Table S7: compilation of QSPRs for direct photolysis and quantum yield

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Symbol** | **Endpoint** | **Equation, method and/or algorithm** | **R2** | **Compound class(es)** | **References** |
| Φ | photolysis quantum yield | log Φ = -0.010 (+-0.004)BS + 0.665(+-0.105)ES + 1.031 (+-0.213) molecular structural descriptors, MLR method | 0.94 | 12 substituted aromatic halides | Peijnenburg (1992), Zhang (2013); Mamy (2014) |
| Φ | photolysis quantum yield | log Φ = a Es molecular structural descriptors, MLR method | 0.81 | 12 substituted aromatic halides | Peijnenburg (1992), Zhang (2013); Mamy (2014) |
| Φ | photolysis quantum yield | log Φ = a BS molecular structural descriptors, MLR method | 0.000 | 12 substituted aromatic halides | Peijnenburg (1992), Zhang (2013); Mamy (2014) |
| Φ | direct photolysis quantum yield | 11 quantum chemical descriptors computed by PM3 Hamiltonian, PLS method | 0.863041 | 13/10 PAHs | Chen (2000) |
| Φ | direct photolysis quantum yield | 11 quantum chemical descriptors computed by PM3 Hamiltonian, PLS method | 0.719104 | 10/9 PAHs (not including phenanthrene, chrysene, or naphthacene) | Chen (2000) |
| Φ | quantum yield | Φ = 10.719(±5.644) × DISPp + 45.996(±10.469)xGm + 34.663(±28.167) × ISH - 13.120(±9.453) × HATS4v - 41.289(±28.553) several molecular descriptors, GA-MLRA approach | 0.874 | 19/9/2 single-benzene ring compounds with various types (hydroxy-, chloro-, nitro-, methyl-, carboxyl-, sulfo-, amino-, etc.) and number (1–4) of substituents | Juretic (2013) |
| Φ | Direct photohydrolysis | log Φ = -1.02 (±0.24) \* sI + 0.30 (±0.I0) \* Es - 0.005 (±0.004) \* BS - 0.4 (±0.3) combinations of several literature-reported parameters, Multiple linear regression | 0.885 | 23 META-SUBSTITUTED HALOBENZENE DERIVATIVES | Stegeman (1993) |
| Φ | quantum yield | log Φ = - 0.007516 MW + 0.660 | 0.529 | 17 Substituted bromo and iodobenzenes | Chen et al (1998b), Mamy (2014) |
| Φ | quantum yield | log Φ = - 0.04814 MW + 4.088 | 0.669 | 7 Substituted fluorobenzenes | Chen et al (1998b), Mamy (2014) |
| Φ | quantum yield | log Φ = - 74.914 BO + 71.363 | 0.348 | 17 Substituted bromo and iodobenzenes | Chen et al (1998b), Mamy (2014) |
| Φ | quantum yield | log Φ = 1.774 EE - 577.087 | 0.664 | 7 Substituted fluorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 0.413 EHOMO + 2.935 | 0.292 | 17 Substituted bromo and iodobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 1.42 EHOMO + 11.829 | 0.651 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 1.904 EHOMO + 17.088 | 0.783 | 7 Substituted fluorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 0.869 ELUMO - 0.621 | 0.336 | 17 Substituted bromo and iodobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 1.137 ELUMO - 1.142 | 0.617 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 1.473 ELUMO - 1.077 | 0.704 | 7 Substituted fluorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 0.913 EN1 - 425.18 | 0.833 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 1.554 EN1 - 1179.43 | 0.651 | 7 Substituted fluorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 0.1797 EN2 + 70.254 | 0.267 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 1.579 NN2 + 323.905 | 0.335 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 8.85 qc - 0.689 | 0.273 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 168.177 qx - 16.879 | 0.672 | 7 Substituted fluorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 48.588 qx + 2.109 | 0.829 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 6.162 TE2 + 71.777 | 0.546 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 0.03706 a + 1.708 | 0.317 | 17 Substituted bromo and iodobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 0.03239 a + 0.611 | 0.268 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 0.1414 a + 6.613 | 0.777 | 15 Substituted fluorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 0.5818 μ - 1.171 | 0.242 | 17 Substituted bromo and iodobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 0.672 (ELUMO + EHOMO) + 5.032 | 0.674 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 0.8462 (ELUMO + EHOMO) + 7.007 | 0.781 | 7 Substituted fluorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 0.4013 (ELUMO + EHOMO) + 2.967 | 0.439 | 17 Substituted bromo and iodobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 1.306 ELUMO + 0.01456 EN2 + 4.812 | 0.807 | 41 Substituted aromatic halides | Chen et al (1998a) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 1.266 EN1 + 1.201 NN2 - 836.861 | 0.902 | 15 Substituted chlorobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 59.63 BO - 0.005774 MW + 57.768 | 0.789 | 17 Substituted bromo and iodobenzenes | Chen et al (1998b) , Mamy (2014) |
| Φ | quantum yield | log Φ = 1.132 ELUMO - 0.05154 EE2 - 0.004623 MW + 9.829 | 0.848 | 41 Substituted aromatic halides | Chen et al (1998a) , Mamy (2014) |
| Φ | quantum yield | log Φ = - 6.347 qC- - 6.177 QH+ + 0.2436 μ + 0.1658 (ELUMO + EHOMO) + 0.105 ELUMO - 0.09202 EHOMO + 0.05059 (ELUMO - EHOMO) + 0.003259 (ELUMO - EHOMO)² - 0.0008944 a - 0.0008147 MW - 0.00188 HOF + 0.00008090 TE - 0.00000961 CCR + 0.0000086 EE - 1.340 | 0.719 | 9 PAHs | Chen et al. (2000) , Mamy (2014) |
| Φ | quantum yield | log Φ = 12.38 BO + 10.28 QH+ - 10.18 qO + 9.863 qC- - 3.786 qCl - 3.160 K + 1.728 qC - 1.634 C + 1.34 qCl-C - 1.115 TE2 - 0.9658 J + 0.8155 EHOMO + 0.5772 NN2 + 0.5561 ELUMO - 0.1807 μ + 0.164 EE1-O - 0.1417 EN1-O - 0.03514 EN2 + 0.02539 EE1-C + 0.02104 EE2 - 0.01554 EN1-C + 0.01069 HOF - 0.00433 a - 0.001379 MW + 0.0001576 TE - 0.00002715 CCR + 0.00002317 EE - 278.5 | 0.972 | 9 PCDDs | Chen et al. (2001c) , Mamy (2014) |
| Φ | quantum yield | log Φ = 15.373 QH+ - 1.943 QO- + 1.462 qC- - 1.257 QBr+ + 0.289 EHOMO + 0.2068 ELUMO + 0.1452 (ELUMO + EHOMO) - 0.000161 CCR + 1.2674 | 0.982 | 11 PBDEs | Niu et al. (2006) , Mamy (2014) |
| DT50 | photolysis half-life value | log t1/2 = -3.681+1.284x10QC - 3.408x10^-2ΔHf - 7.202QCl+ - 1.779ELUMO+1 + 6.914x10^-1EHOMO - 1.188x10QH+ quantum chemical descriptors, PLS algorithm | ? | 7 PCBs | Bao (2011), Zhang (2013) |
| DT50 (Log (1/t0.5)) | photolytic half-life | Log (1/t0.5) = 6.13 (GAP-1) + 23.22(Qhal ) + 0.04(TPSA) - 29.21(Rad-super+) + 4.18(LUMO+) + 28.14 several molecular descriptors. principal component analysis (PCA) and partial least squares (PLS) | 0.932 | 20/6 Brominated compounds | Heimstad (2009) |
| DT50 (Log (1/t0.5)) | photolytic half-life | Log (1/t0.5) = 31.67(Qhal ) + 0.12(TPSA) - 20.49(Hal-BL+) + 7.96(LUMO+) + 0.02(Hf) + 28.33 several molecular descriptors. principal component analysis (PCA) and partial least squares (PLS) | 0.905 | 23/6 Brominated compounds | Heimstad (2009) |
| DT50 | photolysis half-life | log t1/2 = – 2.48522 – 0.742307 EHOMO – 0.427634 ED+ – 0.0258506 log P several molecular descriptors, stepwise multiple linear regression (MLR) | 0.9231 | 14/4 Azo dyes (monoazo and disazo dyes), sulfonephthalein dyes, an oxazine dye and derivatives of fluorescein | Beiknejad (2014) |
| DT50 | photolysis half-live | logt1/2 = –3.91627 + 0.00192 Sm – 0.21510 EHOMO– 1 – 0.04111 – 0.00154 MW + 0.07022 χ – 0.50700 EHOMO – 0.24482 ED+ several molecular descriptors, partial least squares (PLS) | 0.9968 | 14/4 Azo dyes (monoazo and disazo dyes), sulfonephthalein dyes, an oxazine dye and derivatives of fluorescein | Beiknejad (2014) |
| Kphoto (log kb) | photodegradation rate constants | logkb = 6.046 + 54.830EHOMO + 0.272N1 DFT and HF methods, stepwise multiple linear regression analysis | 0.75 | 12 PAHs | Xiang (2014) |
| Kphoto | photolysis rate constant | log kp = 9.770 (ELUMO - EHOMO) - 0.715 (ELUMO - EHOMO)² - 32.738 | 0.848 | 17 PAHs | Chen et al. (1996b) |
| Kphoto | photolysis rate constant | log kp = - 1.2939 EHOMO - 0.05066 (ELUMO - EHOMO)² + 0.01062 ΔHf + 0.00132 MW - 0.001173 CCR - 0.000308 TE - 17.616 | 0.958 | 15 PBDEs | Niu et al. (2006) |
| Kphoto (T1/2ph) | photolysis rate constant | log T1/2ph = - 48.91 qC- - 12.52 QH+ - 1.103 (ELUMO + EHOMO) - 0.7198 EHOMO - 0.4023 ELUMO + 0.3075 (ELUMO - EHOMO) - 0.1167 μ + 0.002008 (ELUMO - EHOMO)² - 0.00144  - 0.0006833 MW + 0.0003194 HOF + 0.0000746 TE - 0.000006315 CCR + 0.000005898 EE - 22.108 | 0.912 | 13 PAHs | Chen et al. (2001e) |
| Kphoto (log kb) | photodegradation rate constant | logkb = 6.046 + 54.830EHOMO + 0.272N1 several molecular descriptors. DFT and HF methods, and stepwise multiple linear regression analysis method | 0.75 | 12 PAHs | Xu (2014) |
| K254nm | Photodegradation rate constant for UV irradiation at 254nm | logk = -0.0075BS + 4.97Es - 8.8s + 55 several molecular descriptors. multiple linear regression | 0.95 | 9 ITHMs (iodinated trihalomethanes) and BTHMs (brominated THMs). | Xiao (2014) |