Demeton-S

Other names:	1-(2-diethoxyphosphorylsulfanylethylsulfanyl)ethane
	Demeton thiolo
	Demetonthiol
	Diethyl S-(2-ethioethyl)thiophosphate
	Disulfoton O-analog
	Disulfoton oxon
	Ethylthionodemeton
	IS
	IS (pesticide)
	Isodemeton
	Isosystox
	Izosystox
	O,O-Diaethyl-S(2-aethylthio-aethyl)-monothiophosphat
	O,O-Diethyl S-(2-(ethylthio)ethyl) phosphorothiolate
	O,O-Diethyl S-(2-eththioethyl)phosphorothioate
	O,O-Diethyl S-[2-(Ethylthio)ethyl] phosphorothioate
	O,O-Diethyl S-[2-(ethylthio)ethyl] thiophosphate
	O,O-Diethyl S-ethyl-2-ethylmercaptophosphorothiolate
	O,O-Diethyl-S-(2-ethylthio-ethyl)-monothiofosfaat
	O,O-Dietil-S-(2-etiltio-etil)-monotiofosfato
	O,O-Dietyl-S-2-etylmerkaptoetyltiofosfat
	Phosphorothioic acid, O,O-diethyl S-[2-(ethylthio)ethyl] ester
	Po-systox
	Systox-thiol
	Thiol systox
	Thioldemeton
	Thiophosphate de O,O-diethyle et de S-(2-ethylthio-ethyle)
Inchi:	InChI=1S/C8H19O3PS2/c1-4-10-12(9,11-5-2)14-8-7-13-6-3/h4-8H2,1-3H3
InchiKey:	GRPRVIYRYGLIJU-UHFFFAOYSA-N
Formula:	C8H19O3PS2
SMILES:	CCOP(=O)(OCC)SCCSCC
Mol. weight [g/mol]:	258.34
CAS:	126-75-0

Physical Properties

Property code	Value	Unit	Source

hvap	76.40	kJ/mol	NIST Webbook
log10ws	-2.11		Aqueous Solubility Prediction Method
logp	3.654		Crippen Method
mcvol	194.350	ml/mol	McGowan Method
rinpol	1738.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.10887e+01
Coeff. B	-9.18962e+03
Temperature range (K), min.	441.79
Temperature range (K), max.	582.46

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126750&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

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