

O-Ethyl S-2-dimethylaminoethyl methylphosphonothiolate

Other names:	S-[2-(Dimethylamino)ethyl] O-ethyl methylphosphonothioate Methyl-phosphonothioic acid S-(2-dimethylamino-ethyl) ester O-ethyl ester Medemo
Inchi:	InChI=1S/C7H18NO2PS/c1-5-10-11(4,9)12-7-6-8(2)3/h5-7H2,1-4H3
InchiKey:	PKDYQTANBZBIRM-UHFFFAOYSA-N
Formula:	C7H18NO2PS
SMILES:	CCOP(C)(=O)SCCN(C)C
Mol. weight [g/mol]:	211.26
CAS:	20820-80-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	2.141		Crippen Method
mcvol	168.020	ml/mol	McGowan Method
rinpol	1442.00		NIST Webbook
rinpol	1442.50		NIST Webbook
rinpol	1442.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20820808&Units=SI
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

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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