1,3-Propanediol,2,2-dimethyl-, bis(diethylphosphate)

Inchi: InChI=1S/C13H30O8P2/c1-7-16-22(14,17-8-2)20-11-13(5,6)12-21-23(15,18-9-3)19-10-4/

InchiKey: ZPBIIRXTRJJZTQ-UHFFFAOYSA-N

Formula: C13H30O8P2

SMILES: CCOP(=O)(OCC)OCC(C)(C)COP(=O)(OCC)OCC

Mol. weight [g/mol]: 376.32

CAS: 116402-41-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.07		Crippen Method
logp	4.408		Crippen Method
mcvol	281.910	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=C116402416&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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