

Demeton-S-methyl

Other names:	Phosphorothioic acid, S-[2-(ethylthio)ethyl] O,O-dimethyl ester Demeton-S-methyl sulfide meta-Isosystox Metaisoseptox Metasystox I Metasystox J Metasystox 55 Methyl demeton thioester Methyl isosystox Methylthionodemeton O,O-Dimethyl S-2-(ethylthio)ethyl phosphorothioate S-[2-(Ethylthio)ethyl] O,O-dimethyl phosphorothioate S-[2-(Ethylthio)ethyl] O,O-dimethyl thiophosphate Demetone-S-methyl S-[2-(Ethylthio)ethyl] O,O-dimethyl phosphorothioate BAY 18436 Bayer 25/154 Demeton-S-metile O,O-Dimethyl-S-(2-aethylthio-aethyl)-monothiophosphat O,O-Dimethyl S-(2-eththioethyl)phosphorothioate Dimethyl S-(2-eththioethyl)thiophosphate O,O-Dimethyl S-ethylmercaptoethyl thiophosphate O,O-Dimethyl 2-ethylmercaptoethyl thiophosphate, thiolo isomer O,O-Dimethyl-S-(2-ethylthio-ethyl)-monothiofosfaat O,O-Dimethyl-S-(3-thia-pentyl)-monothiophosphat O,O-Dimetil-S-(2-etiltio-etil)-monotiofosfato Duratox Ethanethiol, 2-(ethylthio)-, S-ester with O,O-dimethyl phosphorothioate S-(2-(Ethylthio)ethyl) dimethyl phosphorothiolate Methyl-mercaptofos teolery Phosphorothioic acid, O,O-dimethyl S-(2-(ethylthio)ethyl) ester Thiophosphate de O,O-dimethyle et de S-2-ethylthio-ethyle Demetox Methylmercaptofostiol Mifatox Persyst Power DSM Thiometon oxon
Inchi:	InChI=1S/C6H15O3PS2/c1-4-11-5-6-12-10(7,8-2)9-3/h4-6H2,1-3H3
InchiKey:	WEBQKRLKWNIIYKK-UHFFFAOYSA-N

Formula: C6H15O3PS2
SMILES: CCSCCSP(=O)(OC)OC
Mol. weight [g/mol]: 230.28
CAS: 919-86-8

Physical Properties

Property code	Value	Unit	Source
hvap	78.80	kJ/mol	NIST Webbook
log10ws	-3.54		Crippen Method
logp	2.874		Crippen Method
mcvol	166.170	ml/mol	McGowan Method
rinpol	1628.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C919868&Units=SI>

Legend

hvap: Enthalpy of vaporization at standard conditions
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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