2-Methylcyclohexyl methylphosphonofluoridate, diastereomer # 1

Other names: 2-Methylcyclohexyl methylphosphonofluoridate, diastereomer # 1
Inchi: InChI=1S/C8H16FO2P/c1-7-5-3-4-6-8(7)11-12(2,9)10/h7-8H,3-6H2,1-2H3
InchiKey: YBZCCTLVJWWETH-UHFFFAOYSA-N
Formula: C8H16FO2P
SMILES: CC1CCCCC1OP(C)(=O)F
Mol. weight [g/mol]: 194.19

Physical Properties

Property code	Value	Unit	Source
logp	3.374		Crippen Method
mcvol	146.690	ml/mol	McGowan Method
rinpol	1260.20		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1260.20		NIST Webbook
rinpol	1260.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R496061&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices