1,3,5,2,4,6-Triazatriphosphorine, 2-bromo-2,4,4,6,6-pentachloro-2,2,4,4,6,6-hexahyd

Other names:	2-Bromo-2,4,4,6,6-pentachloro-1,3,5,2,4,6-triazatriphosphorine
	Cyclo-bis(dichlorophosphonitrile)- bromochlorophosphonitrile
Inchi:	InChI=1S/BrCl5N3P3/c1-10(2)7-11(3,4)9-12(5,6)8-10
InchiKey:	PSSAXQUUJXHGBY-UHFFFAOYSA-N
Formula:	BrCl5N3P3
SMILES:	ClP1(Cl)=NP(Cl)(Cl)=NP(Cl)(Br)=N1
Mol. weight [g/mol]:	392.11
CAS:	14740-93-3

Physical Properties

Property code	Value	Unit	Source
ie	9.80 ± 0.10	eV	NIST Webbook
log10ws	3.56		Crippen Method
logp	7.427		Crippen Method
mcvol	170.020	ml/mol	McGowan Method

Sources

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=C14740933&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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