

Tetrachlorvinphos

Other names:	(Z)-2-Chloro-1-(2,4,5-trichlorophenyl)ethenyl dimethyl phosphate (Z)-2-Chloro-1-(2,4,5-trichlorophenyl)vinyl dimethyl phosphate (Z)-Tetrachlorvinphos Appex CVMP Debantic Dietreen Dust M ENT 25,841 Gardcide Gardona Gordona Phosphoric acid, (1Z)-2-chloro-1-(2,4,5-trichlorophenyl)ethenyl dimethyl ester Phosphoric acid, 2-chloro-1-(2,4,5-trichlorophenyl)ethenyl dimethyl ester, (Z)- Phosphoric acid, 2-chloro-1-(2,4,5-trichlorophenyl)vinyl dimethyl ester, (Z)- ROL Rabon Rabond SD 8447 Stirifos Stirofos Stirophos Stitifos Tetrachlorvinfos Tetrachlorvinphos, (Z) Vinfos cis-Gardona cis-Tetrachlorvinphos
Inchi:	InChI=1S/C10H9Cl4O4P/c1-16-19(15,17-2)18-10(5-11)6-3-8(13)9(14)4-7(6)12/h3-5H,1-2
InchiKey:	UBCKGWBNUIFUST-YHYXMXQVSA-N
Formula:	C10H9Cl4O4P
SMILES:	<chem>COP(=O)(OC)OC(=CCl)c1cc(Cl)c(Cl)cc1Cl</chem>
Mol. weight [g/mol]:	365.96
CAS:	22248-79-9

Physical Properties

Property code	Value	Unit	Source
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log10ws	-4.52		Aqueous Solubility Prediction Method
log10ws	-4.52		Estimated Solubility Method
logp	5.602		Crippen Method
mcvol	216.600	ml/mol	McGowan Method
tf	369.65 ± 0.20	K	NIST Webbook
tf	369.00 ± 0.20	K	NIST Webbook
tf	370.00 ± 0.20	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22248799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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