

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

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: CIP1(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: <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=C14740933&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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