pinacolyl methylphosphonofluoridate, diastereomer 1

Inchi: InChI=1S/C7H16FO2P/c1-6(7(2,3)4)10-11(5,8)9/h6H,1-5H3
InchiKey: GRXKLBBBQUKJJZ-UHFFFAOYSA-N
Formula: C7H16FO2P
SMILES: CC(OP(C)(=O)F)C(C)(C)C
Mol. weight [g/mol]: 182.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	3.230		Crippen Method
mcvol	143.460	ml/mol	McGowan Method
rinpol	1048.10		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R496145&Units=SI
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

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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