

Phosphoric acid, diethyl p-(methylsulfonyl)phenyl ester

Other names:

O,O-Diethyl O-(p-methylsulfonyl)phenyl phosphate
Phosphoric acid, diethyl 4-(methylsulfonyl)phenyl ester
Fensulfotion oxon sulfone
Diethyl 4-(methylsulfonyl)phenyl phosphate
Dasanit O-analog sulfone

Inchi:

InChI=1S/C11H17O6PS/c1-4-15-18(12,16-5-2)17-10-6-8-11(9-7-10)19(3,13)14/h6-9H,4-

InchiKey:

KUBUBYBFFRVFHD-UHFFFAOYSA-N

Formula:

C11H17O6PS

SMILES:

CCOP(=O)(OCC)Oc1ccc(S(C)(=O)=O)cc1

Mol. weight [g/mol]:

308.29

CAS:

6132-17-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	2.650		Crippen Method
mcvol	214.120	ml/mol	McGowan Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6132178&Units=SI>

Crippen Method:

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

Crippen Method:

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

mcvol:

McGowan's characteristic volume

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