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

Other names: Phosphoric acid, dimethyl 3-methyl-4-(methylsulfonyl)phenyl ester
Phosphoric acid, dimethyl 4-(methylsulfonyl)-m-tolyl ester
Fenoxon sulfone
Dimethyl 4-(methylsulfonyl)-m-tolyl phosphate
Fenthion oxon sulfone

Inchi: InChI=1S/C10H15O6PS/c1-8-7-9(16-17(11,14-2)15-3)5-6-10(8)18(4,12)13/h5-7H,1-4H3

InchiKey: VUTHWSUXEOILTN-UHFFFAOYSA-N

Formula: C10H15O6PS

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

Mol. weight [g/mol]: 294.26

Physical Properties

Property code	Value	Unit	Source
logp	2.178		Crippen Method
mcvol	200.030	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14086352&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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