Diethyl phenylthiomethylphosphonate

Other names:	Phosphonic acid, [(phenylthio)methyl]-, diethyl ester
	Diethyl methylthiobenzyl phosphonate
Inchi:	InChI=1S/C11H17O3PS/c1-3-13-15(12,14-4-2)10-16-11-8-6-5-7-9-11/h5-9H,3-4,10H2,1-
InchiKey:	FBUXEPJJFVDUFE-UHFFFAOYSA-N
Formula:	C11H17O3PS
SMILES:	CCOP(=O)(CSc1ccccc1)OCC
Mol. weight [g/mol]:	260.29
CAS:	38066-16-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	4.002		Crippen Method
mcvol	196.510	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C38066169&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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