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

Inchi: InChI=1S/C11H15O3P/c1-11(2)8-13-15(12,14-9-11)10-6-4-3-5-7-10/h3-7H,8-9H2,1-2H3
InchiKey: IBGSBHZFACCHSP-UHFFFAOYSA-N
Formula: C11H15O3P
SMILES: CC1(C)COP(=O)(c2ccccc2)OC1
Mol. weight [g/mol]: 226.21
CAS: 882-69-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.02		Crippen Method
logp	2.578		Crippen Method
mcvol	169.300	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C882699&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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