1,3-Propanediol, 2,2-dimethyl-, cyclic chloromethyl phosphonate

Inchi: InChI=1S/C6H12ClO3P/c1-6(2)3-9-11(8,5-7)10-4-6/h3-5H2,1-2H3
InchiKey: PJRZVIMIZYGXOX-UHFFFAOYSA-N
Formula: C6H12ClO3P
SMILES: CC1(C)COP(=O)(CCl)OC1
Mol. weight [g/mol]: 198.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	2.449		Crippen Method
mcvol	134.850	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000931&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