

Mecarbam

Other names:	7-Oxa-5-thia-2-aza-6-phosphanonanoic acid, 6-ethoxy-2-methyl-3-oxo-, ethyl ester, 6-sulfide Afos Carbamic acid, (mercaptoacetyl)methyl-, ethyl ester, O,O-diethyl phosphorodithioate Carbamic acid, (mercaptoacetyl)methyl-, ethyl ester, S-ester with O,O-diethyl phosphorodithioate Carbamic acid, (mercaptoacetyl)methyl-, ethyl ester, S-ester with O,O-diethyl phosphorodithioic acid Chiofox Dithiophosphate de O,O-diethyle et de S-N-methyl N-carboethoxy carbamoylmethyle MC 474 MS 1053 MS 1143 Marfotoks Mecarbame Mercarbam Muratox Murfotox Murphotox Murutox N-Ethoxycarbonyl-N-methylcarbamoylmethyl O,O-diethyl phosphorodithioate O,O-Diaethyl-S-(3-methyl-2,4-dioxo-5-oxa-3-aza-heptyl)-dithiophosphat O,O-Diethyl S-(N-ethoxycarbonyl-N-methylcarbamoylmethyl) phosphorodithioate O,O-Diethyl S-(N-ethoxycarbonyl-N-methylcarbamoylmethyl) phosphorothiothionate O,O-Diethyl S-(N-methyl-N-carboethoxycarbamoylmethyl) dithiophosphate O,O-Diethyl-S-(3-methyl-2,4-dioxo-5-oxa-3-aza-heptyl)-dithiofosfaat O,O-Dietil-S-(N-etossi-carbonil-N-metil-carbamoil-metil)-dithiofosfato P 474 Pennsalt TD 72 Pestan Phosphorodithioic acid, O,O-diethyl ester, S-ester with ethyl (mercaptoacetyl)methylcarbamate S-((Ethoxycarbonyl)methylcarbamoyl)methyl O,O-diethyl phosphorodithioate S-(N-Ethoxycarbonyl-N-methylcarbamoylmethyl) O,O-diethyl phosphorodithioate S-(N-Ethoxycarbonyl-N-methylcarbamoylmethyl)-diethyl phosphorodithioate TD 72
Inchi:	InChI=1S/C10H20NO5PS2/c1-5-14-10(13)11(4)9(12)8-19-17(18,15-6-2)16-7-3/h5-8H2,1
InchiKey:	KLGMSAOQDHLCS-UHFFFAOYSA-N
Formula:	C10H20NO5PS2
SMILES:	CCOC(=O)N(C)C(=O)CSP(=S)(OCC)OCC
Mol. weight [g/mol]:	329.37
CAS:	2595-54-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Aqueous Solubility Prediction Method
log10ws	-2.52		Estimated Solubility Method
logp	2.632		Crippen Method
mcvol	235.650	ml/mol	McGowan Method
rinpol	2052.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2052.00		NIST Webbook
rinpol	2044.00		NIST Webbook
rinpol	2044.00		NIST Webbook
rinpol	2010.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

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=C2595542&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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