Carbophenothion sulfone

Other names:	Phosphorodithioic acid, S-[[(4-chlorophenyl)sulfonyl]methyl] O,O-diethyl ester
	Phosphorodithioic acid, S-[[(p-chlorophenyl)sulfonyl]methyl] O,O-diethyl ester
	O,O-Diethyl S-(p-chlorophenylsulfonyl)methyl phosphorodithioate
	R 1776
	S-p-Chlorophenylsulfonylmethyl O,O-diethyl phosphorodithioate
Inchi:	InChI=1S/C11H16ClO4PS3/c1-3-15-17(18,16-4-2)19-9-20(13,14)11-7-5-10(12)6-8-11/h5
InchiKey:	CBXRYOZUHFXMRF-UHFFFAOYSA-N
Formula:	C11H16ClO4PS3
SMILES:	CCOP(=S)(OCC)SCS(=O)(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	374.86
CAS:	16662-85-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.33		Crippen Method
logp	4.102		Crippen Method
mcvol	247.320	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C16662854&Units=SI

Legend

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