Carbophenoxon sulfone

Other names:	Phosphorothioic acid, S-[[(4-chlorophenyl)sulfonyl]methyl] O,O-diethyl ester Phosphorothioic acid, S-[[(p-chlorophenyl)sulfonyl]methyl] O,O-diethyl ester Methanethiol, [(p-chlorophenyl)sulfonyl]-, S-ester with O,O-diethyl phosphorothioate O,O-Diethyl S-(p-chlorophenylsulfonyl)methyl phosphorothioate R 1777 S-(p-Chlorophenylsulfonyl)methyl O,O-diethyl phosphorothioate Carbophenothion oxon sulfone Trithion oxon sulfone S-([(4-Chlorophenyl)sulfonyl]methyl) O,O-diethyl thiophosphate Carbophenothion O-analog sulfone
Inchi:	InChI=1S/C11H16ClO5PS2/c1-3-16-18(13,17-4-2)19-9-20(14,15)11-7-5-10(12)6-8-11/h5
InchiKey:	AQORIFUYBMSEHZ-UHFFFAOYSA-N
Formula:	C11H16ClO5PS2
SMILES:	CCOP(=O)(OCC)SCS(=O)(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	358.80
CAS:	16662-87-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.34		Crippen Method
logp	3.986		Crippen Method
mcvol	236.840	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=C16662876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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