

Phosphoramidic acid, (1-methylethyl)-, ethyl 3-methyl-4-(methylsulfonyl)phenyl ester

Other names: Phosphoramidic acid, isopropyl-, ethyl 4-(methylsulfonyl)-m-tolyl ester

Bay 68138 sulfone

Fenamiphos sulfone

Ethyl 3-methyl-4-(methylsulfonyl)phenyl isopropylamidophosphate

Fenamiphos sulphone

Inchi: InChI=1S/C13H22NO5PS/c1-6-18-20(15,14-10(2)3)19-12-7-8-13(11(4)9-12)21(5,16)17/h

InchiKey: LVNYJXIBJFXIRZ-UHFFFAOYSA-N

Formula: C13H22NO5PS

SMILES: CCOP(=O)(NC(C)C)Oc1ccc(S(C)(=O)=O)c(C)c1

Mol. weight [g/mol]: 335.36

CAS: 31972-44-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.09		Crippen Method
logp	2.920		Crippen Method
mcvol	246.410	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=C31972448&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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