1,3,2-Diazaphosphol-4-ene, 2-chloro-1,3-dibutyl-4,5-dimethyl-

Inchi: InChI=1S/C12H24ClN2P/c1-5-7-9-14-11(3)12(4)15(16(14)13)10-8-6-2/h5-10H2,1-4H3
InchiKey: BOQHZNTZNPUNSU-UHFFFAOYSA-N
Formula: C12H24ClN2P
SMILES: CCCCN1C(C)=C(C)N(CCCC)P1Cl
Mol. weight [g/mol]: 262.76
CAS: 141968-99-2

Physical Properties

Property code	Value	Unit	Source
ie	6.93	eV	NIST Webbook
log10ws	-1.70		Crippen Method
logp	4.921		Crippen Method
mcvol	217.440	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C141968992&Units=SI

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.