Pinacolyl ethylphosphonofluoridate

Inchi: InChI=1S/C8H18FO2P/c1-6-12(9,10)11-7(2)8(3,4)5/h7H,6H2,1-5H3
InchiKey: JAUUZXIIPYQPGA-UHFFFAOYSA-N
Formula: C8H18FO2P
SMILES: CCP(=O)(F)OC(C)C(C)(C)C
Mol. weight [g/mol]: 196.20
CAS: 97931-20-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	3.620		Crippen Method
mcvol	157.550	ml/mol	McGowan Method
rinpol	1141.00		NIST Webbook
rinpol	1141.40		NIST Webbook
rinpol	1141.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97931209&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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