1,2,3-Trimethyltetrahydro-1,3,2-diazaphosphole 2-oxide

Other names: 1,3,2-Diazaphospholidine, 1,2,3-trimethyl-, 2-oxide
c-P(O)CH3N(CH3)CH2CH2N(CH3)

Inchi: InChI=1S/C5H13N2OP/c1-6-4-5-7(2)9(6,3)8/h4-5H2,1-3H3

InchiKey: QBMPOGBYHHUSIF-UHFFFAOYSA-N

Formula: C5H13N2OP

SMILES: CN1CCN(C)P1(C)=O

Mol. weight [g/mol]: 148.14

CAS: 16606-18-1

Physical Properties

Property code	Value	Unit	Source
affp	947.50	kJ/mol	NIST Webbook
basg	915.00	kJ/mol	NIST Webbook
log10ws	-1.22		Crippen Method
logp	0.687		Crippen Method
mcvol	116.740	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16606181&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

affp: Proton affinity

basg: Gas basicity

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:
https://www.chemeo.com/cid/61-596-3/1-2-3-Trimethyltetrahydro-1-3-2-diazaphosphole-2-oxide.pdf
Generated by Cheméo on 2024-04-26 07:55:34.570457605 +0000 UTC m=+16407383.491034920.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.