Chlorpyrifos

Other names:

2-Pyridinol, 3,5,6-trichloro-, O-ester with O,O-diethyl phosphorothioate
Bonidel
Brodan
Chloropyrifos
Chloropyriphos
Chlorpyrifos-ethyl
Chlorpyriphos
Chlorpyriphos-ethyl
Chlorpyrofos
Chlorpyrophos
Coroban
Danusban
Detmol U.A.
Dowco 179
Durmet
Dursban
Dursban 10CR
Dursban 2E
Dursban 4E
Dursban F
Dursban R
ENT 27,311
ENT 27311
Empire 20
Equity
Ethyl chlorpyriphos
Geodinfos
Killmaster
Lentrek
Lock-On
Lorsban
O,O-Diaethyl-O-3,5,6-trichlor-2-pyridylmonothiophosphat
O,O-Diethyl O-(3,5,6-Trichloro-2-pyridyl) phosphorothioate
O,O-Diethyl O-(3,5,6-trichloro-2-pyridinyl)phosphorothioate
O,O-Diethyl O-(3,5,6-trichloropyridin-2-yl) thiophosphate
OMS 971
OMS-0971
Pageant
Phosphorothioic acid, O,O-diethyl O-(3,5,6-trichloro-2-pyridinyl) ester
Phosphorothioic acid, O,O-diethyl O-(3,5,6-trichloro-2-pyridyl) ester

	Piridane
	Pyrinex
	Radar
	Silrifos
	Spannit
	Stipend
	Suscon blue
	Suscon green
	Tafaban
	Terial
	Trichlorpyrphos
	XRM 429
	XRM 5160
	Zidil
	diethoxy-sulfanylidene-(3,5,6-trichloropyridin-2-yl)oxyphosphorane
	m-Chlorpyrifos
	o,o-Diethyl-o-(3,5,6-trichloro-2-pyridyl)phosphorothioate
	suSCon
Inchi:	InChI=1S/C9H11Cl3NO3PS/c1-3-14-17(18,15-4-2)16-9-7(11)5-6(10)8(12)13-9/h5H,3-4H
InchiKey:	SBPBAQFWLVIOKP-UHFFFAOYSA-N
Formula:	C9H11Cl3NO3PS
SMILES:	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	350.59
CAS:	2921-88-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.24		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-5.67		Estimated Solubility Method
log10ws	-5.51		Aqueous Solubility Prediction Method
logp	4.718		Crippen Method
mcvol	215.030	ml/mol	McGowan Method
rinpol	1955.00		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1976.00		NIST Webbook

rinpol	1955.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1967.00		NIST Webbook
rinpol	1971.00		NIST Webbook
rinpol	1982.00		NIST Webbook
tf	316.40 ± 0.10	K	NIST Webbook
tf	315.25 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	24.53	kJ/mol	315.00	NIST Webbook
sfust	81.99	J/mol×K	315.00	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2921882&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

Legend

hfust: Enthalpy of fusion 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
sfust: Entropy of fusion at a given temperature
tf: Normal melting (fusion) point

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