4-Isopropyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]o

Other names: 1,3-Propanediol, 2-(hydroxymethyl)-2-isopropyl-, cyclic phosphite (1:1)
2,6,7-Trioxa-1-phosphabicyclo[2.2.2]octane, 4-(1-methylethyl)-
4-Isopropyl-1,2,6,7-phosphatrioxabicyclo[2.2.2]octane
Inchi: InChI=1S/C7H13O3P/c1-6(2)7-3-8-11(9-4-7)10-5-7/h6H,3-5H2,1-2H3
InchiKey: JKKXVCKZMHGQLJ-UHFFFAOYSA-N
Formula: C7H13O3P
SMILES: CC(C)C12COP(OC1)OC2
Mol. weight [g/mol]: 176.15
CAS: 51486-55-6

Physical Properties

Property code	Value	Unit	Source
log10ws	1.85		Crippen Method
logp	1.933		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
rinpol	1327.00		NIST Webbook

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=C51486556&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices