Chloropyriphos-methyl

Other names:	Chloropyrifos-methyl
	Chlorpyrifos M
	Chlorpyrifos methyl
	Chlorpyriphos-methyl
	Cooper graincote
	Dowco 214
	Dursban methyl
	ENT 27520
	M 3196
	Methyl chlorpyrifos
	Methyl chlorpyriphos
	Methyl dursban
	NSC 60380
	Noltran
	O,O-Dimethyl O-(3,5,6-trichloro-2-pyridyl)phosphorothioate
	O,O-Dimethyl O-(3,5,6-trichloropyridin-2-yl) thiophosphate
	O,O-Dimethyl O-3,5,6-trichloropyridin-2-yl-phosphorothioate
	O,O-dimethyl-O-3,5,6-trichloro-2-pyridyl phosphorothioate (chlorpyrifos methyl)
	OMS-1155
	Phosphorothioic acid, O,O-dimethyl O-(3,5,6-trichloro-2-pyridinyl) ester
	Phosphorothioic acid, O,O-dimethyl O-(3,5,6-trichloro-2-pyridyl) ester
	Reldan
	Reldan 50 EC
	Reldan F
	Trichlormethylfos
	Zertell
	dimethoxy-sulfanylidene-(3,5,6-trichloropyridin-2-yl)oxyphosphorane
Inchi:	InChI=1S/C7H7Cl3NO3PS/c1-12-15(16,13-2)14-7-5(9)3-4(8)6(10)11-7/h3H,1-2H3
InchiKey:	HRBKVYFZANMGRE-UHFFFAOYSA-N
Formula:	C7H7Cl3NO3PS
SMILES:	COP(=S)(OC)Oc1nc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	322.53
CAS:	5598-13-0

Physical Properties

Property code	Value	Unit	Source

log10ws	-4.82		Aqueous Solubility Prediction Method
logp	3.938		Crippen Method
mcvol	186.850	ml/mol	McGowan Method
rinpol	1860.00		NIST Webbook
rinpol	1829.00		NIST Webbook
rinpol	1866.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1902.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	1824.00		NIST Webbook
rinpol	1885.00		NIST Webbook
ripol	2693.00		NIST Webbook
tf	319.16 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	25.92	kJ/mol	318.70	NIST Webbook
hfust	25.92	kJ/mol	318.70	NIST Webbook
hvapt	73.00	kJ/mol	388.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5598130&Units=SI

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

hfust:	Enthalpy of fusion at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point