1,3-Propanediol, 2,2-dimethyl-, bis(cyclic 2,2-dimethyltrimethylene phosphite)

Other names: 2,2'-[(2,2-dimethylpropane-1,3-diyl)bis(oxy)]bis[5,5-dimethyl-1,3,2-dioxaphosphorinane]
Inchi: InChI=1S/C15H30O6P2/c1-13(2,7-16-22-18-9-14(3,4)10-19-22)8-17-23-20-11-15(5,6)12-
InchiKey: KGIIHYQJALVRLD-UHFFFAOYSA-N
Formula: C15H30O6P2
SMILES: CC1(C)COP(OCC(C)(C)COP2OCC(C)(C)CO2)OC1
Mol. weight [g/mol]: 368.34
CAS: 59609-05-1

Physical Properties

Property code	Value	Unit	Source
log10ws	2.66		Crippen Method
logp	4.646		Crippen Method
mcvol	276.630	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=C59609051&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