Vamidothion

Other names: American cyanamid-43073
Dimethyl S-[2-(1-methylcarbamoylethylthio)ethyl] phosphorothiolate
ENT 26,613
Kilval
N-Methyl O,O-dimethylthiolophosphoryl-5-thia-3-methyl-2-valeramide
N-Methyl-3-thia-2-methyl-valeramid der O,O-dimethylthiolphosphorsaeure
NPH 83
O,O-Dimethyl S-2-(1-N-methylcarbamoylethylmercapto)ethyl thiophosphate
O,O-Dimethyl S-[2-(1-methylcarbamoylethylthio)ethyl] phosphorothioate
Phosphorothioic acid, O,O-dimethyl S-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]thio]ethyl] ester
Phosphorothioic acid, O,O-dimethyl ester, S-ester with 2-[(2-mercaptoethyl)thio]-N-methylpropionamide
R.P. 10,465
RP 9895
Trucidor
Vamidoate

Inchi: InChI=1S/C8H18NO4PS2/c1-7(8(10)9-2)15-5-6-16-14(11,12-3)13-4/h7H,5-6H2,1-4H3,(H
InchiKey: LESVOLZBIFDZGS-UHFFFAOYSA-N
Formula: C8H18NO4PS2
SMILES: CNC(=O)C(C)SCCSP(=O)(OC)OC
Mol. weight [g/mol]: 287.34
CAS: 2275-23-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.14		Aqueous Solubility Prediction Method
log10ws	1.14		Estimated Solubility Method
logp	1.988		Crippen Method
mcvol	205.900	ml/mol	McGowan Method
rinpol	2075.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2080.00		NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2275232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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