

Cyclo-heptakis(dichlorophosphonitrile)

Inchi: InChI=1S/Cl14N7P7/c1-22(2)15-23(3,4)17-25(7,8)19-27(11,12)21-28(13,14)20-26(9,10)1
InchiKey: HTERBHRHPXPWDT-UHFFFAOYSA-N
Formula: Cl14N7P7
SMILES: ClP1(Cl)=NP(Cl)(Cl)=NP(Cl)(Cl)=NP(Cl)(Cl)=NP(Cl)(Cl)=NP(Cl)(Cl)=NP(Cl)(Cl)=NP(Cl)(Cl)=N1
Mol. weight [g/mol]: 811.21
CAS: 13827-30-0

Physical Properties

Property code	Value	Unit	Source
ie	9.80 ± 0.05	eV	NIST Webbook
log10ws	8.59		Crippen Method
logp	16.967		Crippen Method
mcvol	384.440	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=C13827300&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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<https://www.cheméo.com/cid/28-746-3/Cyclo-heptakis-dichlorophosphonitrile.pdf>

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