

Omethoate

Other names:	Phosphorothioic acid, O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] ester Phosphorothioic acid, O,O-dimethyl ester, S-ester with 2-mercapto-N-methylacetamide Bayer 45432 BAY 45432 Dimethoate Oxygen analog Dimethoate O-analog Dimethoate PO isologue Dimethoxon Folimat Folimat 4E O,O-Dimethyl S-[(methylcarbamoyl)methyl] phosphorothioate PO-Dimethoate Acetamide, 2-mercapto-N-methyl-, S-ester with O,O-dimethyl phosphorothioate BAYER 45,432 O,O-Dimethyl S-(2-(methylamino)-2-oxoethyl)phosphorothioate O,O-Dimethyl-S-((N-methyl-carbamoyl)-methyl)-monothiofosfaat O,O-Dimethyl-S-(N-methyl-carbamoyl)-methyl-monothiophosphate O,O-Dimethyl-S-(N-methylcarbamoylmethyl)phosphorothioate O,O-Dimethyl S-(N-methylcarbamoylmethyl) phosphorothiolate Dimethyl-S-(N-methyl-carbamoyl-methyl)phosphorothiolate O,O-Dimethyl-S-(N-methyl-carbamoyl-methyl)-thiolphosphate O,O-Dimethyl S-(N-methylcarbamoylmethyl) thiophosphate O,O-Dimethyl-S-(2-oxo-3-azabutyl)-monothiophosphate O,O-Dimetil-S-(N-metil-carbamoil)-metil-monotiofosfato ENT 25,776 O-Analog of dimethoate Omethoat P=O-Rogor S6876 Thiophosphate de O,O-dimethyle et de S-(N-methylcarbamoyl) methyle Dimethoate oxon Dimethoate-met
Inchi:	InChI=1S/C5H12NO4PS/c1-6-5(7)4-12-11(8,9-2)10-3/h4H2,1-3H3,(H,6,7)
InchiKey:	PZXOQEXFMJCDPG-UHFFFAOYSA-N
Formula:	C5H12NO4PS
SMILES:	CN=C(O)CSP(=O)(OC)OC
Mol. weight [g/mol]:	213.19
CAS:	1113-02-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	1.707		Crippen Method
mcvol	147.280	ml/mol	McGowan Method
rinpol	1596.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1640.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C1113026&Units=SI

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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