Thiometon

Other names:	2-Ethylthioethyl O,O-dimethyl phosphorodithioate
	BAY 23129
	BAYER 23129
	Compound M-81
	Dithiometasystox
	Dithiomethon
	Dithiometon
	Dithiophosphate de O,O-dimethyle et de S-(2-ethylthio-ethyle)
	Ekatin
	Ekatin ULV
	Ekatin aerosol
	Ekatine-25
	Ethanethiol, 2-(ethylthio)-, S-ester with O,O-dimethyl phosphorodithioate
	Intrathion
	Intration
	Luxistelm
	M 81
	O,O-Dimethyl S-(2-(ethylthio)ethyl) phosphorodithioate
	O,O-Dimethyl S-(2-Ethylthioethyl) dithiophosphate
	O,O-Dimethyl-S-(2-aethylthio-aethyl)-dithio phosphat
	O,O-Dimethyl-S-(2-ethylmercaptoethyl) dithiophosphate
	O,O-Dimethyl-S-(2-ethylthio-ethyl)-dithiofosfaat
	O,O-Dimethyl-S-2-ethylmerkaptoethylester kyseliny dithiofosforecne
	O,O-Dimetil-S-(etiltio-etil)-ditiofosfato
	Phosphorodithioic acid, O,O-dimethyl S-(2-ethylthio)ethyl ester
	Phosphorodithioic acid, S-[2-(ethylthio)ethyl] O,O-dimethyl ester
	S-(2-(Ethylthio)ethyl) O,O-dimethylphosphorodithionate
	S-(2-(Ethylthio)ethyl)dimethyl phosphorothiolothionate
	S-[2-(Ethylthio)ethyl] O,O-dimethyl phosphorodithioate
	SAN 230
	Thiameton
	Veltin
Inchi:	InChI=1S/C6H15O2PS3/c1-4-11-5-6-12-9(10,7-2)8-3/h4-6H2,1-3H3
InchiKey:	OPASCBHCTNRLRM-UHFFFAOYSA-N
Formula:	C6H15O2PS3
SMILES:	CCSCCSP(=S)(OC)OC
Mol. weight [g/mol]:	246.35
CAS:	640-15-3

Physical Properties

Property code	Value	Unit	Source
hvap	76.80	kJ/mol	NIST Webbook
log10ws	-3.09		Estimated Solubility Method
log10ws	-3.09		Aqueous Solubility Prediction Method
logp	2.990		Crippen Method
mcvol	176.650	ml/mol	McGowan Method
rinpol	1695.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1724.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.86172e+01
Coeff. B	-9.16613e+03
Coeff. C	-1.21000e+00
Temperature range (K), min.	324.76
Temperature range (K), max.	394.51

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C640153&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
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

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