Ronnel

Other names:

Blitex
Dermafos
Dermafosu
Dermaphos
Dimethyl (2,4,5-trichlorophenyl) phosphorothionate
Dimethyl O-(2,4,5-trichlorophenyl) thiophosphate
Dimethyl trichlorophenyl thiophosphate
Dow ET 14
Dow ET 57
ENT 23,284
ET 14
ET 57
Ectoral
Etrolene
Fenchloorfos
Fenchlorfos
Fenchlorfosu
Fenchlorophos
Fenchlorphos
Fenclofos
Gesektin K
Korlan
Korlane
Moorman's Medicated Rid-Ezy
Nanchor
Nanker
Nankor
O,O-Dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate
O,O-Dimethyl O-(2,4,5-trichlorophenyl) phosphorothionate
O,O-Dimethyl O-(2,4,5-trichlorophenyl) thiophosphate
O,O-Dimethyl-O-(2,4,5-trichlorphenyl)-thionophosphat
O-(2,4,5-Trichloor-fenyl)-O,O-dimethyl-monothiofosfaat
O-(2,4,5-Trichlor-phenyl)-O,O-dimethyl-monothiophosphat
O-(2,4,5-Tricloro-fenil)-O,O-dimetil-monotiofosfato
OMS 123
Phenchlorfos
Phenol, 2,4,5-trichloro-, O-ester with O,O-dimethyl phosphorothioate
Phosphorothioic acid, O,O-dimethyl O-(2,4,5-trichlorophenyl) ester
Remelt
Rovan

	Thiophosphate de O,O-dimethyle et de o-(2,4,5-trichlorophenyle)
	Trichlormetaphos
	Trichlorometafos
	Trichlorometaphos
	Trolen
	Trolene
	Trolene 20L
	Viozene
	dimethoxy-sulfanylidene-(2,4,5-trichlorophenoxy)phosphorane
Inchi:	InChI=1S/C8H8Cl3O3PS/c1-12-15(16,13-2)14-8-4-6(10)5(9)3-7(8)11/h3-4H,1-2H3
InchiKey:	JHJOOSLFWRRSGU-UHFFFAOYSA-N
Formula:	C8H8Cl3O3PS
SMILES:	COP(=S)(OC)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	321.55
CAS:	299-84-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-5.72		Estimated Solubility Method
log10ws	-5.72		Aqueous Solubility Prediction Method
logp	4.543		Crippen Method
mcvol	190.960	ml/mol	McGowan Method
rinpol	1880.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1931.00		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1908.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1908.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1936.00		NIST Webbook

tf	315.90 ± 0.10	K	NIST Webbook
tf	314.99 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	18.94	kJ/mol	313.00	NIST Webbook
hfust	18.94	kJ/mol	313.00	NIST Webbook
hvapt	56.80	kJ/mol	335.50	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=C299843&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
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
tf:	Normal melting (fusion) point