Phorate

Other names:	AC 3911
	Agrimet
	American Cyanamid 3,911
	Dithiophosphate de O,O-diethyle et D'ethylthiomethyle
	EI3911
	ENT 24,042
	Experimental Insecticide 3911
	Foraat
	Forate
	Geomet
	Granutox
	L 11/6
	Methanethiol, (ethylthio)-, S-ester with O,O-diethyl phosphorodithioic acid
	O,O-Diaethyl-S-(aethylthio-methyl)-dithiophosphat
	O,O-Diethyl S-Ethylmercaptomethyl dithiophosphate
	O,O-Diethyl S-[(ethylthio)methyl] phosphorodithioate
	O,O-Diethyl S-ethylthiomethyl dithiophosphate
	O,O-Diethyl S-ethylthiomethyl dithiophosphonate
	O,O-Diethyl S-ethylthiomethyl thiothionophosphate
	O,O-Diethyl ethylthiomethyl phosphorodithioate
	O,O-Diethyl-S-(ethylthio-methyl)-dithiofosfaat
	O,O-Dietil-S-(etiltio-metil)-ditiofosfato
	Phorat
	Phorate 10G
	Phosphorodithioic acid, O,O-diethyl S-[(ethylthio)methyl] ester
	Rampart
	Rcra waste number P094
	Thimate
	Thimenox
	Thimet
	Thimet 10G
	Thimet G
	Timet
	VUAgT 182
	Vegfru
	Vegfru foratox
	Volphor
Inchi:	InChI=1S/C7H17O2PS3/c1-4-8-10(11,9-5-2)13-7-12-6-3/h4-7H2,1-3H3
InchiKey:	BULVZWIRKLYCBC-UHFFFAOYSA-N
Formula:	C7H17O2PS3

SMILES: CCOP(=S)(OCC)SCSCC
Mol. weight [g/mol]: 260.38
CAS: 298-02-2

Physical Properties

Property code	Value	Unit	Source
hvap	70.80	kJ/mol	NIST Webbook
log10ws	-4.11		Aqueous Solubility Prediction Method
log10ws	-4.11		Estimated Solubility Method
logp	3.728		Crippen Method
mcvol	190.740	ml/mol	McGowan Method
rinpol	1703.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1686.00		NIST Webbook
ripol	2335.00		NIST Webbook
ripol	2335.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.99169e+01
Coeff. B	-8.51266e+03
Temperature range (K), min.	433.67
Temperature range (K), max.	582.84

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C298022&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

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
ripol:	Polar retention indices