

Phosphorothioic acid, O,O-diethyl O-(p-methylsulfonyl)phenyl ester

Other names:

Dasanit sulfone

Dasanit sulphone

O,O-Diethyl O-(p-methylsulfonyl)phenyl phosphorothioate

Fensulfothion sulfone

Phosphorothioic acid, O,O-diethyl O-(4-(methylsulfonyl)phenyl) ester

Inchi:

InChI=1S/C11H17O5PS2/c1-4-14-17(18,15-5-2)16-10-6-8-11(9-7-10)19(3,12)13/h6-9H,4

InchiKey:

VTFZEBCYVXMEBB-UHFFFAOYSA-N

Formula:

C11H17O5PS2

SMILES:

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

Mol. weight [g/mol]:

324.35

CAS:

14255-72-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.03		Crippen Method
logp	2.766		Crippen Method
mcvol	224.600	ml/mol	McGowan Method

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C14255722&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

mcvol:

McGowan's characteristic volume

Latest version available from:

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