

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]: 194.18

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.15 | | Crippen Method |
| 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

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R496061&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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