Formothion

Other names:	Acetamide, N-formyl-2-mercapto-N-methyl-, S-ester with O,O-dimethyl phosphorodithioate
	Affix
	Anthio
	Anthio 25
	Antio
	CP 53926
	ENT 27,257
	J-38
	N-Formyl-N-methylcarbamoylmethyl O,O-dimethyl phosphorodithioate
	O,O-Dimethyl Dithiophosphorylacetic acid N-methyl-N-formylamide
	O,O-Dimethyl S-(N-formyl-N-methylcarbamoylmethyl) phosphorodithioate
	O,O-Dimethyl S-(N-methyl-N-formylcarbamoylmethyl)phosphorodithioate
	O,O-Dimethyl phosphorodithioate N-formyl-2-mercapto-N-methylacetamide S-ester
	O,O-Dimethyl-S-(3-methyl-2,4-dioxo-3-azabutyl)dithiofosfaat
	O,O-Dimethyl-S-(3-methyl-2,4-dioxo-3-azabutyl)dithiophosphat
	O,O-Dimethyl-S-(N-methyl-N-formylcarbamoylmethyl)dithiophosphat
	O,O-Dimetil-S-(N-formil-N-metilcarbamoilmetil)ditiofosfato
	OMS-968
	Phosphorodithioic acid, O,O-dimethyl ester, N-formyl-2-mercapto-N-methylacetamide S-ester
	Phosphorodithioic acid, O,O-dimethyl ester, S-ester with N-formyl-2-mercapto-N-methylacetamide
	Phosphorodithioic acid, S-[2-(formylmethylamino)-2-oxoethyl] O,O-dimethyl ester
	Phosphorodithioic acid, o,o-dimethyl ester, s-ester with n-formyl-n-methylglycolamide
	S 6900
	S-(2-(Formylmethylamino)-2-oxoethyl) O,O-dimethylphosphorodithioate
	S-(N-Formyl-N-methylcarbamoylmethyl) O,O-dimethyl phosphorodithioate
	S-(N-Formyl-N-methylcarbamoylmethyl) dimethyl phosphorothiolothionate
	SAN 244 I
	SAN 6913 I
	SAN 7107 I
	Sandoz S-6900
	Spencer S-6900
	Toprose
	VEL 4284
Inchi:	InChI=1S/C6H12NO4PS2/c1-7(5-8)6(9)4-14-12(13,10-2)11-3/h5H,4H2,1-3H3
InchiKey:	AIKKULXCBHRFOS-UHFFFAOYSA-N
Formula:	C6H12NO4PS2
SMILES:	COP(=S)(OC)SCC(=O)N(C)C=O
Mol. weight [g/mol]:	257.27
CAS:	2540-82-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Aqueous Solubility Prediction Method
log10ws	-2.00		Estimated Solubility Method
logp	0.852		Crippen Method
mcvol	173.420	ml/mol	McGowan Method
rinpol	1795.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1795.00		NIST Webbook
tf	298.65	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2540821&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point