Phosphoric acid, diethyl 3,5,6-trichloro-2-pyridyl ester

Other names: Diethyl 3,5,6-trichloro-2-pyridyl phosphate
Dursban oxygen analog
Dursban O-analog
Dursbanoxon
Phospyrat ethyl
3,5,6-Trichloro-2-pyridyl diethyl phosphate
Chloropyrifos oxon
Chlorpyrifos oxon
Chloropyrifos oxygen analog
Fospirate-ethyl
Phosphoric acid, diethyl 3,5,6-trichloro-2-pyridinyl ester
O,O-Diethyl O-3,5,6-trichloro-2-pyridyl phosphate
3,5,6-Trichloro-2-pyridyl diethylphosphate (chlorpyrifos oxon)

Inchi: InChI=1S/C9H11Cl3NO4P/c1-3-15-18(14,16-4-2)17-9-7(11)5-6(10)8(12)13-9/h5H,3-4H2

InchiKey: OTMOUPHCTWPNSL-UHFFFAOYSA-N

Formula: C9H11Cl3NO4P

SMILES: CCOP(=O)(OCC)Oc1nc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 334.52

CAS: 5598-15-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	4.602		Crippen Method
mcvol	204.550	ml/mol	McGowan Method
rinpol	1966.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	1971.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	1982.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1971.00		NIST Webbook

rinpol	1950.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1956.00		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1956.00		NIST Webbook
rinpol	1982.00		NIST Webbook
ripol	2717.00		NIST Webbook
tf	314.29 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	15.61	kJ/mol	312.50	NIST Webbook
hsubt	79.00	kJ/mol	388.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5598152&Units=SI

Legend

hfust: Enthalpy of fusion at a given temperature
hsubt: Enthalpy of sublimation 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

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