(kArO-)) | Kinetic rate constant for phenolic anions | logk = 10^10 - log(1 +0.1 exp[(30.1/4)(1+(DG/30.1)^2/0.592)] | - |  | phenolic anions | 23 | Tratnyek (1994) |
| log(KClO2) (log k) | Kinetic rate constant | log k = -4.52Ehomo + 48.77 | 0.76 | 0.7 | phenols | 22 | Rorije (1996) |
| log(KClO2)(log(k)) | Kinetic rate constant | HOMO and HATS3m descriptors | 0.925 | 0.878 | phenols | 21 | Gramatica (2005) |
| EOX | Potential for first-electron transfer step | E\_ox = 0.82(+-0.03) + 0.41(+-0.05)sp+ | 0.97 | - | para-substituted phenoxide ions | 14 | Lind et al (1990), Canonica (2003) |
| EOX | Potential for first-electron transfer step (E\_ox) | E\_ox = 0.79 + 0.34 SIGMA(s+) | 0.94 | - | multisubstituted phenoxide ions | - | Jonsson (1993), Canonica (2003) |
| EOX | Potential for first-electron transfer step (E\_ox) | E\_ox = 0.81(+-0.03) + 0.26(+-0.05) SIGMA(s+) | 0.8 | - | polychlorinated phenoxide ions | 31 | Li (1999), Canonica (2003) |
| EOX | Potential for first-electron transfer step (E\_ox) | E\_ox = 1.02(+-0.03) + 0.33(+-0.05)s+ | 0.96 |  | para-substituted anilines | 12 | Jonsson (1994), Canonica (2003) |
| EOX | Potential for first-electron transfer step (E\_ox) | E\_ox = 2.2 + 0.8 (sp1+ sp4+) + 0.4 sp1+sp4+ |  |  | 1,4-disubstituted benzene derivatives | ? | Jonsson (1993), Canonica (2003) |