1,3,5,2,4,6-Triazatriphosphorine, 2,2,4,4,6,6-hexabromo-2,2,4,4,6,6-hexahydro-

Other names:	Hexabromocyclotriphosphazene
	Phosphonitrile bromide, cyclic trimer
	Phosphononitrile bromide trimer
	Triphosphonitrilic bromide
	2,2,4,4,6,6-Hexabromocyclotriphosphazatriene
	1,3,5,2,4,6-Triazatriphosphorine, 2,2,4,4,6,6-hexabromo-
	2,2,4,4,6,6-hexabromo-2,2,4,4,6,6-hexahydro-1,2,3,4,5,6-triazatriphosphorine
Inchi:	InChI=1S/Br6N3P3/c1-10(2)7-11(3,4)9-12(5,6)8-10
InchiKey:	BISNZAMPUNENFV-UHFFFAOYSA-N
Formula:	Br6N3P3
SMILES:	BrP1(Br)=NP(Br)(Br)=NP(Br)(Br)=N1
Mol. weight [g/mol]:	614.37
CAS:	13701-85-4

Physical Properties

Property code	Value	Unit	Source
ie	9.62 ± 0.03	eV	NIST Webbook
ie	9.60 ± 0.10	eV	NIST Webbook
log10ws	2.17		Crippen Method
logp	8.208		Crippen Method
mcvol	196.320	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13701854&Units=SI
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

Legend

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