

Phosphonothioic acid, methyl-, S-(2-(diethylamino)ethyl) O-ethyl ester

Other names:	S-2-Diethylaminoethyl-O-ethylester kyseliny methylthiofosfonove Edemo Edemo 3 O-Ethyl S-2-(diethylamino)ethyl methylphosphonothiolate S-[2-(Diethylamino)ethyl] O-ethyl methylphosphonothioate Methyl-phosphonothioic acid S-(2-diethylamino-ethyl) ester O-ethyl ester VM
Inchi:	InChI=1S/C9H22NO2PS/c1-5-10(6-2)8-9-14-13(4,11)12-7-3/h5-9H2,1-4H3
InchiKey:	BKWMHKJLXIRTAI-UHFFFAOYSA-N
Formula:	C9H22NO2PS
SMILES:	CCOP(C)(=O)SCCN(CC)CC
Mol. weight [g/mol]:	239.31
CAS:	21770-86-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	2.921		Crippen Method
mcvol	196.200	ml/mol	McGowan Method
rinpol	1594.50		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1594.50		NIST Webbook
rinpol	1594.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C21770865&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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