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
2.	Aspon	dipropoxythiophosphoryloxy-dipropoxy-thioxo-phosphorane
3.	Carbophenothion	[[(4-chlorophenyl)thio]methylthio]-diethoxy-thioxo-phosphorane
4.	Chlorpyrifos	diethoxy-thioxo-[(3,5,6-trichloro-2-pyridyl)oxy]phosphorane
5.	Coumaphos	3-chloro-7-diethoxyphosphinothioyloxy-4-methylchromen-2-one
6.	Crufomate	N-[(4-tert-butyl-2-chlorophenoxy)-methoxyphosphoryl]methanamine
7.	Diazinon	diethoxy-(2-isopropyl-6-methyl-pyrimidin-4-yl)oxy-thioxo-phosphorane
8.	Dichlorvos	2,2-dichloroethenyl dimethyl phosphate
9.	Dimethoate	2-dimethoxyphosphinothioylsulfanyl-N-methylacetamide
10.	Dioxathion	[[3-(diethoxythiophosphorylthio)-1,4-dioxan-2-yl]thio]-diethoxy-thioxo-phosphorane
11.	Disulfoton	diethoxy-[2-(ethylthio)ethylthio]-thioxo-phosphorane
12.	Ethion	[(diethoxythiophosphorylthio)methylthio]-diethoxy-thioxo-phosphorane
13.	Fenithrotin	O, O-dimethyl O-(3-methyl-4-nitrophenyl) phosphorothioate
14.	Fenthion	dimethoxy-[3-methyl-4-(methylthio)phenoxy]-thioxo-phosphorane
15.	Fonofos	ethoxy-ethyl-(phenylthio)-thioxo-phosphorane
16.	Malathion	diethyl 2-dimethoxyphosphinothioylsulfanylbutanedioate
17.	Methyl Parathion	dimethoxy-(4-nitrophenoxy)-thioxo-phosphorane
18.	Monocrotophos	dimethyl [(E)-4-(methylamino)-4-oxobut-2-en-2-yl] phosphate
19.	Parathion	diethoxy-(4-nitrophenoxy)-thioxo-phosphorane
20.	Phorate	diethoxy-[(ethylthio)methylthio]-thioxo-phosphorane
21.	Phosalone	6-chloro-3-(diethoxyphosphinothioylsulfanylmethyl)-1,3-benzoxazol-2-one
22.	Temephos	[4-[(4-dimethoxythiophosphoryloxyphenyl)thio]phenoxy]-dimethoxy-thioxo-phosphorane

TABLE SII. Calculated solvation free energy of transfer from the gas phase to water phase ($\Delta G_{solv(water)}$ / kcal·mol^{-1}) and octanol phase ($\Delta G_{solv(octanol)}$ / 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	$\Delta G_{solv(water)}$	$\Delta G_{solv(octanol)}$	log K_{ow}	log *P* (exp.)	Ref.
1. Acephate	-15.5	-15.5	0.0	-0.8	[1]
2. Aspon	-8.7	-19.1	6.3	6.0	[1]
3. Carbophenothion	-9.3	-16.8	5.5	5.3	[1]
4. Chlorpyrifos	-5.2	-12.5	5.3	5.0	[2]
5. Coumaphos	-11.2	-16.9	4.1	4.5	[3]
6. Crufomate	-9.3	-14.8	4.0	3.4	[1]
7. Diazinon	-8.8	-14.6	3.8	3.8	[1]
8. Dichlorvos	-5.9	-9.3	2.5	1.4	[1]
9. Dimethoate	-15.0	-16.2	0.9	0.8	[1]
10. Dioxathion	-14.4	-22.5	5.9	4.3	[1]
11. Disulfoton	-8.9	-16.1	5.3	4.0	[1]
12. Ethion	-10.4	-18.7	6.0	5.1	[1]
13. Fenithrotion	-6.9	-11.1	3.1	3.3	[1]
14. Fenthion	-7.1	-12.7	4.2	4.1	[4]
15. Fonofos	-9.9	-15.5	4.1	3.9	[1]
16. Malathion	-12.8	-16.7	2.9	2.4	[1]
17. Methyl Parathion	-7.0	-10.6	2.6	2.9	[1]
18. Monocrotophos	-14.7	-15.2	0.4	-0.2	[1]
19. Parathion	-7.5	-12.7	4.2	3.8	[1]
20. Phorate	-7.8	-14.3	4.8	3.6	[1]
21. Phosalone	-11.9	-17.3	4.0	4.4	[1]
22. Temephos	-9.7	-18.3	7.6	6.0	[1]

TABLE SIII. Calculated solvation free energy of transfer from the gas phase to water phase ($\Delta G_{solv(water)}$ / kcal·mol^{-1}) and octanol phase ($\Delta G_{solv(octanol)}$ / 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	$\Delta G_{solv(water)}$	$\Delta G_{solv(octanol)}$	log K_{ow}	log *P* (exp.)	Ref.
1. Acephate	-17.7	-17.1	-0.4	-0.8	[1]
2. Aspon	-10.3	-19.3	5.8	6.0	[1]
3. Carbophenothion	-9.9	-17.0	5.2	5.3	[1]
4. Chlorpyrifos	-5.7	-13.0	5.4	5.0	[2]
5. Coumaphos	-12.2	-17.7	4.1	4.5	[3]
6. Crufomate	-11.9	-15.6	2.7	3.4	[1]
7. Diazinon	-8.8	-14.3	4.0	3.8	[1]
8. Dichlorvos	-7.3	-10.3	2.2	1.4	[1]
9. Dimethoate	-15.2	-16.1	0.7	0.8	[1]
10. Dioxathion	-15.2	-22.3	5.2	4.3	[1]
11. Disulfoton	-9.3	-16.2	5.1	4.0	[1]
12. Ethion	-10.9	-18.3	5.5	5.1	[1]
13. Fenithrotion	-7.9	-11.8	2.8	3.3	[1]
14. Fenthion	-7.7	-13.2	4.0	4.1	[4]
15. Fonofos	-11.3	-16.3	3.7	3.9	[1]
16. Malathion	-13.8	-17.4	2.7	2.4	[1]
17. Methyl Parathion	-7.9	-11.3	2.5	2.9	[1]
18. Monocrotophos	-16.8	-15.7	-0.8	-0.2	[1]
19. Parathion	-8.4	-13.4	3.7	3.8	[1]
20. Phorate	-8.1	-14.0	4.3	3.6	[1]
21. Phosalone	-12.7	-17.8	3.8	4.4	[1]
22. Temephos	-11.1	-19.0	6.6	6.0	[1]

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