Supplemental Information for:

**Density functional theory calculation of lipophilicity for organophosphate type pesticides**

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| TABLE SI. IUPAC names of all 22 OPs pesticides investigated in present study |
|  |  |
| 1. Acephate
 | N-[methoxy(methylsulfanyl)phosphoryl]acetamide |
| 1. Aspon
 | dipropoxythiophosphoryloxy-dipropoxy-thioxo-phosphorane |
| 1. Carbophenothion
 | [[(4-chlorophenyl)thio]methylthio]-diethoxy-thioxo-phosphorane |
| 1. Chlorpyrifos
 | diethoxy-thioxo-[(3,5,6-trichloro-2-pyridyl)oxy]phosphorane |
| 1. Coumaphos
 | 3-chloro-7-diethoxyphosphinothioyloxy-4-methylchromen-2-one |
| 1. Crufomate
 | N-[(4-tert-butyl-2-chlorophenoxy)-methoxyphosphoryl]methanamine |
| 1. Diazinon
 | diethoxy-(2-isopropyl-6-methyl-pyrimidin-4-yl)oxy-thioxo-phosphorane |
| 1. Dichlorvos
 | 2,2-dichloroethenyl dimethyl phosphate |
| 1. Dimethoate
 | 2-dimethoxyphosphinothioylsulfanyl-N-methylacetamide |
| 1. Dioxathion
 | [[3-(diethoxythiophosphorylthio)-1,4-dioxan-2-yl]thio]-diethoxy-thioxo-phosphorane |
| 1. Disulfoton
 | diethoxy-[2-(ethylthio)ethylthio]-thioxo-phosphorane |
| 1. Ethion
 | [(diethoxythiophosphorylthio)methylthio]-diethoxy-thioxo-phosphorane |
| 1. Fenithrotin
 | O, O-dimethyl O-(3-methyl-4-nitrophenyl) phosphorothioate |
| 1. Fenthion
 | dimethoxy-[3-methyl-4-(methylthio)phenoxy]-thioxo-phosphorane |
| 1. Fonofos
 | ethoxy-ethyl-(phenylthio)-thioxo-phosphorane |
| 1. Malathion
 | diethyl 2-dimethoxyphosphinothioylsulfanylbutanedioate |
| 1. Methyl Parathion
 | dimethoxy-(4-nitrophenoxy)-thioxo-phosphorane |
| 1. Monocrotophos
 | dimethyl [(E)-4-(methylamino)-4-oxobut-2-en-2-yl] phosphate |
| 1. Parathion
 | diethoxy-(4-nitrophenoxy)-thioxo-phosphorane |
| 1. Phorate
 | diethoxy-[(ethylthio)methylthio]-thioxo-phosphorane |
| 1. Phosalone
 | 6-chloro-3-(diethoxyphosphinothioylsulfanylmethyl)-1,3-benzoxazol-2-one |
| 1. Temephos
 | [4-[(4-dimethoxythiophosphoryloxyphenyl)thio]phenoxy]-dimethoxy-thioxo-phosphorane |
|  |  |

TABLE SII. Calculated solvation free energy of transfer from the gas phase to water phase (ΔGsolv(water) / kcal·mol−1) and octanol phase (ΔGsolv(octanol) / kcal·mol−1) under standard state conditions, and corresponding log *K*OW values of examined OPs pesticide set at PBE/6-31+G(d,p) level of theory, with experimentally determined log *P*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Organophosphates | ΔGsolv(water) | ΔGsolv(octanol) | log *K*ow | log *P* (exp.) | Ref. |
|  |  |  |  |  |  |
| 1. Acephate
 | -15.5 | -15.5 | 0.0 | -0.8 | [1](#_ENREF_1) |
| 1. Aspon
 | -8.7 | -19.1 | 6.3 | 6.0 | [1](#_ENREF_1) |
| 1. Carbophenothion
 | -9.3 | -16.8 | 5.5 | 5.3 | [1](#_ENREF_1) |
| 1. Chlorpyrifos
 | -5.2 | -12.5 | 5.3 | 5.0 | [2](#_ENREF_2) |
| 1. Coumaphos
 | -11.2 | -16.9 | 4.1 | 4.5 | [3](#_ENREF_3) |
| 1. Crufomate
 | -9.3 | -14.8 | 4.0 | 3.4 | [1](#_ENREF_1) |
| 1. Diazinon
 | -8.8 | -14.6 | 3.8 | 3.8 | [1](#_ENREF_1) |
| 1. Dichlorvos
 | -5.9 | -9.3 | 2.5 | 1.4 | [1](#_ENREF_1) |
| 1. Dimethoate
 | -15.0 | -16.2 | 0.9 | 0.8 | [1](#_ENREF_1) |
| 1. Dioxathion
 | -14.4 | -22.5 | 5.9 | 4.3 | [1](#_ENREF_1) |
| 1. Disulfoton
 | -8.9 | -16.1 | 5.3 | 4.0 | [1](#_ENREF_1) |
| 1. Ethion
 | -10.4 | -18.7 | 6.0 | 5.1 | [1](#_ENREF_1) |
| 1. Fenithrotion
 | -6.9 | -11.1 | 3.1 | 3.3 | [1](#_ENREF_1) |
| 1. Fenthion
 | -7.1 | -12.7 | 4.2 | 4.1 | [4](#_ENREF_4) |
| 1. Fonofos
 | -9.9 | -15.5 | 4.1 | 3.9 | [1](#_ENREF_1) |
| 1. Malathion
 | -12.8 | -16.7 | 2.9 | 2.4 | [1](#_ENREF_1) |
| 1. Methyl Parathion
 | -7.0 | -10.6 | 2.6 | 2.9 | [1](#_ENREF_1) |
| 1. Monocrotophos
 | -14.7 | -15.2 | 0.4 | -0.2 | [1](#_ENREF_1) |
| 1. Parathion
 | -7.5 | -12.7 | 4.2 | 3.8 | [1](#_ENREF_1) |
| 1. Phorate
 | -7.8 | -14.3 | 4.8 | 3.6 | [1](#_ENREF_1) |
| 1. Phosalone
 | -11.9 | -17.3 | 4.0 | 4.4 | [1](#_ENREF_1) |
| 1. Temephos
 | -9.7 | -18.3 | 7.6 | 6.0 | [1](#_ENREF_1) |
|  |  |  |  |  |  |

TABLE SIII. Calculated solvation free energy of transfer from the gas phase to water phase (ΔGsolv(water) / kcal·mol−1) and octanol phase (ΔGsolv(octanol) / kcal·mol−1) under standard state conditions, and corresponding log *K*OW values of examined OPs pesticide set at M062X/6-31+G(d,p) level of theory, with experimentally determined log *P*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Organophosphates | ΔGsolv(water) | ΔGsolv(octanol) | log *K*ow | log *P* (exp.) | Ref. |
|  |  |  |  |  |  |
| 1. Acephate
 | -17.7 | -17.1 | -0.4 | -0.8 | [1](#_ENREF_1) |
| 1. Aspon
 | -10.3 | -19.3 | 5.8 | 6.0 | [1](#_ENREF_1) |
| 1. Carbophenothion
 | -9.9 | -17.0 | 5.2 | 5.3 | [1](#_ENREF_1) |
| 1. Chlorpyrifos
 | -5.7 | -13.0 | 5.4 | 5.0 | [2](#_ENREF_2) |
| 1. Coumaphos
 | -12.2 | -17.7 | 4.1 | 4.5 | [3](#_ENREF_3) |
| 1. Crufomate
 | -11.9 | -15.6 | 2.7 | 3.4 | [1](#_ENREF_1) |
| 1. Diazinon
 | -8.8 | -14.3 | 4.0 | 3.8 | [1](#_ENREF_1) |
| 1. Dichlorvos
 | -7.3 | -10.3 | 2.2 | 1.4 | [1](#_ENREF_1) |
| 1. Dimethoate
 | -15.2 | -16.1 | 0.7 | 0.8 | [1](#_ENREF_1) |
| 1. Dioxathion
 | -15.2 | -22.3 | 5.2 | 4.3 | [1](#_ENREF_1) |
| 1. Disulfoton
 | -9.3 | -16.2 | 5.1 | 4.0 | [1](#_ENREF_1) |
| 1. Ethion
 | -10.9 | -18.3 | 5.5 | 5.1 | [1](#_ENREF_1) |
| 1. Fenithrotion
 | -7.9 | -11.8 | 2.8 | 3.3 | [1](#_ENREF_1) |
| 1. Fenthion
 | -7.7 | -13.2 | 4.0 | 4.1 | [4](#_ENREF_4) |
| 1. Fonofos
 | -11.3 | -16.3 | 3.7 | 3.9 | [1](#_ENREF_1) |
| 1. Malathion
 | -13.8 | -17.4 | 2.7 | 2.4 | [1](#_ENREF_1) |
| 1. Methyl Parathion
 | -7.9 | -11.3 | 2.5 | 2.9 | [1](#_ENREF_1) |
| 1. Monocrotophos
 | -16.8 | -15.7 | -0.8 | -0.2 | [1](#_ENREF_1) |
| 1. Parathion
 | -8.4 | -13.4 | 3.7 | 3.8 | [1](#_ENREF_1) |
| 1. Phorate
 | -8.1 | -14.0 | 4.3 | 3.6 | [1](#_ENREF_1) |
| 1. Phosalone
 | -12.7 | -17.8 | 3.8 | 4.4 | [1](#_ENREF_1) |
| 1. Temephos
 | -11.1 | -19.0 | 6.6 | 6.0 | [1](#_ENREF_1) |
|  |  |  |  |  |  |

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