

1,3,5,2,4,6-Triazatriphosphorine, 2,4-dibromo-2,4,6,6-tetrachloro-2,2,4,4,6,6-hexahy

Other names:	2,2,4,4,6,6-Hexahydro-2,4-dibromo-2,4,6,6-tetrachloro-1,3,5,2,4,6-triazatriphosphorine Cyclo-bis(bromochlorophosphonitrile)- dichlorophosphonitrile
Inchi:	InChI=1S/Br2Cl4N3P3/c1-10(3)7-11(2,4)9-12(5,6)8-10
InchiKey:	NZOPHDJOTZVWNN-UHFFFAOYSA-N
Formula:	Br2Cl4N3P3
SMILES:	CIP1(Cl)=NP(Cl)(Br)=NP(Cl)(Br)=N1
Mol. weight [g/mol]:	436.56
CAS:	15964-99-5

Physical Properties

Property code	Value	Unit	Source
ie	9.80 ± 0.10	eV	NIST Webbook
log10ws	3.28		Crippen Method
logp	7.584		Crippen Method
mcvol	175.280	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C15964995&Units=SI

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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