

Prothoate

Other names:	Phosphorodithioic acid, O,O-diethyl S-[2-[(1-methylethyl)amino]-2-oxoethyl] ester Phosphorodithioic acid, O,O-diethyl ester, S-ester with N-isopropyl-2-mercaptoacetamide American Cyanamid 18,682 Fac 20 Fak-40 Fostion FAC O,O-Diethyl S-(N-Isopropylcarbamoylmethyl) phosphorodithioate O,O-Diethyldithiophosphorylacetic acid, N-monoisopropylamide Prothoat Trimethoate AC 18682 Acetamide, N-isopropyl-2-mercapto-, S-ester with O,O-diethyl phosphorodithioate American cyanamid 18682 O,O-Diethyl S-(N-isopropylcarbamoylmethyl) dithiophosphate O,O-Diethyl S-isopropylcarbamoylmethyl phosphorodithioate EI 18682 ENT 24,652 Isopropyl diethyldithiophosphorylacetamide L 343 N-Monoisopropylamide of O,O-diethyldithiophosphorylacetic acid Oleofac Protoat Telefos FAC (pesticide)
Inchi:	InChI=1S/C9H20NO3PS2/c1-5-12-14(15,13-6-2)16-7-9(11)10-8(3)4/h8H,5-7H2,1-4H3,(H
InchiKey:	QTXHFDHVLBDJIO-UHFFFAOYSA-N
Formula:	C9H20NO3PS2
SMILES:	CCOP(=S)(OCC)SCC(=O)NC(C)C
Mol. weight [g/mol]:	285.36
CAS:	2275-18-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.02		Crippen Method
logp	2.542		Crippen Method

mcvol	214.120	ml/mol	McGowan Method
rinpol	1873.00		NIST Webbook
rinpol	1881.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2275185&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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