1,1-Di(phosphonic acid diethyl ester)-1-hydroxy ethane

Inchi: InChI=1S/C10H24O7P2/c1-6-14-18(12,15-7-2)10(5,11)19(13,16-8-3)17-9-4/h11H,6-9H2,

InchiKey: GHERDGLHLZPTDX-UHFFFAOYSA-N

Formula: C10H24O7P2

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

Mol. weight [g/mol]: 318.24

CAS: 20427-93-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.27		Crippen Method
logp	3.185		Crippen Method
mcvol	233.770	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20427934&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume