

Diethyl methylphosphonothioate

Other names:	Phosphonothioic acid, methyl-, O,O-diethyl ester Diethyl methylphosphonothionate O,O-Diethyl methylphosphonothioate Diethyl phosphonothioate O,O'-Diethyl methylphosphonothioate Methylthiophosphonic acid, O,O-diethyl ester
Inchi:	InChI=1S/C5H13O2PS/c1-4-6-8(3,9)7-5-2/h4-5H2,1-3H3
InchiKey:	GEDUXIUTPVHAAV-UHFFFAOYSA-N
Formula:	C5H13O2PS
SMILES:	CCOP(C)(=S)OCC
Mol. weight [g/mol]:	168.19
CAS:	6996-81-2

Physical Properties

Property code	Value	Unit	Source
log10ws	2.65		Crippen Method
logp	1.999		Crippen Method
mcpvol	129.860	ml/mol	McGowan Method
rinpol	1028.00		NIST Webbook
rinpol	1028.00		NIST Webbook

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=C6996812&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
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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