Phosphoric acid, dimethyl 3-methyl-4-(methylthio)phenyl ester

Other names: Fenthion O-analog
Bayoxon
m-Cresol, 4-(methylthio)-, dimethyl phosphate
Fenoxon
Fenthion oxon
Phosphoric acid, dimethyl 4-(methylthio)-m-tolyl ester
BAY 35570
Bayer 35570
Dimethyl 3-methyl-4-(methylthio)phenyl phosphate
Dimethyl 4-(methylthio)-m-tolyl phosphate
ENT 25564
Fenthoxon

Inchi: InChI=1S/C10H15O4PS/c1-8-7-9(5-6-10(8)16-4)14-15(11,12-2)13-3/h5-7H,1-4H3

InchiKey: ZNRZGJAHNMGWQN-UHFFFAOYSA-N

Formula: C10H15O4PS

SMILES: COP(=O)(OC)Oc1ccc(SC)c(C)c1

Mol. weight [g/mol]: 262.26

CAS: 6552-12-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	3.497		Crippen Method
mcvol	188.290	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=C6552121&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