

# 1,3,5,2,4,6-Triazatriphosphorine, 2,2,4,4,6-pentabromo-6-chloro-2,2,4,4,6,6-hexahydro-

**Other names:** 2,2,4,4,6,6-Hexahydro-6-chloro-2,2,4,4,6-pentabromo-1,3,5,2,4,6-triazatriphosphorine  
Cyclo-bis(dibromophosphonitrile)bromo- chlorophosphonitrile

**Inchi:** InChI=1S/Br5ClN3P3/c1-10(2)7-11(3,4)9-12(5,6)8-10

**InchiKey:** BGYSZBSLCSDYFJ-UHFFFAOYSA-N

**Formula:** Br<sub>5</sub>ClN<sub>3</sub>P<sub>3</sub>

**SMILES:** CIP1(Br)=NP(Br)(Br)=NP(Br)(Br)=N1

**Mol. weight [g/mol]:** 569.91

**CAS:** 15608-37-4

## Physical Properties

Property code	Value	Unit	Source
ie	9.50 ± 0.10	eV	NIST Webbook
log10ws	2.45		Crippen Method
logp	8.052		Crippen Method
mcvol	191.060	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](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=C15608374&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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