

Pinacolyl methylphosphonate-A, methylated

Other names: Methyl-phosphonic acid pinacolyl ester methyl ester, diastereomer 1
Inchi: InChI=1S/C8H19O3P/c1-7(8(2,3)4)11-12(6,9)10-5/h7H,1-6H3
InchiKey: IVTOWMZA ZSBKOT-UHFFFAOYSA-N
Formula: C8H19O3P
SMILES: COP(C)(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 194.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	2.907		Crippen Method
mcvol	161.650	ml/mol	McGowan Method
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook

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=R266518&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/98-808-7/Pinacolyl-methylphosphonate-A-methylated.pdf>

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