Table S1: compilation of QSPRs for sorption to environmental matrices (supplemented from Mamy et al. (2015)

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| --- | --- | --- | --- | --- |
| Endpoint | QSPR equation and specifics | r2 | Specifications of training/test set | Reference |
| Ktoc | log Ktoc = 0.29 naromatic-C | - | PAH | Arp et al. (2009) |
| Ktoc | log Ktoc = 0.40 nCl | - | Chlorobenzenes | Arp et al. (2009) |
| Ktoc | log Ktoc = 0.36 nCl | - | PCDD | Arp et al. (2009) |
| Ktoc | log Ktoc = 0.42 nCl | - | PCDF | Arp et al. (2009) |
| Ktoc | log Ktoc = 0.45 (nCl - 0.5 northo-Cl) | - | PCB | Arp et al. (2009) |
| Koc | log Koc = 0.44 1χ + 0.34 | 0.504 | 56 miscellaneous organic compounds | Bahnick and Doucette (1988) |
| Koc | log Koc = 0.53 1χ - 2.09 Δ1χv + 0.64 | 0.939 | 56 Miscellaneous organic compounds | Bahnick and Doucette (1988) |
| Koc | log Koc = 0.53 (+-0.04) 1x - 2.09 (+-0.22)D 1xv + 0.64 | 0.94 | 56 Wide variety | Bahnick and Doucette (1988) |
| Koc | log Koc = a Δ3χ + b | 0.69 | 94 miscellaneous organic compounds, “not likely to be applicable for chemicals with log Kow < 1.7” | Baker et al. (1997) |
| Koc | log Koc = a 1χ + b | 0.348 | 94 miscellaneous organic compounds | Baker et al. (1997) |
| Koc | log Koc = a 1χv + b | 0.397 | PAHs; chlorinated phenols | Baker et al. (1997) |
| Koc | log Koc = a 2χv + b | 0.524 | 94 miscellaneous organic compounds | Baker et al. (1997) |
| Koc | log Koc = a 3χv + b | 0.531 | 94 Miscellaneous organic compounds | Baker et al. (1997) |
| Koc | log Koc = a Δ2χ + b | 0.579 | 94 Miscellaneous organic compounds | Baker et al. (1997) |
| Koc | log Koc = a 1χv + b Δ1χv + b | 0.366 | 14 Miscellaneous organic compounds | Baker et al. (1997) |
| Koc | log Koc = a 1χ + b 1χv + c Δ0χv + d | 0.532 | 14 Miscellaneous organic compounds | Baker et al. (1997) |
| Koc | log Koc = 3.36 Vi/100 - 2.09 Sb2H + 0.93 | 0.72 | 68 Miscellaneous organic compounds | Baker et al. (1997) |
| Koc | log Koc = 0.903 log Kow + 0.094 | 0.91 | 72, wide variety | Baker et al. (1997) |
| Koc | log Koc = 0.28 1χ + 3.19 | 0.388 | 18 POP | Baker et al. (2001) |
| Koc | log Koc = 0.33 1χ - 5.29 4χvc + 0.99 3χc + 1.62 | 0.84 | 18 POP | Baker et al. (2001) |
| Kp | log Kp = 0.93 log Kow + 1.09 log fOC + 0.32Cfa - 0.55Cfb + 0.25 | 0.966 | Using 229 Kp values for 53 chemicals, tested on 87 chemicals having 500 Kp values. Only Kp values for soils having a %OC >0.1 were included. Dataset contained both ionized and non-ionized chemicals. | Bintein and Devillers 1994 |
| Koc | log Koc = 0.51[log S + (0.01MP - 0.25)] + 0.8 | 0.77 | 38 Variety, mostly pesticides | Briggs (1981) |
| Kom | log Kom = 0.0062 (P - 100 n) + 0.58 | 0.846 | 38 Substituted benzenes | Briggs (1981) |
| Kom | log Kom = 0.0062 (P-100N) + 0.58 | r=0.92 | 38 or 36 chemicals? | Briggs, 1981 |
| Koc | log Koc = 0.54 \* L + -0.98 \* S + -0.42 \* A + -3.34 \* B + 1.20 \* V + 0.02 | 0.93 | 79/50 pesticides and other multifunctional organic chemicals | Bronner (2011) |
| Koc | log Koc = 2.99 \* V + -0.61 \* S + -0.21 \* A + -3.44 \* B + 0.81 \* E + -0.29 | 0.92 | 129 pesticides and other multifunctional organic chemicals | Bronner, 2011 |
| Koc | log Koc = 0.937 log Kow - 0.006 | 0.95 | 9 Triazines | Brown (1981) |
| Kds | log Kds = a 1χ + b | <0.180 | 11 Naphthoic acids, 5 quinolines | Burgos and Pisutpaisal (2006) |
| Kds | log Kds = a 1χv + b | <0.130 | 11 Naphthoic acids, 5 quinolines | Burgos and Pisutpaisal (2006) |
| Kds | log Kds = a 3χv + b | <0.060 | 11 Naphthoic acids, 5 quinolines | Burgos and Pisutpaisal (2006) |
| Kds | log Kds = a 4χv + b | <0.020 | 11 Naphthoic acids, 5 quinolines | Burgos and Pisutpaisal (2006) |
| Kds | log Kds = a 4χvpc + b | <0.220 | 11 Naphthoic acids, 5 quinolines | Burgos and Pisutpaisal (2006) |
| Kocs | log Kocs = 0.0202 a - 0.363 μ - 5.220 q- - 4.722 | 0.93 | 22 Alkyl(1-phenylsulfonyl)-cycloalkane-carboxylates | Chen et al. (1996a) |
| Koc | log Koc = -0.557 log S + 4.277 (S in m moles/L) | 0.99 | 15 Chlorinated hydrocarbons | Chiou (1979) |
| Koc | log Koc = 0.904 log Kow - 0.539 | 0.99 | 12 PAHs, Chlorinated hydrocarbons | Chiou (1983) |
| Kom | log Kom = -0.729 log S + 0.001 (S is in moles/L for supercooled liquid) | 0.99 | 12 PAHs, chlorinated hydrocarbons | Chiou, 1983 |
| Koc | log Koc = 8.74(+-1.26) - 0.39mu(+-0.15) - 0.74EHOMO (+-0.13) - 3.18qH(+-0.14) - 2.72q(+-0.62) + 1.29TE(+-0.09) | r = 0.924 | 70 or 65?? polychlorinated organic compounds (i.e., pesticides, PCBs, furans, and dioxins) | Dai (1999) |
| Koc | log Koc = 5.99 - 1.02mu - 9.24qH + 0.49q | 0.8636 | 14 substituted benzaldehydes | Dai (2000) |
| Koc | log Koc = 0.526 1χ + 0.641 | 0.571 | 65 PCOCs | Dai et al. (1999) |
| Koc | log Koc = - 0.39 μ - 0.74 EHOMO - 3.18 QH+ - 2.72 q- + 1.29 TE + 8.74 | 0.854 | 65 PCOC | Dai et al. (1999) |
| Kocs | log Kocs = - 0.89 μ - 5.80 QH+ - 1.26 3χpc + 0.28 2χv + 5.28 | 0.922 | 14 Substituted benzaldehydes | Dai et al. (2000) |
| Koc | log Koc = 0.51 + 0.60 Nφ + 1.02 × 10-2 MW - 0.48 NN - 0.25 NO + 0.61 NS | 0.94 | Ntrain = 82, Ntest = 43. Polar and non-polar organic compounds | Delgrado (2003) |
| Kocs | log Kocs = 0.022 Vm - 0.10 | 0.99 | 5 Chlorobenzenes | Djohan et al. (2005) |
| Koc | log Koc = 1.4 log k9 + 2.5 | 0.87 | 30 compounds, octadecylsilane column | Doucette (2003) |
| Koc | log Koc = 2.0 log k9 + 3.0 | 0.91 | 48 compounds, trimethylammoniumpropylic column | Doucette (2003) |
| KCEC | Log KCEC,illite = 1.55(+-0.14)Vx - 0.15(+-0.05)NAi + 1.26(+-0.28) | 0.93 | 21 CXHYN amines (15mM NaCl, pH 6) | Droge (2013) |
| KCEC | Log KCEC,kaolinite = 1.16(+-0.17)Vx - 0.13(+-0.06)NAi + 2.07(+-0.34) | 0.83 | 22 CXHYN amines, (15mM NaCl, pH 6) | Droge (2013) |
| KCEC | Log KCEC, clays = 1.22(+-0.15)Vx - 0.22(+-0.05)NAi + 2.09(+-0.05) | 0.9 | 23 CXHYN amines, (15mM NaCl, pH 6) | Droge (2013) |
| Doc | Log Doc = 0.00892 Vc + 0.0328 A + 0.257 | 0.84 | 30 CxHyN model amines (pH 4.5) , >90% of species ionized | Droge (2013) |
| KLs | log KL (illite) = 0.45 #C + 0.11 #EO - 1.82 | 0.92 | 9 Alcohol ethoxylates | Droge et al. (2009) |
| KII | log KII (illite) = 0.51 #C - 0.023 #EO - 2.88 | 0.98 | 9 Alcohol ethoxylates | Droge et al. (2009) |
| KLs | log KL (sediment) = 0.42 #C + 0.14 #EO - 2.59 | 0.91 | 9 Alcohol ethoxylates | Droge et al. (2009) |
| KII | log KII (sediment) = 0.55 #C - 0.065 #EO - 4.06 | 0.97 | 9 Alcohol ethoxylates | Droge et al. (2009) |
| Koc | log Koc = 3.71 \* V + 1.27 \* S + -0.10 \* A + -3.94 \* B + 0.31 \* E + -1.04 | 0.91 | - | Endo |
| Koc | log Koc = 3.51 \* V + 0.19 \* S + 0.02 \* A + -3.83 \* B + 0.43 \* E + -0.82 | 0.9 | - | Endo |
| Koc | log Koc = 1.501 Vm/100 + 14.487 q- - 0.108 μtot - 12.476 | 0.96 | 28 Alkyl(1-phenylsulfonyl) cycloalkane-carboxylates | Famini and Wilson (1997) |
| Koc | log Koc = 3.185 Vi/100 - 0.510 π\* - 1.525 Sb2H + 0.851 | 0.982 | 18 Phenylthiocarbamates | Feng et al. (1996) |
| Koc | log Koc = log(øn10^0.37og(Pn+1.70) + øion 10^pKa^0.65 f^0.14) | 0.76 (training); 0.55 (validation) | Full training set of 65 bases | Franco and Trapp (2008) |
| Koc | log Koc = log(øn 10^0.50 log(Pn)+1.13 + ømin 10^0.11 log(Pn) + 1.54 + øplus 10^pKa^0.65 f^0.14) | 0.04 to 0.80 | 6 amphoters | Franco and Trapp (2008) |
| Koc | log Koc = log(øn 10^0.54log(Pn + 1.11) + øion 10^0.11log(Pn + 1.54)) | 0.54 (0.44) | N = 93, organic acids (combined regression) | Franco and Trapp (2008) |
| Koc | log Koc = 0.544 log Kow + 1.377 | 0.74 | 45, Variety, mostly pesticides | Fugate (1989) |
| Koc | log Koc = 0.02 TSA - 0.29 | 0.83 | 36 non polar (chlorobenzenes, PAH, PCB) | Fugate (1989) in Doucette (2003) |
| Koc | log Koc = 6.786/(exp(1.573 + 0.282 log S - 0.301 log Kow)+1) | - | 119 nonpolar and polar organics, 66 polychlorinated biphenyls (PCBs) | Gao (1996) |
| Koc | log Koc 5 1.937 log k9 2.982 | 0.824 | 47 Mainly pesticides, cyanopropyl column | Gawlik (1998) |
| Koc | log Koc = 1.688 log k9 2.593 | 0.824 | 47 Mainly pesticides, cyanopropyl column | Gawlik (2000) |
| Koc | log Koc = 0.567 1xv - 0.29 | 0.86 | 12 Alcohols | Gerstl (1987) |
| Koc | log Koc = 1.146 3xv + 0.54 | 0.83 | 14 PAHs, heterocyclic PAHs | Gerstl (1987) |
| Koc | log Koc = 0.679 log Kow + 0.663 | 0.831 | N = 419, mainly non-ionic organic chemicals | Gerstl (1990) |
| Koc | log Koc = 0.545 log Kow + 0.943 | 0.713 | 57, ureas | Gerstl (1990) |
| Koc | log Koc = 0.433 log Kow + 0.919 | 0.863 | 39 Carbamates | Gerstl (1990) |
| Koc | log Koc = (-0.508 log S + 0.953) - Fc | 0.757 | 419 Wide variety | Gerstl (1990) |
| Koc | log Koc = 20.38 log S + 1.177 (S is in moles/L) | 0.616 | 57 Ureas | Gerstl (1990) |
| Koc | log Koc = -0.410 log S + 0.978 (S is in moles/L) | 0.601 | 39 Carbamates | Gerstl (1990) |
| Koc | log Koc = 0.529 log Kow - 0.916 | 0.664 | 38 nonhalogenated aromatics | Gerstl (1990) |
| Kfoc\* | log Kfoc = 0.519 1χv - 1.76 5χv + 0.732 4χvpc + 0.487 | 0.711 | 21 Acetalinides | Gerstl (1990) |
| Kfoc\* | log Kfoc = 1.22 1χv - 1.06 3χv - 0.621 3χvc - 1.18 | 0.758 | 12 Amides | Gerstl (1990) |
| Kfoc\* | log Kfoc = - 0.207 0χ + 0.969 0χv - 0.712 3χv - 0.184 | 0.847 | 73 Halogenated aromatic hydrocarbons | Gerstl (1990) |
| Kfoc\* | log Kfoc = - 1.04 0χ + 1.16 2χ + 1.39 1χv + 0.767 | 0.673 | 38 Non-halogenated aromatic hydrocarbons | Gerstl (1990) |
| Kfoc\* | log Kfoc = - 1.25 3χ + 1.11 4χpc + 0.946 1χv + 0.890 | 0.624 | 20 Dinitroanilines | Gerstl (1990) |
| Kfoc\* | log Kfoc = 0.365 4χpc + 0.135 0χv - 0.094 3χv + 1.15 | 0.877 | 17 Non-aromatic halogenated hydrocarbons | Gerstl (1990) |
| Kfoc\* | log Kfoc = 1.91 2χv - 1.54 3χv + 1.95 3χvc + 0.801 | 0.826 | 20 PAH | Gerstl (1990) |
| Kfoc\* | log Kfoc = - 0.492 0χ + 0.776 5χ + 0.44 0χc + 1.94 | 0.535 | > 400 Miscellaneous organic compounds | Gerstl (1990) |
| Koc | log Koc = 1.151 5χv + 1.70 | 0.633 | 97 miscellaneous organic compounds | Gerstl and Helling (1987) |
| Kom | log Kom = 1.94 - 0.492 0x + 0.776 5x + 0.440 0xc | 0.535 | 419 Wide variety | Gerstl, 1990 |
| Koc | log Koc = 0.443 1χv + 0.29 | 0.477 | Non acidic pesticides | Gertsl and Helling (1987) |
| Koc | log Koc = 0.567 1χv - 0.29 | 0.864 | 11 aliphatic alcohols | Gertsl and Helling (1987) |
| Koc | log Koc = 1.146 3χv + 0.54 | 0.827 | 14 Miscellaneous organic compounds (pesticides) | Gertsl and Helling (1987) |
| Koc | log Koc = 1.336 5χv - 2.746 4χvc + 1.58 | 0.633 | 97 Miscellaneous organic compounds | Gertsl and Helling (1987) |
| Koc | log Koc = 0.400 1χv + 17.53 0χvc + 0.47 | 0.575 | Non acidic pesticides | Gertsl and Helling (1987) |
| Koc | log Koc = 1.953 3χv - 4.010 3χvc - 0.17 | 0.905 | 14 Miscellaneous organic compounds | Gertsl and Helling (1987) |
| Koc | log Koc = 1.146 3χv - 2.078 5χvc + 0.81 | 0.841 | 14 Miscellaneous organic compounds | Gertsl and Helling (1987) |
| Koc | log Koc = 0.333407 HTp + 0.936504 MATS6e + 0.78916 G3v + 0.122569 Mor(05)m + 4.201647 G1m + 1.210337 MATS4p - 0.711055 BEHm2 + 1.72965 | ? | 62 Pesticides | Goudarzi et al. (2009) |
| Koc | log Koc = -1.92(+-0.11) + 2.07(+-0.06)VED1 - 0.31(+-0.01)nHAcc - 0.31(+-0.02)MAXDP - 0.39(+-0.05)CIC0 | 0.82 | 642 heterogeneous non-ionic organic compounds | Gramatica (2006) |
| Koc | log Koc = 0.009 MW + 0.277 nNO - 0.192 nHA + 0.325 CIC - 0.265 MAXDP + 0.052 Ts + 1.355 | 0.843 | 141/20 non-ionic organic pesticides | Gramatica et al. (2000) |
| Koc | log Koc = 0.61 1χ - 0.093 DELS - 0.711 | 0.965 | 13 Triazines | Gramatica et al. (2000) |
| Koc | log Koc = 0.299 nX - 0.497 nO - 0.446 nNO + 0.006 ξC + 2.016 | 0.948 | 29 Carbamates | Gramatica et al. (2000) |
| Koc | log Koc = 1.515 IEdeg - 0.972 IC - 0.298 MAXDP - 6.028 η1u + 0.166 Ts + 5.328 | 0.889 | 28 Organophosphates | Gramatica et al. (2000) |
| Koc | log Koc = 0.015 MW + 0.272 nCl + 0.484 NoRING - 0.067 λ1v - 1.283 η2s - 0.033 | 0.911 | 43 Phenylureas | Gramatica et al. (2000) |
| Koc | log Koc = 0.87 + 0.26 VP0 - 0.23 nHBAcc + 0.08 nAromBond - 0.19 MAXDP | 0.79 | 643 heterogeneous non-ionic chemicals | Grammatica (2014) |
| Kf | log Kf = 0.0067 (P - 45 N) - 0.65 | 0.83 | 29 Aromatic herbicides | Hance (1969) |
| Koc | log Koc = 0.0252 TSA - 0.677 | 0.92 | 48 PCBs | Hansen et al. (1999a) |
| Kd | log Kd = 0.0265 TSA - 3.62 | 0.95 | 48 PCBs | Hansen et al. (1999a) |
| Koc | log Koc = -0.686 log S + 4.273 (S in mol/L) | 0.93 | 22 PAHs, heterocyclic PAHs, aromatic amines, chlorinated hydrocarbons | Hassett (1980) |
| Ktoc | log Ktoc = 0.52 (nCl - northo-Cl) + 5.13 | - | 209 PCBs | Hawthorne et al. (2011) |
| Ktoc | log Ktoc = 0.53 (nCl - northo-Cl) + 4.98 | - | PCBs | Hawthorne et al. (2011) |
| Kocs | log Kocs = 2.175 Vi/100 - 0.666 π\* - 1.260 Sb2H - 1.821 | 0.976 | 28 Phenylsulfonyl acetates | He et al. (1995) |
| Koc | log Koc = 2.70 log k9 + 2.04 | 0.992 | 7 Aromatic and aliphatic hydrocarbons, cyanopropyl column | Hodson (1988) |
| Koc | log Koc = 0.22 + 0.015TSA - 0.041(N-TSA) - 2 0.25(O-TSA) - 0.045(ARN-TSA) | 0.49 | 167 nonpolar and polar compounds | Holt (1992) |
| Koc | log Koc = 3.782 + 3.138RRT | 0.92 | 168 nonpolar and polar compounds | Holt (1992) |
| Kp | log Kp = 1.35 1χ + 0.15 | 0.979 | 6 Halogenated aliphatics | Hsieh and Mukherjee (2003) |
| Kd | log Kd = 0.074 VdW - 3.11 | 0.83 | 6 Non polar, non ionizable organic compounds | Hu et al. (1995) |
| Kd | log Kd = 0.052 VdW - 4.80 | 0.88 | 15 Non polar, non ionizable organic compounds | Hu et al. (1995) |
| Kd | log Kd = 1.44 1χv - 2.42 | 0.93 | 6 Non polar, non ionizable organic compounds | Hu et al. (1995) |
| Kd | log Kd = 1.00 1χv - 4.19 | 0.94 | 15 Non polar, non ionizable organic compounds | Hu et al. (1995) |
| Koc | log Koc = 0.35 1χ + ΣaiSi + 0.622 | 0.82 | 143 Nonionic pesticides | Huuskonen (2003) |
| Koc | log Koc = 0.84 + (0.60)logKow | 0.4 | 19 PhACs | Huuskonen (2003) |
| Koc | log Koc = -0.54log S + 0.81 | 0.8 | Ntrain = 403 Ntest = 165, mainly nonionic pesticides and herbicides | Huuskonen (2003) |
| Koc | log Koc = -0.35log S - 0.18HBA + 0.24NAR + 0.004MW - 0.55Iacid+ 0.88 | 0.85 | Ntrain = 403 Ntest = 165, mainly nonionic pesticides and herbicides | Huuskonen (2003) |
| Koc | log Koc = 0.60log P + 0.84 | 0.79 | Ntrain = 403 Ntest = 165, mainly nonionic pesticides and herbicides | Huuskonen (2003) |
| Koc | log Koc = 0.48log P + 0.26NAR - 0.07ROT + 0.002MW - 0.77Iacid + 0.56 | 0.86 | Ntrain = 403 Ntest = 165, mainly nonionic pesticides and herbicides | Huuskonen (2003) |
| Koc | log Koc = [(0.47 ± 0.46)] + [(0.79 ± 0.13)logKow] | 0.41 | 13 PhACs | Hyland et al. (2012) |
| Kd | log kd = 0.06 log D + 1.07 log OC + 0.99 GATS7v + 2.45 | 0.721 | 78 acidic pesticides in 36 temperate soils | Kah and Brown (2007) |
| Kd | log kd = 0.13 log D + 1.02 log OC - 1.51 | 0.392 | 6 ionizable pesticides measured under different soil properties | Kah and Brown (2007) |
| Kd | log kd = 0.06 log D + 1.07 log OC + 0.99 GATS7v + 2.45 | 0.872 | 6 ionizable pesticides measured under different soil properties | Kah and Brown (2007) |
| Kd | log kd = 1.09 log OC + 0.11 Mg + 3.36 BELv3 | 0.807 | 4 basic pesticides measured under different soil properties | Kah and Brown (2007) |
| Koc | log Koc = 0.0085 MW + 0.132 | 0.628 | 15 pesticides | Kanazawa (1989) |
| Koc | log Koc = -0.356 log S + 3.01 (S in ppm) | 0.79 | 15 Pesticides | Kanazawa (1989) |
| Koc | log Koc = 0.402 log Kow + 1.071 | 0.69 | 15 pesticides | Kanazawa J. (1989) |
| Koc | log Koc = 1.00 log Kow - 0.21 | 1 | 10 PAHs, aromatics | Karickhoff (1979) |
| Koc | log Koc = log S + 0.44 | 0.94 | 10 PAHs, aromatics | Karickhoff (1979) |
| Koc | log Koc = 0.989 log Kow - 0.346 | 0.997 | 5 PAHs | Karickhoff (1981) |
| Koc | log Koc = -0.83 log S - 0.01(MP - 25) - 0.93 (S in mole fraction) | 0.93 | 47 PAHs, chlorinated hydrocarbons, pesticides | Karickhoff (1984) |
| Koc | log Koc = -0.55 log S + 3.64 (S in mg/L) | 0.71 | 106 Variety, mostly pesticides | Kenaga and Goring (1980) |
| Ks/w | log Ks/w = 0.33 #C + 0.06 #EO - 1.7 | 0.88 | 11 Alcohol ethoxylates | Kiewiet et al. (1996) |
| Koc | log Koc = 0.673 1χ | 0.95 | 18 halogenated aromatics | Koch (1983) in Doucette (2003) |
| Kom | log Kom = 0.673 1x | 0.95 | 18, Halogenated aromatics | Koch, 1983 |
| Koc | log Koc = 1.8 log k9 + 2.4 | 0.98 | 48 Mainly pesticides, amines, triazines, cyanopropyl nolumn | Kordel (1993) |
| Kh | log Kh = 0.023 TSA (non planar configuration) - 1.491 | 0.919 | 26 PCB | Lara and Ernst (1989) |
| Kh | log Kh = 0.028 TSA (planar configuration) - 2.093 | 0.954 | 26 PCB | Lara and Ernst (1989) |
| Koc | log Koc = 1.002 + 0.582 log Kow | 0.765 | 42 substituted anilines and phenols | Liu (2005) |
| Koc | log Koc = 0.244 + 0:538 log Kow - 0.141Ehomo + 0.025a - 0.092mu | 0.775 | 42 substituted anilines and phenols | Liu (2005) |
| Koc | log Koc = 0.0011 MW + 0.729 | 0.532 | 42 Substituted anilines and phenols | Liu and Yu (2005) |
| Koc | log Koc = 0.745 1χv + 0.263 | 0.507 | 42 substituted anilines and phenols | Liu and Yu (2005) |
| Koc | log Koc = - 0.779 ELUMO + 2.559 | 0.35 | 42 Substituted anilines and phenols | Liu and Yu (2005) |
| Koc | log Koc = - 0.523 EHOMO - 2.074 | 0.126 | 42 Substituted anilines and phenols | Liu and Yu (2005) |
| Koc | log Koc = 1.823 q + 3.126 | 0.035 | 42 Substituted anilines and phenols | Liu and Yu (2005) |
| Koc | log Koc = 0.032 a + 0.137 | 0.319 | 42 Substituted anilines and phenols | Liu and Yu (2005) |
| Koc | log Koc = - 0.191 μ + 2.720 | 0.018 | 42 Substituted anilines and phenols | Liu and Yu (2005) |
| Koc | log Koc = 0.153 0χv + 0.222 n34 + 0.122 nCl - 0.764 O2S - 0.901 O2P + 0.318 C4C4C1N - 0.729 O1C + 0.216 C4C4C1O + 0.482 C1S1C - 0.259 C2O1N1C + 0.043 C4C4C + 0.732 | 0.772 | 120 Pesticides | Lohninger (1994) |
| Koc | log Koc = 0.1880 Lu + 0.7856 | 0.788 | 11 phthalates | Lu (2009) |
| Koc | log Koc = 0.2382 Lu - 0.1798 DAI(CH3-) - 0.0350 DAI (~CH~) + 0.1787 DAI (~C») + 0.1147 DAI (-C») + 0.1456 DAI(-O-) + 1.0501 | 0.9 | 32 POP | Lu et al. (2006) |
| Koc | log Koc = 0.94 log Kow + 0.02 | - | 9 s-triazines and dinitroaniline herbicides | Lyman (1982) |
| Koc | log Koc = 0.524 log Kow + 0.855 | 0.84 | 30 substituted phenylureas and alkyl-N-phenylcarbamates | Lyman (1982) |
| Koc | log Koc = 0.681 log Kow + 1.886 | 0.83 | 22 heterogeneous pesticides | Lyman (1982) |
| Kd | log Kd = 0.70 (+-0.07) log γsat -10.68 (+-0.17) | 0.94 | N = 16, sorption of the PAHs, chlorobenzenes, and biphenyl to r-Al2O3 | Mader, 1997 |
| Kd | log Kd = 0.98 (+-0.10) log γsat -11.39 (+-0.25) | 0.92 | N = 16, sorption of the PAHs, chlorobenzenes, and biphenyl to r-Fe2O3 | mader, 1997 |
| Kd | log Kd = 2.61 + (0.67) log(Kow) | 0.6 | 15 PhACs | Matter-Muller et al. (1980) |
| Koc | log Koc = 0.53 1x0.63 + Sum Pf N | 0.96 | 189 Wide variety | Meylan (1992) |
| Koc | log Koc = 0.53 1χ + 62 | 0.956 | 64 non polar organic compounds | Meylan et al. (1992) |
| Koc | log Koc = -0.58 log S + 4.24 (S in mmol/L) | 0.41 | 15 Apolar hydrocarbons | Mingelgrin (1983) |
| Koc | log Koc =-1.6463+0.7032(0.0556)0cv 1 | 0.8001 | 42 polar organic chemicals: substituted anilines & phenols | Mishra and Sachan (2012) |
| Koc | log Koc =-2.1222+1.5017(0.1160)1cv 2 0.8073 | 0.8025 | 43 polar organic chemicals: substituted anilines & phenols | Mishra and Sachan (2012) |
| Koc | log Koc =-1.1276+1.5637(0.0938)2cv 3 0.8742 | 0.8711 | 44 polar organic chemicals: substituted anilines & phenols | Mishra and Sachan (2012) |
| Koc | log Koc =-1.1710-0.0023(0.0016)W+0.6781(0.1222)2cv 4 | 0.8805 | 45 polar organic chemicals: substituted anilines & phenols | Mishra and Sachan (2012) |
| Koc | log Koc =- 1.6296+0.2921(0.1766)Jhetp+1.4313(0.1218)2cv 5 | 0.8825 | 46 polar organic chemicals: substituted anilnes & phenols | Mishra and Sachan (2012) |
| Koc | log Koc =-0.6691-0.4258(0.2127)0cv+2.4512(0.4525)2cv 6 0.8860 | 0.8801 | 47 polar organic chemicals: substituted anilnes & phenols | Mishra and Sachan (2012) |
| Koc | log Koc=2.0683-6.1021(1.3431)Jhetv+5.2394(1.0984)Jhetp+1.2807(0.1047)2cv | 0.9239 | 48 polar organic chemicals: substituted anilines & phenols | Mishra and Sachan (2012) |
| KL | log KL = -54.47 9χ + 183.75 | 0.999 | 9 Dye tracers | Mon et al. (2006) |
| Koc | log Koc = a 0χ + b | 0.317 | 66 pesticides, polar, non polar | Müller and Kördel (1996) |
| Koc | log Koc = a 0χv + b | 0.381 | 66 Pesticides, polar, non polar | Müller and Kördel (1996) |
| Koc | log Koc = a 1χ + b | 0.324 | 66 pesticides, polar and non polar organic compounds | Müller and Kördel (1996) |
| Koc | log Koc = a 1χv + b | 0.374 | 66 pesticides, polar and non polar organic compounds | Müller and Kördel (1996) |
| Koc | log Koc = a 2χ + b | 0.354 | 66 pesticides, polar and non polar organic compounds | Müller and Kördel (1996) |
| Koc | log Koc = a 2χv + b | 0.395 | 66 pesticides, polar and non polar organic compounds | Müller and Kördel (1996) |
| Kdoc | log(Kdoc) SP = 0.40 \* L + -0.72 \* S + 0.49 \* A + -3.42 \* B + 2.65 \* V + -0.92 | 0.97 | - | Neale (2012) |
| Kdoc | log(Kdoc) SP = 3.94 \* V + -0.52 \* S + 0.63 \* A + -3.40 \* B + 0.29 \* E + -0.85 | 0.971 | 52 chemicals | Neale (2012) |
| Kdoc | log(Kdoc) SP = 0.34 \* L + -0.69 \* S + 0.02 \* A + -2.43 \* B + 1.54 \* V + -0.82 | 0.82 | - | Neale (2012) |
| Kdoc | log(Kdoc) SP = 2.86 \* V + -0.63 \* S + 0.05 \* A + -2.48 \* B + 0.63 \* E + -1.21 | 0.845 | 34 polar and non-polar compounds | Neale (2012) |
| Koc | log Koc = 2.28 \* V + -0.72 \* S + 0.15 \* A + -1.98 \* B + 1.10 \* E + 0.14 | 0.98 | 75 chemicals, including apolar, monopolar, and bipolar compounds | Nguyen et al. 2005 |
| Koc | log Koc = 0.64 Vx + 1.12 R2 - 0.69 Sa2H - 1.60 Sb2O + 1.20 | 0.929 | 28 Miscellaneous organic compounds | Poole and Poole (1999) |
| Koc | log Koc = 2.58 Vx + 0.80 R2 - 0.42 p\* - 0.43 Sa2H - 2.08 Sb2O - 0.02 | 0.933 | 55 Miscellaneous organic compounds | Poole and Poole (1999) |
| Koc | log Koc = 1.76 \* V + -0.39 \* S + -0.39 \* A + -1.51 \* B + 0.95 \* E + 0.55 | 0.94 | 138 compounds | Poole and Poole, 1999 |
| Koc | log Koc = 0.893 log k9 + 1.803 | 0.971 | 11 Aromatics, humic acid column | Pussemier (1990) |
| Koc | log Koc = 1.029 log Kow - 0.18 | 0.94 | 13 Chlorinated hydrocarbons, pesticides | Rao (1980) |
| Koc | log Koc = 0.064 + 0.541 log Kow | 0.57 | 18, six pollutants | Rao (2001) |
| Koc | log Koc = 0.006 + 0.541 log Kow + 1.09 IS | 0.57 | N = 18 | Rao (2001) |
| Koc | log Koc = 1.615 + 2.419 (Vi/100) - 1.821pi - 2.102b | 0.74 | N = 18 | Rao (2001) |
| Koc | log Koc = 1.557 + 2.419 (Vi/100) - 1.821pi - 2.102 b + 1.095 IS | 0.75 | N = 18 | Rao (2001) |
| Koc | log Koc = 0.0195 VdW - 0.9944 | 0.68 | 71 herbicides | Reddy and Locke (1994a) |
| Koc | log Koc = 0.0162 VdW + 0.0219 a - 0.0502 μ - 0.3607 EHOMO - 3.9898 | 0.7 | 71 Herbicides | Reddy and Locke (1994a) |
| Koc | log Koc = - 0.0306 VdW + 0.00013 (VdW)² - 0.3116 μ + 0.05009 μ² - 0.5716 ELUMO + 3.6424 | 0.7 | 44 Substituted phenylureas | Reddy and Locke (1994b) |
| Kom | log Kom = 0.55 1χ + 0.45 | 0.973 | 37 PAH, halogenated hydrocarbons | Sabljic (1984) |
| Koc | log Koc = 0.55 1x | 0.95 | 72 Polynuclear aromatic hydrocarbons, (PAHs), halogenated hydrocarbons | Sabljic (1987) |
| Kom | log Kom = 0.528 1χ - 0.996 Pf + 0.551 | 0.972 | 143 Polar organic compounds | Sabljic (1987) |
| Kom | log Kom = 53 1χ + 0.54 | 0.952 | 72 PAH, heteroPAH, chlorobenzenes, alkylbenzenes, amino and hydroxy | Sabljic (1987) |
| Koc | log Koc = 0.81 log Kow + 0.10 | 0.887 | 81, predominantly hydrophobics | Sabljic (1995) |
| Koc | log Koc = 0.63 log Kow + 0.90 | 0.865 | 54, Substituted phenols, anilines, and nitrobenzenes, chlorinated benzonitriles | Sabljic (1995) |
| Koc | log Koc = 0.47 log Kow + 1.09 | 0.681 | 216 Agricultural chemicals: acetamilides, carbamates, esters, phenylureas, phosphates, triazines, triazoles, and uracils | Sabljic (1995) |
| Koc | log Koc = 0.52 1x + 0.70 | 0.96 | 81 Hydrophobics | Sabljic (1995) |
| Koc | log Koc = 1.08 + 0.57 log Kow | 0.737 | 24 phenols and benzonitriles | Sabljic (1995) |
| Koc | log Koc = 0.47 log Kow + 0.50 | 0.72 | 36 alcohols and organic acids | Sabljic (1995) |
| Koc | log Koc = 0.40 log Kow + 1.12 | 0.51 | 21 acetanilides | Sabljic (1995) |
| Koc | log Koc = 0.39 log Kow + 0.50 | 0.77 | 13 alcohols | Sabljic (1995) |
| Koc | log Koc = 0.33 log Kow + 1.25 | 0.46 | 28 amides | Sabljic (1995) |
| Koc | log Koc = 0.365 log Kow + 1.14 | 0.58 | 43 carbamates | Sabljic (1995) |
| Koc | log Koc = 0.38 log Kow + 1.92 | 0.83 | 20 dinitroanilines | Sabljic (1995) |
| Koc | log Koc = 0.49 log Kow + 1.05 | 0.76 | 25 esters | Sabljic (1995) |
| Koc | log Koc = 0.77 log Kow + 0.55 | 0.7 | 10 nitrobenzenes | Sabljic (1995) |
| Koc | log Koc = 0.49 log Kow + 1.05 | 0.62 | 52 phenylureas | Sabljic (1995) |
| Koc | log Koc = 0.49 log Kow + 1.17 | 0.73 | 41 phosphates | Sabljic (1995) |
| Koc | log Koc = 0.30 log Kow + 1.50 | 0.32 | 16 triazines | Sabljic (1995) |
| Koc | log Koc = 0.47 log Kow + 1.405 | 0.66 | 15 triazoles | Sabljic (1995) |
| Kh | log Kh = - 0.25 (1χ)² + 5.30 1χ - 21.42 | 0.948 | 26 PCB | Sabljic et al. (1989) |
| Kh | log Kh = - 0.22 (1χ)² + 4.83 1χ - 0.16 noCl - 19.44 | 0.99 | 26 PCB | Sabljic et al. (1989) |
| Koc | log Koc = 0.52 1χ + 0.70 | 0.961 | 81 hydrophobic organic compounds containing C, H, F, Cl, Br or I atoms | Sabljic et al. (1995) |
| Koc | log Koc = 0.10 + (0.81)logKow | 0.4 | 11 PhACs | Sabljic et al. (1995) |
| Kom | log Kom = 0.55 1x | 0.94 | 37 0.940 PAHs, halogenated, hydrocarbons, chlorophenols | Sabljic, 1984 |
| Koc | Koc = (+-0.034)1.034CRI + (+-0.113)0.441 | 0.982 | 36 chlorinated biphenyls, phenols and benzenes | Sacan and Balcioglu (1996) |
| Kd | log Kd = [-1.71 ± 0.29] + [(0.41 ± 0.08)logKow] | 0.4 | 19 PhACs | Sathyamoorthy and Ramsburg (2013) |
| Kd | log Kd = [-2.49 ± 0.30] + [(0.63 ± 0.08)logKow] | 0.6 | 15 PhACs (limited Kow range) | Sathyamoorthy and Ramsburg (2013) |
| Kd | log Kd = [ 3.12 ± 0.29] + [(0.63 ± 0.07)logD] + [(0.30 ± 0.06)nHBA] + [( 0.07 ± 0.03)nRB] | 0.73 | 19 uncharged PhACs | Sathyamoorthy and Ramsburg (2013) |
| Kd | log Kd = [5.88 ± 1.69] + [(0.37 ± 0.05)log D] + [(0.30 ± 0.05)nHBA] + [( 3.56 ± 0.78)logMV] | 0.6 | 16 negatively charged PhACs | Sathyamoorthy and Ramsburg (2013) |
| Kd | log Kd = (7.65 ± 2.24) + [(0.34 ± 0.04)]log(KOW)] + [(1.65 ± 0.31)]log(Pi.Energy)] + [( 4.34 ± 0.94)]log(vdWSA)] + [(0.05 ± 0.02)]log(nRB)] | 0.54 | 32 positively charged PhACs | Sathyamoorthy and Ramsburg (2013) |
| Kd | log Kd = (4.54 ± 1.36) + [(0.39 ± 0.04)logD] + [(0.32 ± 0.04)nHBA] + [( 2.41 ± 0.59)logMV] + [( 0.86 ± 0.25)log(TPSA) | 0.64 | 16 negatively charged and uncharged PhACs | Sathyamoorthy and Ramsburg (2013) |
| Koc | log Koc = 0.00321 MW + 0.255 ε - 0.0139 Si + ΣajFj + ΣbkIk + 0.936 | 0.852 | 571 Non-ionic organic compounds | Schüürmann et al. (2006) |
| Koc | log Koc = 0.44 2χv - 0.24 NoNP - 0.45 | 0.941 | 11 Amides | Sekusak and Sabljic (1992) |
| Koc | log Koc = 0.25 1χ - 0.99 NoPP - 4.23 | 0.941 | 16 Dinitroanilines | Sekusak and Sabljic (1992) |
| Koc | log Koc = 1.27 F1χv - 14.18 NoRING - 0.25 NoPP - 2.32 | 0.902 | 15 Triazoles | Sekusak and Sabljic (1992) |
| Koc | log Koc = 0.28 1χv - 0.49 Δ1 + 3.33 FG + 0.70 | 0.846 | 21 Acetalinides | Sekusak and Sabljic (1992) |
| Koc | Koc = 0.35 Kow | 0.89 | Hydrophobic chemicals | Seth (1999) |
| Koc | log Koc = 1.03 log Kow - 0.61 | 0.95 | 117. Wide variety | Seth et al. (1999) |
| Koc | log Koc = 0.695 + (0.602)logKow | 0.41 | 13 PhACs | Stevens-Garmon et al. (2011) |
| Koc | log Koc = 0.95 log kw9 + 1.781 | 0.986 | 10 Aromatics, humic acid column | Szabo (1990) |
| Koc | log Koc = 1.441 log kw9 + 1.488 | 0.947 | 10 Aromatics, Ethylsilica column | Szabo (1990) |
| Koc | log Koc = 0.656 1χv + 0.574 1χ + 0.259 2χ + 10.716 6χch + 0.734 | 0.624 | 400 Miscellaneous organic compounds | Tao and Lu (1999) |
| Koc | log Koc = 0.389 Sester + 0.058 Salkyl - 9.353 | 0.822 | 8 Phthalates | Thomsen et al. (1999) |
| Koc | log Koc = 0.96 -0.26\*Polarity parameter (AM1) / distance +1.07E-002\*ALFA polarizability (DIP) (AM1) -1.99\*Max net atomic charge (AM1) for C atoms +1.30E-002\*WNSA1 Weighted PNSA (PNSA1\*TMSA/1000) (Zefirov) | 0.756 | 142 non-ionic organic pesticides | Tulp et al. (2015) |
| Koc | log Koc = 1.034 CRI + 0.441 | 0.964 | 36 PCBs, chlorinated phenols, and chlorinated benzenes | Türker Saçan and Balcioğlu (1996) |
| Kds | log Kds = 0.331 #C - 0.00897 #EO - 1.126 | 0.64 | 31 Alcohol ethoxylates and 4 alcohols | Van Compernolle et al. (2006) |
| Koc | log Koc = a Vm + b | 0.012 to 0.902 | 10 esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Koc | log Koc = a 1χ + b | 0.006 to 0.921 | 10 esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Koc | log Koc = a 1χv + b | 0.01 to 0.883 | 10 esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Koc | log Koc = a ALP + b | 0.05 to 0.921 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Koc | log Koc = 0.27 ALP - 0.41 | 0.883 | 10 Esters (in Podzol) | Von Oepen et al. (1991) |
| Koc | log Koc = 0.23 ALP + 0.11 | 0.921 | 10 Esters (in Alfisol) | Von Oepen et al. (1991) |
| Koc | log Koc = a DN + b | 0.017 to 0.902 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Koc | log Koc = a Qave + b | 0.002 to 0.705 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Koc | log Koc = a Qtot + b | 0.08 to 0.921 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Kocs | log Kocs = a Vm + b | 0.185 to 0.846 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Kocs | log Kocs = a 1χ + b | 0.073 to 0.624 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Kocs | log Kocs = a 1χv + b | 0.211 to 0.828 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Kocs | log Kocs = a ALP + b | 0.126 to 0.883 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Kocs | log Kocs = 0.22 ALP - 0.07 | 0.883 | 10 Esters | Von Oepen et al. (1991) |
| Kocs | log Kocs = a DN + b | 0.193 to 0.828 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Kocs | log Kocs = a Qave + b | 0.032 to 0.533 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Kocs | log Kocs = a Qtot + b | 0.044 to 0.757 | 10 Esters, 8 acids, 10 amides, 8 amines | Von Oepen et al. (1991) |
| Kd | Regressions with pharmacological volume of distribution (Vd) | 0.39 to 0.76 (median: 0.5) | 21 pharmaceuticals | Williams (2009) |
| Koc | log Koc = 0.21(+-0.09) + 2.09(+-0.10)Vx + 0.74(+-0.04)R - 0.31(+-0.09)a - 2.27(+-0.11)b | r=0.977 | 131 compounds | Winget (2000) |
| Koc | log Koc = 4.90 Vi/100 + 0.54 π\* - 2.70 Sb2H + 0.19 Sa2H - 0.87 | 0.984 | 38 Hydrophobic organic compounds | Xu et al. (2002) |