Cyclo-tris(diphenoxyphosphonitrile)

Other names:	2,2,4,4,6,6-hexahydro-2,2,4,4,6,6-hexaphenoxy-1,3,5,2,4,6-triazatriphosphorine
	2,2,4,4,6,6-hexaphenoxy-1,3,5,2.lambda.5,4.lambda.5,6.lambda.5-triazatriphosphinine
Inchi:	InChI=1S/C36H30N3O6P3/c1-7-19-31(20-8-1)40-46(41-32-21-9-2-10-22-32)37-47(42-33
InchiKey:	RNFJDJUURJAICM-UHFFFAOYSA-N
Formula:	C36H30N3O6P3
SMILES:	c1ccc(OP2(Oc3ccccc3)=NP(Oc3ccccc3)(Oc3ccccc3)=NP(Oc3ccccc3)(Oc3ccccc3)=N2)c
Mol. weight [g/mol]:	693.56
CAS:	1184-10-7

Physical Properties

Property code	Value	Unit	Source
hfus	51.07	kJ/mol	Solubilities of Phenylphosphinic Acid, Methylphenylphosphinic Acid, Hexachlorocyclotriphosphazene, and Hexaphenoxycyclotriphosphazene in Selected Solvents
ie	8.83 ± 0.05	eV	NIST Webbook
log10ws	-3.34		Crippen Method
logp	12.313		Crippen Method
mcvol	491.220	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1184107&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of Phenylphosphinic Acid, Methylphenylphosphinic Acid, Hexachlorocyclotriphosphazene, and Hexaphenoxycyclotriphosphazene in Selected Solvents:	https://www.doi.org/10.1021/je1009812
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume