Phosphorothioic acid, O,O-dimethyl O-[3-methyl-4-(methylsulfonyl)phenyl] ester

Other names: m-Cresol, 4-(methylsulfonyl)-, O-ester with O,O-dimethyl phosphorothioate
Fenthion sulfone
Phosphorothioic acid, O,O-dimethyl O-[4-(methylsulfonyl)-m-tolyl] ester
O,O-Dimethyl O-(4-(methylsulfonyl)-m-tolyl) phosphorothioate
O,O-Dimethyl O-((4-methylthio)-m-tolyl)phosphorothioate sulfone
Fenthione sulfone

Inchi: InChI=1S/C10H15O5PS2/c1-8-7-9(15-16(17,13-2)14-3)5-6-10(8)18(4,11)12/h5-7H,1-4H3

InchiKey: ZDHYERRNXRANLI-UHFFFAOYSA-N

Formula: C10H15O5PS2

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

Mol. weight [g/mol]: 310.33

CAS: 3761-42-0

Physical Properties

Property code	Value	Unit	Source
log10ws	1.39		Crippen Method
logp	2.295		Crippen Method
mcvol	210.510	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=C3761420&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume