Phosphorodiamidic acid, tetramethyl-, pentachlorophenyl ester

Other names:	Bis(N,N-dimethylamino) pentachlorophenyl phosphate
	Phenol, pentachloro-, tetramethylphosphorodiamidate
	TH 184F
	Pentachlorophenyl tetramethylphosphorodiamidate
	Phosphorodiamidic acid, N,N,N',N'-tetramethyl-, O-pentachlorophenyl ester
Inchi:	InChI=1S/C10H12Cl5N2O2P/c1-16(2)20(18,17(3)4)19-10-8(14)6(12)5(11)7(13)9(10)15/h
InchiKey:	RBBJXBKKZWSEHR-UHFFFAOYSA-N
Formula:	C10H12Cl5N2O2P
SMILES:	CN(C)P(=O)(Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)N(C)C
Mol. weight [g/mol]:	400.45
CAS:	1440-97-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.68		Crippen Method
logp	5.564		Crippen Method
mcvol	241.360	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1440977&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume