1,3,2-Dioxaphosphorinane,2-methoxy-4,6-dimethy

Inchi: InChI=1S/C6H13O3P/c1-5-4-6(2)9-10(7-3)8-5/h5-6H,4H2,1-3H3/t5-,6-/m1/s1
InchiKey: GNWZQVMWSLTQMZ-PHDIDXHHSA-N
Formula: C6H13O3P
SMILES: COP1OC(C)CC(C)O1
Mol. weight [g/mol]: 164.14
CAS: 41821-91-4

Physical Properties

Property code	Value	Unit	Source
affp	946.60	kJ/mol	NIST Webbook
basg	914.10	kJ/mol	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	1.46		Crippen Method
logp	2.074		Crippen Method
mcvol	122.610	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41821914&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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume