Cyclooctyl isopropylphosphonofluoridate

Inchi: InChI=1S/C11H22FO2P/c1-10(2)15(12,13)14-11-8-6-4-3-5-7-9-11/h10-11H,3-9H2,1-2H3
InchiKey: QYQMMSKFTOXOQI-UHFFFAOYSA-N
Formula: C11H22FO2P
SMILES: CC(C)P(=O)(F)OC1CCCCCCC1
Mol. weight [g/mol]: 236.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.76		Crippen Method
logp	4.687		Crippen Method
mcvol	188.960	ml/mol	McGowan Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U298268&Units=SI

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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