Mesulfenfos

Other names:	Phosphorothioic acid, O,O-dimethyl O-(4-(methylsulfinyl)-m-tolyl) ester
	O,O-Dimethyl O-(4-(methylsulfinyl)-m-tolyl) phosphorothioate
	O,O-Dimethyl O-((4-methylthio)-m-tolyl)phosphorothioate sulfoxide
	Fensulfoxide
	Fenthion sulfoxide
	Phosphorothioic acid, O,O-dimethyl O-(3-methyl-4-(methylsulfinyl)phenyl) ester
	Mesulfenos
	Mesulfenphos
Inchi:	InChI=1S/C10H15O4PS2/c1-8-7-9(5-6-10(8)17(4)11)14-15(16,12-2)13-3/h5-7H,1-4H3
InchiKey:	DLAPIMGBBDILHJ-UHFFFAOYSA-N
Formula:	C10H15O4PS2
SMILES:	COP(=S)(OC)Oc1ccc(S(C)=O)c(C)c1
Mol. weight [g/mol]:	294.33
CAS:	3761-41-9

Physical Properties

Property code	Value	Unit	Source
log10ws	1.59		Crippen Method
logp	2.629		Crippen Method
mcvol	204.640	ml/mol	McGowan Method
rinpol	2305.50		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2210.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3761419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices