

Benzoyl-phosphonic acid diethyl ester

Inchi: InChI=1S/C11H15O4P/c1-3-14-16(13,15-4-2)11(12)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3
InchiKey: TZAMQIAPGYOUKF-UHFFFAOYSA-N
Formula: C11H15O4P
SMILES: CCOP(=O)(OCC)C(=O)c1ccccc1
Mol. weight [g/mol]: 242.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	3.093		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
rinpol	1667.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1667.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R205197&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/91-082-0/Benzoyl-phosphonic-acid-diethyl-ester.pdf>

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