4-Methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octa

Other names:	Trimethylolethane cyclic phosphite
	1,3-Propanediol, 2-(hydroxymethyl)-2-methyl-, cyclic phosphite (1:1)
	2-(Hydroxymethyl)-2-methyl-1,3-propanediol, cyclicphosphite (1:1)
	2,6,7-Trioxa-1-phosphabicyclo(2.2.2)octane, 4-methyl-
Inchi:	InChI=1S/C5H9O3P/c1-5-2-6-9(7-3-5)8-4-5/h2-4H2,1H3
InchiKey:	OMAIORNZIIDXOB-UHFFFAOYSA-N
Formula:	C5H9O3P
SMILES:	CC12COP(OC1)OC2
Mol. weight [g/mol]:	148.10
CAS:	1449-91-8

Physical Properties

Property code	Value	Unit	Source
affp	882.80	kJ/mol	NIST Webbook
basg	850.30	kJ/mol	NIST Webbook
ie	9.95	eV	NIST Webbook
ie	9.95	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	2.45		Crippen Method
logp	1.297		Crippen Method
mcvol	97.660	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=C1449918&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume