

Diethyl 1-hydroxybutylphosphonate

Other names:	Phosphonic acid, (1-hydroxybutyl)-, diethyl ester
Inchi:	InChI=1S/C8H19O4P/c1-4-7-8(9)13(10,11-5-2)12-6-3/h8-9H,4-7H2,1-3H3
InchiKey:	QGNCNQNIDOVSQB-UHFFFAOYSA-N
Formula:	C8H19O4P
SMILES:	CCCC(O)P(=O)(OCC)OCC
Mol. weight [g/mol]:	210.21
CAS:	17477-67-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	2.371		Crippen Method
mcvol	167.520	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17477677&Units=SI
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

Legend

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

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