

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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/54-366-6/1-1-Di-phosphonic-acid-diethyl-ester-1-hydroxy-ethane.pdf>

Generated by Cheméo on 2024-04-20 02:20:23.740647772 +0000 UTC m=+15868872.661225087.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.