2-(Dimethylamino)-1,3-dimethyltetrahydro-1,3,2-di 2-oxide

Other names: 1,3,2-Diazaphospholidin-2-amine, N,N,1,3-tetramethyl-2-oxide
c-OP(N(CH3)2)N(CH3)CH2CH2N(CH3)
c-OP{N(CH3)2}N(CH3)CH2CH2N(CH3)

Inchi: InChI=1S/C6H16N3OP/c1-7(2)11(10)8(3)5-6-9(11)4/h5-6H2,1-4H3

InchiKey: PTUNVBFYPJJYOY-UHFFFAOYSA-N

Formula: C6H16N3OP

SMILES: CN(C)P1(=O)N(C)CCN1C

Mol. weight [g/mol]: 177.18

CAS: 7778-06-5

Physical Properties

Property code	Value	Unit	Source
affp	961.70	kJ/mol	NIST Webbook
basg	929.30	kJ/mol	NIST Webbook
log10ws	-1.20		Crippen Method
logp	0.533		Crippen Method
mcvol	140.810	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=C7778065&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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