Demeton-O-methyl

Other names:	Phosphorothioic acid, O-[2-(ethylthio)ethyl] O,O-dimethyl ester
	Methyl-O-demeton
	O-[2-(Ethylthio)ethyl] O,O-dimethyl phosphorothioate
	O-[2-(Ethylthio)ethyl] O,O-dimethyl thiophosphate
	O,O-Dimethyl O-[2-(ethylthio)ethyl] phosphorothioate
	O,O-Dimethyl O-[2-(ethylthio)ethyl] thiophosphate
	Demeton-O-metile
	O,O-Dimethyl-O-(2-aethylthio-aethyl)monothiophosphat
	O,O-Dimethyl 2-ethylmercaptoethyl thiophosphate, thiono isomer
	O,O-Dimethyl-O-(2-ethyl-thio-ethyl)-monothiofosfaat
	O,O-Dimethyl O-ethylmercaptoethyl thiophosphate
	O,O-Dimetil-O-(2-etiltio-etil)-monotiofosfato
	ENT 18,862
	Ethanol, 2-(ethylthio)-, O-ester with O,O-dimethyl phosphorothioate
	«beta»-Ethylmercaptoethyl dimethyl thionophosphate
	2-(Ethylthio)ethyl dimethyl phosphorothionate
	Methyl-demeton-O
	O-Methyldemeton
	Thiophosphate de O,O-dimethyle et de O-2-ethylthio-ethyle
	Metasystox thiono
Inchi:	InChI=1S/C6H15O3PS2/c1-4-12-6-5-9-10(11,7-2)8-3/h4-6H2,1-3H3
InchiKey:	ZVZQKNVMDKSGGF-UHFFFAOYSA-N
Formula:	C6H15O3PS2
SMILES:	CCSCCOP(=S)(OC)OC
Mol. weight [g/mol]:	230.28
CAS:	867-27-6

Physical Properties

Property code	Value	Unit	Source
hvap	71.00	kJ/mol	NIST Webbook
log10ws	2.27		Crippen Method
logp	2.273		Crippen Method
mcvol	166.170	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C867276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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