4-Ethyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane 1-oxide

Other names: 2,6,7-Trioxa-1-phosphabicyclo[2.2.2]octane, 4-ethyl-, 1-oxide
1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-, cyclic phosphate
4-Aethyl-1-phospha-2,6,7-trioxabicyclo(2.2.2)octan-1-oxid
2-Ethyl-2-(hydroxymethyl)-1,3-propanediol, cyclic phosphate (1:1)
4-Ethyl-1-phospha-2,6,7-trioxabicyclo(2.2.2)octane-1-oxide
2-(Hydroxymethyl)-2-ethyl-1,3-propanediol, cyclic phosphate (1:1)
TMP-P
Trimethyolpropane phosphate
Trimethylopropane phosphate
1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-, cyclic phosphate (1:1)
Trimethylolpropane phosphate

Inchi: InChI=1S/C6H11O4P/c1-2-6-3-8-11(7,9-4-6)10-5-6/h2-5H2,1H3

InchiKey: BYEFHDZWRALTEN-UHFFFAOYSA-N

Formula: C6H11O4P

SMILES: CCC12COP(=O)(OC1)OC2

Mol. weight [g/mol]: 178.12

CAS: 1005-93-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	1.568		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1005932&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

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