4-ISOPROPYL-2,6,7-TRIOXA-1-PHOSPHABICYCLO 1-OXIDE

Other names: 1,3-Propanediol, 2-(hydroxymethyl)-2-isopropyl-, cyclic phosphate (1:1)
2-(Hydroxymethyl)-2-isopropyl-1,3-propanediol, cyclic phosphate (1:1)
4-Isopropyl-2,6,7-trioxa-1-fosfabicyklo(2.2.2)oktan-1-oxid
2,6,7-Trioxa-1-phosphabicyclo(2.2.2)octan-1-oxide, 4-isopropyl-
2,6,7-Trioxa-1-phosphabicyclo[2.2.2]octane, 4-(1-methylethyl)-, 1-oxide
4-Isopropylbicyclophosphate
Isopropyl bicyclic phosphate
4-Isopropyl-1-phospha-2,6,7-trioxabicyclo(2,2,2)octane 1-oxide
Isopropylbicyclophosphate

Inchi: InChI=1S/C7H13O4P/c1-6(2)7-3-9-12(8,10-4-7)11-5-7/h6H,3-5H2,1-2H3

InchiKey: CIEZMYRJRCLYNF-UHFFFAOYSA-N

Formula: C7H13O4P

SMILES: CC(C)C12COP(=O)(OC1)OC2

Mol. weight [g/mol]: 192.15

Physical Properties

Property code	Value	Unit	Source
logp	1.814		Crippen Method
mcvol	131.710	ml/mol	McGowan Method

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51052723&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume