Cis-chlorfenvinphos

Other names:	Phosphoric acid, 2-chloro-1-(2,4-dichlorophenyl)ethenyl diethyl ester, (Z)- Phosphoric acid, 2-chloro-1-(2,4-dichlorophenyl)vinyl diethyl ester, (Z)- cis-Isomer of chlorfenvinphos Chlorfenvinphos (cis) «beta»-Chlorfenvinphos Chlorfenvinphos, «beta»- (Z)-2-Chloro-1-(2,4-dichlorophenyl)ethenyl diethyl phosphate (Z)-Chlorfenvinfos (Z)-Chlorfenvinphos Chlorfenvinphos (Z), «beta» Chlorfenvinphos Z
Inchi:	InChI=1S/C12H14Cl3O4P/c1-3-17-20(16,18-4-2)19-12(8-13)10-6-5-9(14)7-11(10)15/h5-8
InchiKey:	FSAVDKDHPDSCTO-WQLSENKSSA-N
Formula:	C12H14Cl3O4P
SMILES:	CCOP(=O)(OCC)O/C(=C\Cl)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	359.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Cheméo Relay (1.0)
logp	5.728		Crippen Method
mcvol	232.540	ml/mol	McGowan Method
rinpol	2069.00		NIST Webbook
rinpol	2071.00		NIST Webbook
tf	307.79	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18708877&Units=SI

Legend

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