Methyl trithion

Other names: Phosphorodithioic acid, S-[[(4-chlorophenyl)thio]methyl] O,O-dimethyl ester
Phosphorodithioic acid, S-[[(p-chlorophenyl)thio]methyl] O,O-dimethyl ester
Methyl carbophenothion
Carbophenothion methyl
S-[[(p-Chlorophenyl)thio]methyl] O,O-dimethyl phosphorodithioate
Stauffer R 1492
Dimethyl (((p-chlorophenyl)thio)methyl) dithiophosphate
ENT 25,599
Geigy g-29288
Methanethiol, ((p-chlorophenyl)thio)-, S-ester with O,O-dimethyl phosphorodithioate
O,O-Dimethyl-S-(((p-chlorophenyl)thio)methyl)phosphorodithioate
O,O-Dimethylthiophosphoric acid p-chlorophenyl ester
R-1492
Tri-Me
S-(((4-Chlorophenyl)thio)methyl) O,O-dimethylphosphorodithioate
ENT 25586
G-29288
NSC 231692
Trithion-methyl

Inchi: InChI=1S/C9H12ClO2PS3/c1-11-13(14,12-2)16-7-15-9-5-3-8(10)4-6-9/h3-6H,7H2,1-2H3
InchiKey: OUCCVXVYGFBXSV-UHFFFAOYSA-N
Formula: C9H12ClO2PS3
SMILES: COP(=S)(OC)SCSc1ccc(Cl)cc1
Mol. weight [g/mol]: 314.81
CAS: 953-17-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.54		Crippen Method
logp	4.640		Crippen Method
mcvol	207.400	ml/mol	McGowan Method
rinpol	2187.00		NIST Webbook
rinpol	2247.00		NIST Webbook
ripol	3045.00		NIST Webbook
ripol	3045.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C953173&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
ripol:	Polar retention indices