

1,3,2-Diazaphosphol-4-ene, 2,4-dichloro-1,3-dicyclohexyl-

Inchi: InChI=1S/C14H23Cl2N2P/c15-14-11-17(12-7-3-1-4-8-12)19(16)18(14)13-9-5-2-6-10-13/
InchiKey: UKOPYDZPWJFKBJ-UHFFFAOYSA-N
Formula: C14H23Cl2N2P
SMILES: ClC1=CN(C2CCCCC2)P(Cl)N1C1CCCCC1
Mol. weight [g/mol]: 321.23
CAS: 115072-85-0

Physical Properties

Property code	Value	Unit	Source
ie	7.19	eV	NIST Webbook
log10ws	-3.20		Crippen Method
logp	5.773		Crippen Method
mcvol	236.140	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=C115072850&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

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