

Acetic acid, diisopropylphosphono-

Inchi: InChI=1S/C8H17O5P/c1-6(2)12-14(11,5-8(9)10)13-7(3)4/h6-7H,5H2,1-4H3,(H,9,10)
InchiKey: NWYWXXQNZRWXDJ-UHFFFAOYSA-N
Formula: C8H17O5P
SMILES: CC(C)OP(=O)(CC(=O)O)OC(C)C
Mol. weight [g/mol]: 224.19
CAS: 118729-24-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	2.114		Crippen Method
mcvol	169.090	ml/mol	McGowan Method

Sources

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=C118729241&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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