

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:

FSAVDKDHPDSTO-WQLSENKSSA-N

Formula:

C12H14Cl3O4P

SMILES:

CCOP(=O)(OCC)OC(=CCl)c1ccc(Cl)cc1Cl

Mol. weight [g/mol]:

359.57

CAS:

18708-87-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.01		Crippen Method
logp	5.728		Crippen Method
mcvol	232.540	ml/mol	McGowan Method
rinpol	2069.00		NIST Webbook
rinpol	2071.00		NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C18708877&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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