

Phosphonic acid, acetyldiethyl ester

Inchi: InChI=1S/C6H13O4P/c1-4-9-11(8,6(3)7)10-5-2/h4-5H2,1-3H3
InchiKey: YOHJPFQGGNEGSE-UHFFFAOYSA-N
Formula: C6H13O4P
SMILES: CCOP(=O)(OCC)C(C)=O
Mol. weight [g/mol]: 180.14
CAS: 919-19-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.799		Crippen Method
mcvol	135.040	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=C919197&Units=SI>

Legend

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

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