

O,S-Diethyl methylphosphonothioate

Other names:	Phosphonothioic acid, methyl-, O,S-diethyl ester O,S-Diethyl methylthiophosphonate OSDMP LG 61 Methylphosphonothioic acid O,S-diethyl ester O-Ethyl S-ethyl methylphosphonothioate Phosphonothioic acid, methyl, diethyl ester Phosphonothioic acid, P-methyl-, O,S-diethyl ester O,S-Diethyl methylphosphonothiolate Methylthiophosphonic acid, O,S-diethyl ester
Inchi:	InChI=1S/C5H13O2PS/c1-4-7-8(3,6)9-5-2/h4-5H2,1-3H3
InchiKey:	AIMOGGQLCCAPQJ-UHFFFAOYSA-N
Formula:	C5H13O2PS
SMILES:	CCOP(C)(=O)SCC
Mol. weight [g/mol]:	168.19
CAS:	2511-10-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	2.599		Crippen Method
mcvol	129.860	ml/mol	McGowan Method
rinpol	1174.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1174.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2511106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices

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