

Phosphoramidothioic acid, O,O-diethyl ester

Other names:	O,O-Diethyl phosphoramidothioate O,O-diethyl thiophosphoramidate
Inchi:	InChI=1S/C4H12NO2PS/c1-3-6-8(5,9)7-4-2/h3-4H2,1-2H3,(H2,5,9)
InchiKey:	LAGRCNJEUAJJQC-UHFFFAOYSA-N
Formula:	C4H12NO2PS
SMILES:	CCOP(N)(=S)OCC
Mol. weight [g/mol]:	169.18
CAS:	17321-48-1

Physical Properties

Property code	Value	Unit	Source
log10ws	2.64		Crippen Method
logp	1.243		Crippen Method
mvol	125.750	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=C17321481&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
mvol:	McGowan's characteristic volume

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