

1,3,5,2,4,6-Triazatriphosphorine, 2,4,6-tribromo-2,4,6-trichloro-2,2,4,4,6,6-hexahydr

Inchi: InChI=1S/Br3Cl3N3P3/c1-10(4)7-11(2,5)9-12(3,6)8-10
InchiKey: IQZOEXNRIFPZGP-UHFFFAOYSA-N
Formula: Br3Cl3N3P3
SMILES: ClP1(Br)=NP(Cl)(Br)=NP(Cl)(Br)=N1
Mol. weight [g/mol]: 481.01
CAS: 16032-52-3

Physical Properties

Property code	Value	Unit	Source
ie	9.70 ± 0.10	eV	NIST Webbook
log10ws	3.01		Crippen Method
logp	7.740		Crippen Method
mcvol	180.540	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16032523&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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