

Cyclohexyl methyl ethylphosphonate

Other names:	Ethylphosphonic acid, cyclohexyl methyl ester Cyclohexyl ethylphosphonate, methylated
Inchi:	InChI=1S/C9H19O3P/c1-3-13(10,11-2)12-9-7-5-4-6-8-9/h9H,3-8H2,1-2H3
InchiKey:	AUJSOZMLPGLDLR-UHFFFAOYSA-N
Formula:	C9H19O3P
SMILES:	CCP(=O)(OC)OC1CCCCC1
Mol. weight [g/mol]:	206.22
CAS:	170275-49-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	3.195		Crippen Method
mcvol	164.880	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=C170275497&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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