

Fenthion O-analog sulfone

Other names:	Phosphoric acid, dimethyl 3-methyl-4-(methylsulfonyl)phenyl ester
	Phosphoric acid, dimethyl 4-(methylsulfonyl)-m-tolyl ester
	Fenoxon sulfone
	Dimethyl 4-(methylsulfonyl)-m-tolyl phosphate
	Fenthion oxon sulfone
Inchi:	InChI=1S/C10H15O6PS/c1-8-7-9(16-17(11,14-2)15-3)5-6-10(8)18(4,12)13/h5-7H,1-4H3
InchiKey:	VUTHWSUXEOILTU-UHFFFAOYSA-N
Formula:	C10H15O6PS
SMILES:	<chem>COP(=O)(OC)Oc1ccc(S(C)(=O)=O)c(C)c1</chem>
Mol. weight [g/mol]:	294.26
CAS:	14086-35-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	2.178		Crippen Method
mcvol	200.030	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14086352&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

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