Demeton-S-methyl sulfone

Other names:	Phosphorothioic acid, S-[2-(ethylsulfonyl)ethyl] O,O-dimethyl ester Metasystox i sulfone Metasystox R sulfone O,O-Dimethyl S-[2-(ethylsulfonyl)ethyl] monothiophosphate O,O-Dimethyl S-[2-(ethylsulfonyl)ethyl] thiophosphate O,O-Dimethyl S-2-(ethylsulfonyl)ethyl phosphorothioate Oxydemetonmethyl sulfone S-[2-(Ethylsulfonyl)ethyl] O,O-dimethyl phosphorothioate Phosphorothioic acid, O,O-dimethyl S-(2-(ethylsulfonyl)ethyl) ester BAYER 20315 Demeton-S-methylsulfon Demeton-S-methyl-sulphone O,O-Dimethyl-S-(2-aethylsulfonyl-aethyl)-thiolphosphat O,O-Dimethyl S-(2-ethsulfonylethyl)phosphorothioate Dimethyl S-(2-ethsulfonylethyl)thiophosphate O,O-Dimethyl S-ethyl-2-sulfonylethyl phosphorothiolate O,O-Dimethyl S-ethylsulphonylethyl phosphorothiolate Dioxydemeton-S-methyl E 158 Isometasystox sulfone Isomethylsystox sulfone M 3/158 Metaisosystox-solfon 20 315 Sulfone, demeton-S-methyl- Demethon S-methyl sulfone demeton-S-methylsulphon
Inchi:	InChI=1S/C6H15O5PS2/c1-4-14(8,9)6-5-13-12(7,10-2)11-3/h4-6H2,1-3H3
InchiKey:	PZIRJMYRYORVIT-UHFFFAOYSA-N
Formula:	C6H15O5PS2
SMILES:	CCS(=O)(=O)CCSP(=O)(OC)OC
Mol. weight [g/mol]:	262.28
CAS:	17040-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method

logp	1.555		Crippen Method
mcvol	177.910	ml/mol	McGowan Method
rinpol	1850.00		NIST Webbook
rinpol	1871.00		NIST Webbook
rinpol	1889.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17040196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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