

# 4-Methyl-2,6,7-trioxa-1-phosphabicyclo(2.2.2)octane

<b>Other names:</b>	4-Methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane 1-sulphide Phosphorothioic acid, cyclic O,O,O-ester with 2-(hydroxymethyl)-2-methyl-1,3-propanediol, 2-(Hydroxymethyl)-2-methyl-1,3-propanediol, cyclic phosphorothioate (1:1) 1,3-Propanediol, 2-(hydroxymethyl)-2-methyl, cyclic phosphorothioate (1:1) 2,6,7-Trioxa-1-phosphabicyclo(2.2.2)octane, 4-methyl-, 1-sulfide 1,3-Propanediol, 2-(hydroxymethyl)-2-methyl-, cyclic O,O,O-ester with phosphorothioic acid
<b>Inchi:</b>	InChI=1S/C5H9O3PS/c1-5-2-6-9(10,7-3-5)8-4-5/h2-4H2,1H3
<b>InchiKey:</b>	OKSHJMXSMVSYAW-UHFFFAOYSA-N
<b>Formula:</b>	C5H9O3PS
<b>SMILES:</b>	CC12COP(=S)(OC1)OC2
<b>Mol. weight [g/mol]:</b>	180.16
<b>CAS:</b>	3196-56-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	3.02		Crippen Method
logp	1.294		Crippen Method
mcvol	114.010	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3196563&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3196563&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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