sec-Butyl methylphosphonofluoridate, diastereomer # 1

Other names: sec-Butyl methylphosphonofluoridate, diastereomer # 1
Inchi: InChI=1S/C5H12FO2P/c1-4-5(2)8-9(3,6)7/h5H,4H2,1-3H3
InchiKey: INIUKZAEJHEEFF-UHFFFAOYSA-N
Formula: C5H12FO2P
SMILES: CCC(C)OP(C)(=O)F
Mol. weight [g/mol]: 154.12

Physical Properties

Property code	Value	Unit	Source
logp	2.594		Crippen Method
mcvol	115.280	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R496170&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:
https://www.chemeo.com/cid/70-844-7/sec-Butyl-methylphosphonofluoridate-diastereomer-1.pdf
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