Hexamethylcyclotriphosphazene

Other names: Cyclo-tris(dimethylphosphonitrile)
Inchi: InChI=1S/C6H18N3P3/c1-10(2)7-11(3,4)9-12(5,6)8-10/h1-6H3
InchiKey: DEBZEVJNWCNATM-UHFFFAOYSA-N
Formula: C6H18N3P3
SMILES: CP1(C)=NP(C)(C)=NP(C)(C)=N1
Mol. weight [g/mol]: 225.15
CAS: 6607-30-3

Physical Properties

Property code	Value	Unit	Source
ie	8.35 ± 0.05	eV	NIST Webbook
log10ws	8.19		Crippen Method
logp	4.127		Crippen Method
mcvol	175.860	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=C6607303&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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