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