

Fenoxon sulfoxide

Other names:	Phosphoric acid, dimethyl 3-methyl-4-(methylsulfinyl)phenyl ester Phosphoric acid, dimethyl 4-(methylsulfinyl)-m-tolyl ester Fenthion O-analog sulfoxide BAY 35681 Bayer 35681 Dimethyl 3-methyl-4-(methylsulfinyl)phenyl phosphate Dimethyl 4-(methylsulfinyl)-m-tolyl phosphate ENT 25565 Fenthion oxon sulfoxide
Inchi:	InChI=1S/C10H15O5PS/c1-8-7-9(5-6-10(8)17(4)12)15-16(11,13-2)14-3/h5-7H,1-4H3
InchiKey:	GTZCKTIZOGTWQO-UHFFFAOYSA-N
Formula:	C10H15O5PS
SMILES:	<chem>COP(=O)(OC)Oc1ccc(S(C)=O)c(C)c1</chem>
Mol. weight [g/mol]:	278.26
CAS:	6552-13-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	2.512		Crippen Method
mcvol	194.160	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6552132&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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