

Phosphonic acid, di-isooctyl ester

Inchi: InChI=1S/C16H35O3P/c1-13(9-15(3,4)5)11-18-20(17)19-12-14(2)10-16(6,7)8/h13-14,20
InchiKey: OFOUIYGUOUTLLP-UHFFFAOYSA-N
Formula: C16H35O3P
SMILES: CC(CO[PH](=O)OCC(C)CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 306.42
CAS: 79373-12-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	5.554		Crippen Method
mcvol	274.370	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=C79373129&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/115-216-4/Phosphonic-acid-di-isooctyl-ester.pdf>

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