

1,3,2-Diazaphospholidine,2-methoxy-1,3-dimethyl

Inchi: InChI=1S/C5H13N2OP/c1-6-4-5-7(2)9(6)8-3/h4-5H2,1-3H3
InchiKey: UXHWCDZLFXZF EI-UHFFFAOYSA-N
Formula: C5H13N2OP
SMILES: COP1N(C)CCN1C
Mol. weight [g/mol]: 148.14
CAS: 7137-86-2

Physical Properties

Property code	Value	Unit	Source
ie	7.40	eV	NIST Webbook
ie	8.12	eV	NIST Webbook
ie	8.12	eV	NIST Webbook
log10ws	3.14		Crippen Method
logp	0.737		Crippen Method
mcvol	116.740	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7137862&Units=SI>
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>

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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